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École Doctorale Mathématiques et Sciences et Technologies de l'Information et de la Communication (MSTIC)

THÈSE DE DOCTORAT

Discipline: Mathématiques

présentée par

Boris NECTOUX

Analyse spectrale et analyse semi-classique pour la métastabilité en dynamique moléculaire

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Thèse dirigée par Éric Cancès et Tony Lelièvre au CERMICS, École des Ponts Paristech

Soutenue le 20 novembre 2017 devant le jury composé de:

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Titre: Analyse spectrale et analyse semi-classique pour la métastabilité en dynamique moléculaire.

Résumé: Dans cette thèse, nous étudions le comportement asymptotique précis à basse température de l'événement de sortie d'un domaine métastable $\Omega \subset \mathbb{R}^d$ (point de sortie et temps de sortie) pour le processus de Langevin suramorti. En pratique, le processus de Langevin suramorti peut par exemple simuler l'évolution des positions des atomes d'une molécule ou la diffusion d'impuretés interstitielles dans un cristal. Nos résultats principaux concernent le comportement asymptotique précis de la distribution de la loi du point de sortie de Ω. Dans la limite d'une petite température, ces résultats permettent de justifier l'utilisation de la formule d'Eyring-Kramers pour modéliser les événements de sortie de Ω. La loi d'Eyring-Kramers est par exemple utilisée pour calculer les taux de transition entre les états d'un système dans un algorithme de Monte-Carlo cinétique afin de simuler efficacement les différents états visités par le système. L'analyse repose de manière essentielle sur la distribution quasi stationnaire associée au processus de Langevin suramorti dans Ω. Nos preuves utilisent des outils d'analyse semi-classique. La thèse se décompose en trois chapitres indépendants. Le premier chapitre (rédigé en français) est une introduction aux résultats obtenus. Les deux autres chapitres (rédigées en anglais) sont consacrés aux énoncés mathématiques.

Mots-clés: Dynamique moléculaire, Loi d'Eyring-Kramers, processus de Langevin suramorti, analyse semi-classique, régime d'une petite température, évènement de sortie, distribution de sortie, métastabilité, distribution quasi stationnaire.

Title: Spectral analysis and semi-classical analysis for metastability in molecular dynamics.

Abstract: This thesis is dedicated to the study of the sharp asymptotic behaviour in the low temperature regime of the exit event from a metastable domain $\Omega \subset \mathbb{R}^d$ (exit point and exit time) for the overdamped Langevin process. In practice, the overdamped Langevin dynamics can be used to describe for example the motion of the atoms of a molecule or the diffusion of interstitial impurities in a crystal. The obtention of sharp asymptotic approximations of the first exit point density in the small temperature regime is the main result of this thesis. These results justify the use of the Eyring-Kramers law to model the exit event. The Eyring-Kramers law is used for example to compute the transition rates between the states of a system in a kinetic Monte-Carlo algorithm in order to sample efficiently the state-to-state dynamics. The cornerstone of our analysis is the quasi stationary distribution associated with the overdamped Langevin dynamics in Ω. The proofs are based on tools from semi-classical analysis. This thesis is divided into three independent chapters. The first chapter (in French) is dedicated to an introduction to the mathematical results. The other two chapters (in English) are devoted to the precise statements and proofs.

Key words: Molecular dynamics, Eyring-Kramers law, overdamped Langevin, semi-classical analysis, small temperature regime, exit event, first exit point density, metastability, quasi stationary distribution.

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Introduction générale de la thèse

Dans toute cette thèse, nous considérons le processus de Langevin suramorti:

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

où $f : \mathbb{R}^d \to \mathbb{R}$ est l'énergie potentielle du système considéré ($d \in \mathbb{N}^*$), $h > 0$ est sa température et $(B_t)_{t\geq 0}$ un mouvement brownien standard dans $\mathbb{R}^d$. Soit $\Omega \subset \mathbb{R}^d$ un ouvert borné et τ_Ω le premier temps de sortie de Ω:

$$\tau_\Omega := \inf\{t \geq 0, X_t \notin \Omega\}.$$

Cette thèse a pour objectif:

1. l'obtention à basse température ($h \to 0$) du comportement asymptotique précis de la loi du point de sortie X_{τ_Ω} et du temps moyen de sortie $\mathbb{E}\big[\tau_\Omega\big]$.

2. l'étude à basse température du comportement asymptotique précis des taux de transition entre régions métastables du processus (1). Cette étude permettra notamment de dégager un cadre d'hypothèses sous lequel la loi d'Eyring-Kramers peut être utilisée pour évaluer ces taux de transitions.

Cette thèse est constituée de trois chapitres:

1. Le Chapitre A est une introduction (rédigée en français) consacrée aux résultats obtenus. Dans ce chapitre, nous expliquons comment les méthodes de Monte-Carlo cinétique et la loi d'Eyring-Kramers sont utilisées en pratique pour simuler efficacement (i.e. sur des longues périodes de temps) les transitions entre régions métastables (ou états) d'un système. A la fin de cette introduction, nous présentons les résultats obtenus dans cette thèse; ces résultats font l'objet des deux autres chapitres de ce manuscrit.

2. Le Chapitre B (rédigé en anglais) est consacré à l'étude à basse température du comportement asymptotique précis de toute la distribution de sortie du domaine Ω du processus (1) dans le cas où le potentiel f ne contient qu'un seul point critique x_0 dans Ω avec $\min_{\overline{\Omega}} f = \min_\Omega f = f(x_0)$. Cette étude aboutit notamment à l'obtention de la loi d'Eyring-Kramers pour toutes les transitions démarrant du domaine Ω.

   Les articles supports de ce chapitre sont [1] et [2].

3. Le Chapitre C (rédigé en anglais) est consacré à l'étude à basse température de la concentration de la loi du point de sortie X_{τ_Ω} sur les minima de f sur $\partial\Omega$. Nos résultats permettent de prouver des formules obtenues de manière formelle dans la littérature et de généraliser considérablement les résultats connus jusqu'ici. Nous avons notamment dégagé un cadre d'hypothèse nécessaire et suffisant pour assurer que la loi de X_{τ_Ω} se concentre sur les points d'énergie les plus bas de$f$ sur $\partial\Omega$.

   L'article support de ce chapitre est [4], il est en cours de rédaction.

Les trois chapitres de cette thèse sont indépendants et peuvent donc être lus séparément. Les Chapitres B et C comportent chacun une introduction des résultats démontrés. Les techniques de preuves utilisées sont majoritairement issues de l'analyse semi-classique. Enfin, l'utilisation de la distribution quasi stationnaire associée à Ω et au processus (1) a été fondamentale dans notre approche.

Articles écrits pendant la thèse

[1] G. Di Gesù, T. Lelièvre, D. Le Peutrec, and B. Nectoux. Jump markov models and transition state theory: the quasi-stationary distribution approach. *Faraday Discussions*, 195:469–495, 2017.

[2] G. Di Gesù, T. Lelièvre, D. Le Peutrec, and B. Nectoux. Sharp asymptotics of the first exit point density. *preprint arXiv:1706.08728*, 2017.

[3] B. Nectoux. Sharp estimate of the mean exit time of a bounded domain in the zero white noise limit. *preprint arXiv:1710.07510*, 2017.

[4] G. Di Gesù, T. Lelièvre, D. Le Peutrec, and B. Nectoux. The exit from a metastable state: concentration of the exit point on the low energy saddle points, 2017. In preparation.

Chapter A

Introduction

Cette introduction comporte cinq sections dépendantes:

- La Section A.1 a pour but d'énoncer la loi d'Eyring-Kramers, d'introduire la notion de métastabilité énergétique et d'expliquer les problématiques liées à la séparation des échelles de temps.
- La Section A.2 a pour but de présenter les méthodes de Monte-Carlo cinétique, d'expliquer comment ces méthodes sont utilisées en pratique pour échantillonner les différents états visités par un système et d'en justifier l'utilisation. Nous expliquons aussi comment la loi d'Eyring-Kramers est utilisée dans les algorithmes de Monte-Carlo cinétique ainsi que dans l'algorithme *temperature accelerated dynamics*.
- En Section A.3, nous donnons une expression exacte des taux de transition entre les états pour la dynamique de Langevin suramortie (1). Ensuite, nous expliquons la stratégie adoptée pour prouver la loi d'Eyring-Kramers.
- En Section A.4, nous présentons les résultats obtenus le Chapitres B. Nous fournissons aussi une explication des preuves et des outils utilisés.
- En Section A.5, nous présentons les résultats obtenus le Chapitres C. Nous donnons un schéma des preuves et une explication des outils utilisés.

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A.1 L'équation de Langevin suramortie et la loi d'Eyring-Kramers

A.1.1 L'équation de Langevin suramortie

L'équation de Langevin suramortie (1) est l'équation centrale de cette thèse. Elle peut être vue comme une perturbation stochastique des trajectoires déterministes

$$\frac{d}{dt}x(t) = -\nabla f(x(t)).$$

Elle est couramment utilisée pour modéliser l'évolution des positions des atomes d'une molécule dans un milieu ou l'évolution des impuretés dans un cristal (cf. par exemple [64, Sections 2 et 3]).

A.1.1.1 Mouvement d'une molécule

Une molécule est un agrégat, électriquement neutre, d'atomes reliés entre eux par des liaisons (majoritairement covalentes et appelées liaisons moléculaires). Dans de nombreuses situations d'intérêt, la position des atomes évolue (agitation thermique, forces extérieures, etc.). Ces modifications se font par exemple lorsque des liaisons covalentes au sein de la molécule se forment ou se brisent ou bien lorsque la molécule change de forme. Ces transformations de la molécule (ou changements de configuration de la molécule) sont appelées réactions.

Les atomes d'une molécule ne sont pas immobiles et vibrent (ou oscillent) autour d'une position d'équilibre stable. Ces vibrations sont causées par des forces aléatoires extérieures provenant des nombreuses collisions avec les atomes voisins. Ces vibrations peuvent être modélisées par un mouvement brownien. Soit $f : \mathbb{R}^d \to \mathbb{R}$ le potentiel engendré par les liaisons moléculaires ($d = 3N$ où N est le nombre de particules constituant la molécule). Un modèle possible pour l'évolution de la position des N particules de la molécule est donné par l'équation de Langevin suramortie (1).

Remarque A.1. *On peut réduire la dimension $d = 3N$ en ne considérant que les degrés de liberté de la molécule qui suffisent à décrire entièrement les réactions considérées. Cette réduction se fait à l'aide de coordonnées de réaction $\xi : \mathbb{R}^{3N} \to \mathbb{R}^p$ dont l'intérêt est d'autant plus grand que p est petit devant $3N$ (cf. par exemple [52, Section 1.3.2.2]).*

Remarque A.2. *L'équation différentielle stochastique généralement utilisée en dynamique moléculaire pour décrire l'évolution des atomes d'une molécule est l'équation de Langevin:*

$$\begin{cases} dq_t = p_t dt, \\ dp_t = -\nabla f(q_t)dt - \gamma\, p_t dt + \sqrt{h}\, dB_t, \end{cases} \tag{A.1}$$

où q_t est le vecteur position des particules, p_t le vecteur vitesse des particules et $\gamma > 0$ est la constante de viscosité du milieu. La force γp_t est une force de type frottement visqueux qui modélise les frictions entre les atomes de la molécule et les atomes du bain thermique (cette force ralentit les particules de la molécule). L'équation de Langevin suramortie (1) *s'obtient à partir de l'équation de Langevin* (A.1) *dans la limite grande*

friction ($\gamma \to \infty$) avec le changement d'échelle temporel $\frac{t}{\gamma}$. Ceci justifie la qualification de "suramortie" donnée à l'équation (1)*. L'équation de Langevin suramortie décrit alors en première approximation le mouvement des particules d'une molécule dont le terme de friction est grand.*

A.1.1.2 Mouvement des impuretés dans un cristal

Un cristal est un assemblage d'atomes formant un réseau périodique dans l'espace. Il est généralement constitué d'une cellule de référence répétée dans toutes les directions. Les impuretés en insertion (ou impureté interstitielle, défaut interstitiel) du cristal sont des atomes (appelés atomes interstitiels) logés dans les sites interstitiels du réseau cristallin (cf. Figure A.1 pour une représentation schématique). Ces impuretés peuvent se déplacer.
Une impureté interstitielle est maintenue dans un état stable grâce aux forces interatomiques du réseau cristallin. Ces forces dérivent d'une énergie potentielle que l'on note f. Les atomes du réseau ne sont pas immobiles: la structure cristalline vibre. L'agitation thermique responsable de la vibration du réseau cristallin est modélisée par un mouvement brownien. Cette agitation induit un mouvement aléatoire de l'impureté interstitielle. Le mouvement de l'impureté interstitielle peut être modélisé par un processus de Langevin suramorti (1) et dans ce cas le vecteur $X_t \in \mathbb{R}^3$ représente la position de l'atome interstitiel, f l'énergie potentielle des forces d'interaction avec les atomes du réseau cristallin, h la température du cristal (cf. par exemple [69, Chapter 6]).

Remarque A.3. *D'autres types d'impuretés peuvent exister au sein d'un cristal comme un site vacant du réseau (où il manque un atome) ou bien la présence en un site d'un atome étranger à la structure (impureté substitutionnelle). Les impuretés dans un cristal peuvent être volontairement introduites, le plus souvent afin d'améliorer la conductivité du cristal et dans ce cas on parle de dopage.*

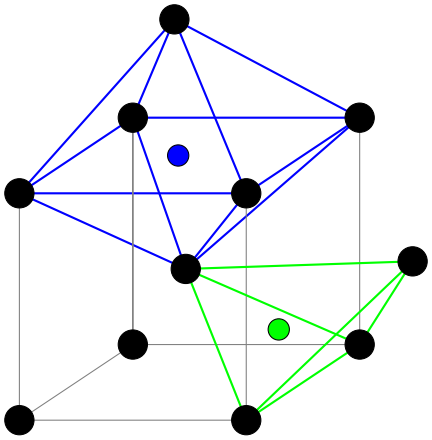

Figure A.1: Représentation schématique de la cellule de référence d'une structure cubique centrée composée d'un seul type d'atome (par exemple le chrome Cr) représenté par des ronds noir. Cette structure possède deux types de sites interstitiels: les sites octaédriques (en bleu) et les sites tétraédriques (en vert) représentés sur la figure.

A.1.1.3 Evolution des systèmes considérés et définition d'une réaction

Dans toute la suite, les systèmes considérés sont supposés avoir une évolution modélisée par le processus de Langevin suramorti (1) (bien que l'essentiel de ce que nous allons expliquer en Section A.1 et A.2 s'applique aussi lorsqu'ils sont modélisés par la dynamique (A.1)). L'espace des phases de tels systèmes est $\mathbb{R}^d$. La fonction $f : \mathbb{R}^d \to \mathbb{R}$ désigne l'énergie potentielle du système et h sa température. Nous parlons de processus pour désigner implicitement le processus (1) décrivant l'évolution du système. Parfois, lorsqu'aucune confusion n'est possible, nous confondons l'état du système et le domaine qui le représente dans l'espace des phases. Une réaction est par définition la transition d'un état du système à un autre état.

Nous allons maintenant présenter une des lois majeures de la cinétique chimique: la loi d'Eyring-Kramers. Cette loi permet de relier le temps moyen d'une réaction à la température du système.

A.1.2 La loi d'Eyring-Kramers

Cette section est organisée comme suit. En Section A.1.2.1, nous énonçons la loi d'Eyring-Kramers. En Section A.1.2.2, nous montrons comment elle peut s'obtenir rigoureusement dans un cas unidimensionnel.

A.1.2.1 Enoncé de la loi d'Eyring-Kramers

La loi d'Eyring-Kramers, en référence à Henry Eyring et Hendrik Anthony Kramers, donne la dépendance du temps moyen pour passer d'un état à un autre (temps de réaction) en la température h (cf. par exemple [33]). Considérons un système dont l'évolution est régie par le processus de Langevin suramorti (1). Supposons que le système est initialement dans un état stable, noté 1 et repéré dans l'espace des phases par le bassin d'attraction du minimum local $x_1 \in \mathbb{R}^d$ de l'énergie potentielle f pour la dynamique de gradient

$$\frac{d}{dt}x(t) = -\nabla f(x(t)). \tag{A.2}$$

Considérons ensuite un autre état stable, noté 2, voisin de l'état 1 et repéré dans l'espace des phases par le bassin d'attraction du minimum local $x_2 \in \mathbb{R}^d$ de l'énergie potentielle f pour la dynamique (A.2). Soit la réaction ou changement d'état du système

$$1 \to 2 \tag{A.3}$$

Remarque A.4. *Afin de présenter la formule d'Eyring-Kramers, nous nous plaçons dans le cas simple où il n'y a qu'un seul point selle (ici $z_{1,2}$) qui sépare les états* 1 *et* 2*. Dans cette thèse, nous traiterons le cas des systèmes possédant plusieurs états séparés par plusieurs points selles certains pouvant être au même niveau d'énergie.*

La réaction (A.3) nécessite un apport d'énergie minimal $\Delta_{1\to 2} f > 0$ pour se réaliser, cette quantité d'énergie est appelée énergie d'activation de la réaction (A.3). Supposons désormais qu'il existe un unique point selle $z_{1,2} \in \mathbb{R}^d$ dont l'énergie correspond à l'énergie minimale à traverser pour aller de l'état 1 à l'état 2, i.e.

$$\Big\{ z \in \mathbb{R}^d,\ f(z) = \inf_{\gamma \in \mathcal{P}(x_1,x_2)} \sup_{t\in[0,1]} f(\gamma(t)) \Big\} = \{z_{1,2}\},$$

où $\mathcal{P}(x_1, x_2)$ est l'ensemble des courbes $\gamma \in C^0([0,1], \mathbb{R}^d)$ telles que $\gamma(0) = x_1$ et $\gamma(1) = x_2$. Dans ce cas, l'énergie d'activation est définie par

$$\Delta_{1\to 2} f = f(z_{1,2}) - f(x_1).$$

Sur la Figure A.2 est représenté le graphe d'un potentiel f en dimension 2 correspondant à cette situation.

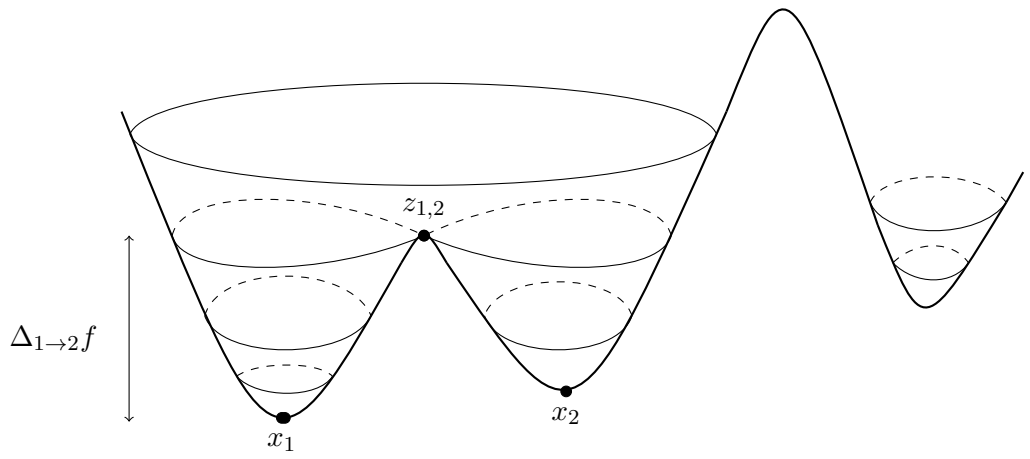

Figure A.2: Représentation schématique en dimension 2 du potentiel f. Le système est initialement dans l'état 1 (bassin d'attraction de x_1 pour la dynamique(A.2)).

Notons $\mathcal{T}_{1\to 2}$ le temps moyen à la température h pour que la réaction (A.3) se réalise. La formule d'Eyring-Kramers pour le temps moyen de réaction $\mathcal{T}_{1\to 2}$ est:

$$\mathcal{T}_{1\to 2} \sim_{h\to 0} A_{1,2}\, e^{\frac{2}{h}(f(z_{1,2}) - f(x_1))}, \tag{A.4}$$

où $A_{1,2}$ est un préfacteur dépendant de la dynamique considérée, ici (1), et de la géométrie locale du potentiel f en x_1 et $z_{1,2}$. L'obtention d'un équivalent de $\mathcal{T}_{1\to 2}$ dans la limite d'une petite température est l'objet de la théorie de l'état de transition. Sous l'hypothèse que les matrices hessiennes de f en x_1 et en $z_{1,2}$ sont inversibles (cf. par exemple [55, 71]):

$$A_{1,2} = \frac{2\pi}{|\lambda(z_{1,2})|} \frac{\sqrt{|\det \mathrm{Hess} f(z_{1,2})|}}{\sqrt{\det \mathrm{Hess} f(x_1)}}, \tag{A.5}$$

où $\lambda(z_{1,2}) < 0$ est l'unique valeur propre négative de la matrice hessienne de f en $z_{1,2}$. L'expression (A.5) obtenue pour $A_{1,2}$ indique qu'au premier ordre, il suffit de ne prendre en compte que la géométrie locale du potentiel f aux points $z_{1,2}$ et x_1. Il traduit la facilité ou la difficulté avec laquelle le processus (1) arrive à sortir du puits de potentiel en x_1 et à passer le col $z_{1,2}$ pour arriver en x_2. Pour une revue complète sur l'obtention de la formule d'Eyring-Kramers et la théorie de l'état de transition (ainsi que sa généralisation à l'équation de Langevin (A.1)), le lecteur peut se référer à [33].

Remarque A.5. *La trajectoire empruntée par le système lors d'une réaction (passage d'un état à un autre) est appelée trajectoire réactive. A température nulle, c'est la trajectoire qui minimise l'énergie sur toutes les trajectoires qui vont de l'état initial à l'état final en temps arbitraire. Elle permet de comprendre les états intermédiaires (le mécanisme de réaction) par lequel passe le système pendant la réaction.*

A.1.2.2 Un calcul en dimension un pour obtenir la formule d'Eyring-Kramers

Le but de cette section est de montrer comment obtenir rigoureusement la formule d'Eyring-Kramers en dimension un dans un cadre géométrique extrêmement simple.

Considérons un système dont l'évolution est modélisée par le processus de Langevin suramorti (1) en dimension un et dont le potentiel $f : \mathbb{R} \to \mathbb{R}$ est celui dont le graphe est représenté sur la Figure A.3. Dans cet exemple, f est une fonction C^∞, paire, $\lim_{\pm\infty} f = +\infty$ et f a cinq points critiques. Les points $x_1 = 0$, $x_2 < 0$, $x_3 = -x_2 > 0$ sont les trois minima locaux de f et les points $z_{1,2} < 0$, $z_{1,3} = -z_{1,2} > 0$ sont les deux maxima locaux (ce sont deux points selles). Le système considéré a donc trois états: l'état 1 repéré dans l'espace des phases par le domaine $\Omega_1 = (z_{1,2}, z_{1,3})$, l'état 2 repéré par le domaine $\Omega_2 = (-\infty, z_{1,2})$ et l'état 3 repéré par le domaine $\Omega_3 = (z_{1,3}, +\infty)$. Dans la suite, $(X_t)_{t\geq 0}$ désigne le processus de Langevin suramorti (1) en dimension un pour le potentiel f de la figure A.3.

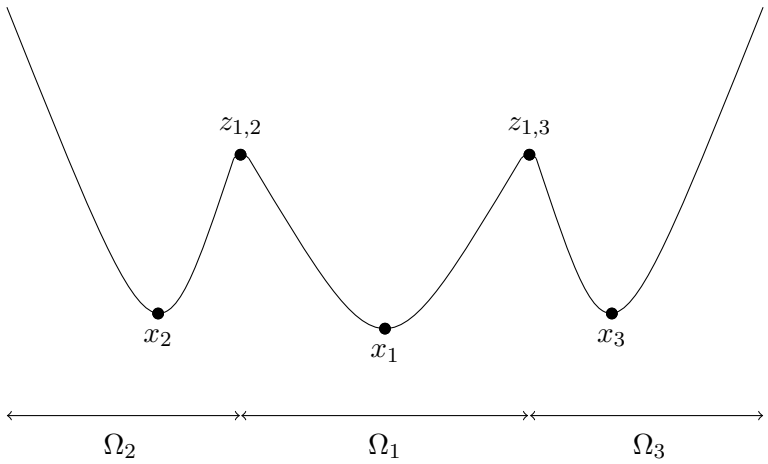

Figure A.3: Graphe du potentiel f du système considéré pour un calcul en dimension un.

Comme en Section A.1.2.1, $\mathcal{T}_{1\to 2}$ désigne le temps moyen de la réaction $1 \to 2$ et $\mathcal{T}_{1\to 2\cup 3}$ le temps moyen de la réaction $1 \to 2 \cup 3$. Soit $\tau^x_{\Omega_1}$ le premier moment où le processus $(X_t)_{t\geq 0}$ démarrant en x quitte le domaine $\Omega_1 = (z_{1,2}, z_{1,3})$:

$$\tau^x_{\Omega_1} = \inf\{t \geq 0, X_t \notin \Omega_1 \text{ when } X_0 = x\}.$$

Les temps moyens $\mathcal{T}_{1\to 2\cup 3}$ et $\mathbb{E}^x\big[\tau_{\Omega_1}\big]$ sont liés par la relation

$$\mathcal{T}_{1\to 2\cup 3} = 2\,\mathbb{E}^x\big[\tau_{\Omega_1}\big],$$

où la notation $\mathbb{E}^x$ désigne l'espérance sachant $X_0 = x$. En effet, quand $X_0 = x \in \Omega_1$, le processus $(X_t)_{t\geq 0}$ quitte Ω_1 en $z_{1,2}$ ou $z_{1,3}$ (car $X_{\tau_{\Omega_1}} \in \{z_{1,2}, z_{1,3}\}$, les trajectoires

du processus (1) étant continues) et il a ensuite une chance sur deux, dans la limite $h \to 0$, de revenir en Ω_1 ou de tomber dans $\Omega_2 \cup \Omega_3$. En effet, soient $A_1 = (-\infty, x_1)$ et $A_3 = (x_3, +\infty)$. Il est possible de montrer que (cf. [3, Section 3.1]),

$$\mathbb{P}^{z_{1,3}}[\tau_{A_1} < \tau_{A_3}] = \frac{\displaystyle\int_{z_{1,3}}^{x_3} e^{\frac{2}{h}f}}{\displaystyle\int_{x_1}^{x_3} e^{\frac{2}{h}f}},$$

où $\mathbb{P}^{z_{1,3}}$ désigne la probabilité sachant $X_0 = z_{1,3}$, $\tau_{A_1} = \inf\{t \geq 0, X_t \notin A_1\}$ et $\tau_{A_3} = \inf\{t \geq 0, X_t \notin A_3\}$. Ainsi, en utilisant une méthode de Laplace, on a bien dans la limite $h \to 0$:

$$\mathbb{P}^{z_{1,3}}[\tau_{A_1} < \tau_{A_3}] = \frac{1}{2} + O(h). \tag{A.6}$$

De plus, les temps moyens $\mathcal{T}_{1\to 2\cup 3}$ et $\mathcal{T}_{1\to 2}$ sont liés par la relation

$$\mathcal{T}_{1\to 2\cup 3} = \frac{1}{2}\mathcal{T}_{1\to 2},$$

par symétrie (le potentiel f est pair). Ainsi, nous avons:

$$\mathcal{T}_{1\to 2} = 4\,\mathbb{E}^x\big[\tau_{\Omega_1}\big]. \tag{A.7}$$

Nous allons donc maintenant chercher un équivalent précis de $\mathbb{E}^x\big[\tau_{\Omega_1}\big]$ dans la limite d'une petite température.
A l'aide de la formule de Dynkin [48, Théorème 11.2], l'unique solution du problème elliptique

$$\Big(\frac{h}{2}\frac{d^2}{dx^2} - \frac{d}{dx}f(x)\frac{d}{dx}\Big)v(x) = -1 \text{ pour tout } x \in \Omega_1 \text{ et } v(z_{1,2}) = 0 \text{ et } v(z_{1,3}) = 0, \tag{A.8}$$

est la fonction

$$x \in \Omega_1 \mapsto \mathbb{E}^x\big[\tau_{\Omega_1}\big].$$

En effet, soit $v \in C^\infty([z_{1,2}, z_{1,3}], \mathbb{R})$ l'unique solution problème (A.8). La formule de Dynkin appliquée à la fonction v pour le processus (1) et pour le temps d'arrêt τ_{Ω_1} s'écrit pour $x \in \Omega_1$

$$\mathbb{E}^x\big[v(X_{\tau_{\Omega_1}})\big] - v(x) = \mathbb{E}^x\left[\int_0^{\tau_{\Omega_1}} \Big(\frac{h}{2}\frac{d^2}{dx^2} - \frac{d}{dx}f(x)\frac{d}{dx}\Big)v(X_s)ds\Big)\right].$$

Ainsi, puisque v est solution du problème (A.8), il vient:

$$v(x) = \mathbb{E}^x\big[\tau_{\Omega_1}\big].$$

Le problème (A.8) se réécrit sous la forme:

$$\frac{h}{2}e^{\frac{2}{h}f(x)}\frac{d}{dx}\Big(e^{-\frac{2}{h}f}\frac{d}{dx}v\Big)(x) = -1 \text{ pour tout } x \in \Omega_1 \text{ et } v(z_{1,2}) = 0 \text{ et } v(z_{1,3}) = 0.$$

En intégrant deux fois, il existe deux constantes C_0 et C_1 telles que pour tout $x \in \Omega_1$:

$$v(x) = C_1 + C_0\int_{z_{1,2}}^{x} e^{\frac{2}{h}f(y)}dy - \frac{2}{h}\int_{z_{1,2}}^{x}\int_{z_{1,2}}^{y} e^{\frac{2}{h}(f(y)-f(t))}dt\,dy.$$

Puisque $v(z_{1,2}) = 0$, nous en déduisons que $C_1 = 0$ et puisque $v(z_{1,3}) = 0$, nous obtenons

$$C_0 = \frac{2}{h} \frac{\displaystyle\int_{z_{1,2}}^{z_{1,3}} \int_{z_{1,2}}^{y} e^{\frac{2}{h}(f(y)-f(t))} dt\, dy}{\displaystyle\int_{z_{1,2}}^{z_{1,3}} e^{\frac{2}{h}f(y)} dy}.$$

Ainsi, nous obtenons pour tout $x \in \Omega_1$:

$$v(x) = \frac{2}{h} \left(\int_{z_{1,2}}^{z_{1,3}} \int_{z_{1,2}}^{y} e^{\frac{2}{h}(f(y)-f(t))} dt\, dy \, \frac{\displaystyle\int_{z_{1,2}}^{x} e^{\frac{2}{h}f}}{\displaystyle\int_{z_{1,2}}^{z_{1,3}} e^{\frac{2}{h}f}} - \int_{z_{1,2}}^{x} \int_{z_{1,2}}^{y} e^{\frac{2}{h}(f(y)-f(t))} dt\, dy \right). \tag{A.9}$$

Supposons maintenant que les points x_1, $z_{1,2}$ et $z_{1,3}$ sont des points critiques de f non dégénérés: c'est-à-dire que $f''(y) \neq 0$ pour tout $y \in \{x_1, z_{1,2}, z_{1,3}\}$. Puisque les deux maxima de f sur $[z_{1,2}, z_{1,3}]$ sont $z_{1,2}$ et $z_{1,3}$ et puisque f est une fonction paire, à l'aide d'une méthode de Laplace, nous obtenons pour tout $x \in \Omega_1$ dans la limite $h \to 0$:

$$\frac{\displaystyle\int_{z_{1,2}}^{x} e^{\frac{2}{h}f}}{\displaystyle\int_{z_{1,2}}^{z_{1,3}} e^{\frac{2}{h}f}} = \frac{1}{2} + O(h). \tag{A.10}$$

De plus, comme le maximum de la fonction

$$(t, y) \in \Big((z_{1,2}, z_{1,3}) \times [z_{1,2}, z_{1,3}] \Big) \cap \{t \leq y\} \mapsto f(y) - f(t)$$

est atteint uniquement en $t = x_1$ et $y = z_{1,3}$, une méthode de Laplace implique quand $h \to 0$:

$$\int_{z_{1,2}}^{z_{1,3}} \int_{z_{1,2}}^{y} e^{\frac{2}{h}(f(y)-f(t))} dt\, dy = \frac{\pi}{2\sqrt{f''(x_1)|f''(z_{1,3})|}}\, h\, e^{\frac{2}{h}(f(z_{1,3})-f(x_1))} \big(1 + O(h)\big). \tag{A.11}$$

Enfin, pour tout $x \in (z_{1,2}, z_{1,3})$ il existe $r > 0$ tel que pour tout $(t, y) \in \Big((z_{1,2}, z_{1,3}) \times [z_{1,2}, x] \Big) \cap \{t \leq y\}$:

$$f(y) - f(t) \leq f(z_{1,3}) - f(x_1) + r. \tag{A.12}$$

En utilisant (A.9), (A.11), (A.10) (A.12) et le fait que $f''(z_{1,3}) = f''(z_{1,2})$, nous obtenons pour $x \in \Omega_1 = (z_{1,2}, z_{1,3})$ dans la limite $h \to 0$:

$$\begin{aligned} v(x) &= \frac{1}{h} \int_{z_{1,2}}^{z_{1,3}} \int_{z_{1,2}}^{y} e^{\frac{2}{h}(f(y)-f(t))} dt\, dy \big(1 + O(h)\big) \\ &= \frac{\pi}{2\sqrt{f''(x_1)|f''(z_{1,2})|}} e^{\frac{2}{h}(f(z_{1,3})-f(x_1))} \big(1 + O(h)\big). \end{aligned} \tag{A.13}$$

La relation précédente est même valide uniformément sur les compacts $[a, b] \subset (z_{1,2}, z_{1,3})$: c'est-à-dire qu'il existe une constante $C > 0$ telle que $\sup_{x \in [a,b]} |O(h)| \leq Ch$. En conclusion, en utilisant (A.13) et (A.7), nous obtenons quand $h \to 0$:

$$\mathcal{T}_{1 \to 2} = \frac{2\pi}{\sqrt{f''(x_1)|f''(z_{1,2})|}} e^{\frac{2}{h}(f(z_{1,2})-f(x_1))} \big(1 + O(h)\big).$$

Cette relation est la formule d'Eyring-Kramers (A.4) pour la réaction $1 \to 2$ dans cet exemple unidimensionnel pour le potentiel f représenté sur la figure A.3.

A.1.3 Métastabilité et séparation des échelles de temps

La dynamique de Langevin suramortie (1) contient deux termes: le terme $-\nabla f(X_t)$ qui envoie le processus vers les minima locaux de f et le forçage aléatoire $\sqrt{h}\, dB_t$ qui fait passer le processus d'un minimum local de f à un autre. Si la température h est petite, le processus $(X_t)_{t\geq 0}$ reste piégé pendant un long moment dans un voisinage d'un bassin d'attraction d'un minimum local de f, que l'on appelle état métastable, avant d'aller dans une autre région de l'espace. On dit alors que le processus $(X_t)_{t\geq 0}$ est métastable. Le processus a de longues périodes d'inactivité durant lesquelles aucune transition entre les états métastables n'a lieu. Le temps typique d'équilibration dans une région métastable est bien inférieur au temps de sortie de cette région, il y a une séparation entre ces deux échelles de temps (cf. par exemple [8, Chapter 8]). Dans l'espace des configurations, le passage d'un état métastable à un autre état métastable correspond à un changement de configuration macroscopique du système que l'on a appelé réaction. Pour avoir accès aux différentes configurations du système, il est donc nécessaire de simuler la trajectoire du processus sur de longues périodes de temps. En pratique il est parfois impossible d'observer ces réactions en simulant directement l'évolution du système à partir de son équation d'évolution (1).

Cette séparation des temps caractéristiques est un des problèmes majeurs de la simulation en dynamique moléculaire car pour en comprendre l'évolution macroscopique, il faut aussi bien avoir accès à l'état dans lequel se trouve le système qu'aux mécanismes qui permettent le passage d'un état du système à un autre (les mécanismes réactionnels, cf. Remarque A.5). La transition entre deux états est un événement rare à basse température.

Plusieurs enjeux liés à cette séparation des échelles de temps apparaissent alors:

- Le premier enjeu concerne l'échantillonnage des trajectoires réactives (cf. Remarque A.5). Les trajectoires réactives ne sont pas accessibles à partir d'une simulation directe de toute la trajectoire du système à cause de cette séparation entre le temps caractéristique de vibration et le temps moyen pour observer une réaction. Par exemple, la méthode TPS, (pour *Transition Path Sampling*), ou la méthode AMS (pour *Adaptative Multilevel Splitting*), ont pour objectif de construire des méthodes pour échantillonner de manière efficace les trajectoires réactives. Ces méthodes ne seront pas développées dans la suite de ce manuscrit et si le lecteur est intéressé, il peut consulter par exemple [14], [21] ou [70] pour la méthode TPS et [11, 12] pour la méthode AMS.

- Le second enjeu est de simuler de manière correcte les états successifs visités (comme les étapes successives lors du repliement d'une protéine, les ruptures ou les formations successives de liaisons au sein d'une molécule, les différents sites interstitiels visités par un atome dans un cristal...) ainsi que les temps associés. Afin de contourner les problèmes liés à la métastabilité, des méthodes ont été développées pour ne simuler que l'évolution du système à l'échelle macroscopique

c'est-à-dire ne simuler que les changements d'état. En Section A.2, nous présentons deux de ces méthodes qui reposent sur l'utilisation la formule d'Eyring-Kramers.

A.2 Utilisation de la formule d'Eyring-Kramers: méthodes de Monte-Carlo cinétique et algorithme *temperature accelerated dynamics*

L'objectif de cette section est de présenter deux algorithmes utilisés en dynamique moléculaire qui ont pour objectif d'accélérer l'observation d'une transition entre deux états et qui reposent sur l'utilisation de la loi d'Eyring-Kramers. Les deux algorithmes que nous présentons sont l'algorithme de Monte-Carlo cinétique et l'algorithme *temperature accelerated dynamics*. La section est organisée comme suit.

1. En Section A.2.1, nous expliquons dans un premier temps comment les méthodes de Monte-Carlo cinétique sont utilisées en pratique pour simuler efficacement la dynamique d'état à état par le système. Dans un second temps, nous expliquons comment la formule d'Eyring-Kramers est utilisée pour calculer les taux de transition entre les états dans un algorithme de Monte-Carlo cinétique.

2. En Section A.2.2, nous expliquons comment la formule d'Eyring Kramers est utilisée dans l'algorithme *temperature accelerated dynamics* pour extrapoler à basse température l'événement de sortie d'un domaine métastable observé à une plus haute température.

A.2.1 Méthodes de Monte-Carlo cinétique et utilisation de la formule d'Eyring-Kramers

Nous rappelons que nous considérons un système à la température h, d'énergie potentielle $f : \mathbb{R}^d \to \mathbb{R}$ et dont l'évolution est modélisée par le processus de Langevin suramorti (1).
L'accès aux réactions qui ont lieu au sein du système ainsi qu'aux temps de réaction (i.e. les états successifs visités par le système ainsi que les temps passés dans chacun des états) est un des objectifs majeurs de la simulation en dynamique moléculaire. Toutefois, comme nous l'avons vu, la dynamique de Langevin suramortie (1) est une dynamique métastable. Ainsi, il est impossible en pratique d'avoir accès aux différentes réactions du système en simulant naïvement la trajectoire du processus. En pratique, les états successifs visités par le système ainsi que le temps passé dans chacun de ces états peuvent être approchés en construisant une chaîne de Markov en temps continu et à valeurs dans l'espace des états du système. En dynamique moléculaire de tels processus sont appelés *kinetic Monte Carlo models* [73] ou *Markov state models* [9, 65, 66]. En français, on parle de méthodes (ou algorithmes) de Monte-Carlo cinétique. Cette section a trois objectifs principaux:

- Le premier objectif est d'expliquer comment sont utilisées les méthodes de Monte-Carlo cinétique pour simuler efficacement les états successifs visités par le système ainsi que le temps passé dans chacun de ces états.

- Le second objectif est d'expliquer comment la formule d'Eyring-Kramers (A.4) est utilisée pour calculer les taux de transition entre les états dans les algorithmes de Monte-Carlo cinétique.

- Le dernier objectif est de justifier l'utilisation des méthodes de Monte-Carlo cinétique: pourquoi est-il possible de modéliser la dynamique d'état à état par un processus markovien de sauts?

La section est organisée comme suit. En Section A.2.1.1 nous définissons la dynamique d'état à état. En Section A.2.1.2, nous rappelons comment sont construits les algorithmes de Monte-Carlo cinétique. Ensuite, en Section A.2.1.3, nous expliquons comment la formule d'Eyring-Kramers et les méthodes de Monte-Carlo cinétique sont utilisées pour simuler efficacement la dynamique d'état à état du système. Enfin, en Section A.2.1.4, nous expliquerons pourquoi il est possible d'approcher certaines parties de la trajectoire de la dynamique d'état à état avec une méthode de Monte-Carlo cinétique.

A.2.1.1 La dynamique d'état à état

Supposons que l'espace des phases du système se décompose en un nombre dénombrable de domaines métastables (cf. Figure A.4 pour une représentation schématique):

$$\mathbb{R}^d = \cup_{j=1}^{N} \Omega_j, \tag{A.14}$$

où $N \in \mathbb{N} \cup \{+\infty\}$. Chaque domaine Ω_j correspond à un état j du système et l'on note l'ensemble des états

$$\mathcal{E} = \{1, ..., N\}. \tag{A.15}$$

Soit la fonction $S : \mathbb{R}^d \to E$ qui a chaque point de l'espace des phases associe l'état dans lequel il se trouve:

$$S(x) = i \text{ si } x \in \Omega_i.$$

La dynamique d'état à état[1] est la dynamique à valeurs dans l'ensemble des états $\mathcal{E}$ définie par:

$$\big(S(X_t)\big)_{t \geq 0}.$$

Remarque A.6. *En pratique, chaque domaine Ω_j peut être défini comme le bassin d'attraction pour la dynamique de gradient (cf. [72]):*

$$\frac{d}{dt} x(t) = -\nabla f(x(t)).$$

De manière générale, la question du découpage de l'espace des phases en des régions métastables n'est pas une question simple et doit être le plus souvent traitée au cas par cas.

[1] Parfois appelée le processus trace.

A.2.1.2 Principe des méthodes de Monte-Carlo cinétique

Dans cette section, nous expliquons comment construire un algorithme de Monte-Carlo cinétique. Les méthodes de Monte-Carlo cinétique ont pour objet de générer une dynamique markovienne $(Z_t)_{t\geq 0}$ à valeurs dans l'espace discret $\mathcal{E}$. Les deux ingrédients principaux d'une méthode de Monte-Carlo cinétique sont l'espace d'état discret

$$\mathcal{E} = \{1, ..., N\}$$

et les taux de transition entre les états

$$(k_{i,j})_{(i,j)\in\{1,...,N\}^2, i\neq j} \in \big(\mathbb{R}_+\big)^{(N-1)\times(N-1)}.$$

L'état j est voisin de l'état i si et seulement si $k_{i,j} > 0$. La dynamique générée à l'aide de ces deux ingrédients est un processus markovien $(Z_t)_{t\geq 0}$ à valeur dans l'espace $\mathcal{E}$ dont le générateur infinitésimal est $L \in \big(\mathbb{R}_+\big)^{(N-1)\times(N-1)}$ où $L_{i,j} = k_{i,j}$ pour $(i,j) \in \{1, ..., N\}^2$, $i \neq j$. Pour simuler le processus de sauts $(Z_t)_{t\geq 0}$, il suffit de simuler la suite des temps passés dans chaque état, que l'on note $(T_n)_{n\geq 0}$, et la chaîne de Markov subordonnée notée $(Y_n)_{n\geq 0}$ définie comme la suite des états successifs visités par $(Z_t)_{t\geq 0}$. Supposons qu'à l'instant $t = 0$, $Y_0 = 1$. La construction de la chaîne de Markov $(Z_t)_{t\geq 0}$ se fait en itérant sur $n \geq 0$ les deux étapes suivantes: étant donné un état Y_n,

1. simuler le temps T_n passé dans l'état Y_n à l'aide d'une loi exponentielle de paramètre $\sum_{j=1,\, j\neq Y_n}^{N} k_{Y_n,j}$, c'est-à-dire que pour tout $i \in \{1, ..., N\}$ et $t > 0$:

$$\mathbb{P}\big[T_n > t \big| Y_n = i\big] = e^{-t\sum_{j=1,\, j\neq i}^{N} k_{i,j}}.$$

2. simuler indépendamment de T_n, le prochain état visité Y_{n+1} selon la loi:

$$\mathbb{P}\big[Y_{n+1} = l | Y_n = i\big] = \frac{k_{i,l}}{\sum_{j=1,\, j\neq i}^{N} k_{i,j}}.$$

Le processus markovien $(Z_t)_{t\geq 0}$ est alors défini par

$$\forall n \geq 0,\, \forall t \in \Big[\sum_{m=0}^{n-1} T_m,\, \sum_{m=0}^{n} T_m\Big),\, Z_t = Y_n, \tag{A.16}$$

avec la convention $\sum_{m=0}^{-1} T_m = 0$.

Remarque A.7. *Voici une manière équivalente de construire la chaîne de Markov $(Z_t)_{t\geq 0}$ qui sera notamment utile pour comprendre l'algorithme* temperature accelerated dynamics *en Section A.2.2. Etant donné un état Y_n, soient $N-1$ variables aléatoires $(\tau_{Y_n,\ell})_{\ell\in\{1,...,N\},\, \ell\neq Y_n}$, indépendantes telles que pour tout $\ell \in \{1, ..., N\}$, $\ell \neq Y_n$*

$$\tau_{Y_n,\ell} \sim \mathcal{E}(k_{Y_n,\ell}),$$

où $\mathcal{E}(k_{Y_n,\ell})$ désigne la loi exponentielle de paramètre $k_{Y_n,\ell}$. Alors:

1. *Le temps T_n passé dans l'état Y_n (défini à l'étape 1) a la même loi que*

$$\min_{\ell\in\{1,...,N\},\, \ell\neq Y_n} \tau_{Y_n,\ell}.$$

2. *Le prochain état visité Y_{n+1} (défini à l'étape 2) a la même loi que*

$$\underset{\ell\in\{1,\dots,N\},\,\ell\neq Y_n}{\arg\min}\ \tau_{Y_n,\ell}$$

qui est bien indépendant du temps $\min_{\ell\in\{1,\dots,N\},\,\ell\neq Y_n}\tau_{Y_n,\ell}$ *passé dans l'état* Y_n.

Nous allons désormais montrer comment sont utilisées les méthodes de Monte-Carlo cinétique pour simuler approximativement la dynamique d'état à état $\big(S(X_t)\big)_{t\geq 0}$ définie en Section A.2.1.1.

A.2.1.3 Méthodes de Monte-Carlo cinétique en dynamique moléculaire

Si l'on veut approcher la dynamique d'état à état $\big(S(X_t)\big)_{t\geq 0}$ en utilisant un algorithme de Monte-Carlo cinétique, il faut deux ingrédients, comme mentionné ci-dessus: une collection dénombrable d'états et les taux de transition entre les états (cf. par exemple [10, 29, 73, 74] pour l'utilisation de ces algorithmes en dynamique moléculaire). Les différents états du système ont été définis lorsque nous avons divisé l'espace des phases en domaines métastables (cf. (A.14) et (A.15)):

$$\mathcal{E}=\{1,\dots,N\}.$$

Il ne manque alors plus que les taux de transition pour pouvoir utiliser un algorithme de Monte-Carlo cinétique. En pratique, les taux de transition sont calculés avec la formule d'Eyring-Kramers (cf. Section A.1.2). Soyons un peu plus précis sur ce point. Rappelons que pour chaque $i\in\{1,\dots,N\}$, l'état i correspond à un domaine métastable $\Omega_i\subset\mathbb{R}^d$. Supposons que:

- Dans chaque domaine Ω_j, $j\in\{1,\dots,N\}$, il y a un unique minimum global du potentiel f noté x_j.
- Pour chaque paire d'états (i,j) telle que $i\neq j$ et $\partial\Omega_j\cap\partial\Omega_i\neq\emptyset$, il existe un unique point selle $z_{i,j}\in\partial\Omega_j\cap\partial\Omega_i$ de plus basse énergie sur $\partial\Omega_j\cap\partial\Omega_i$. On a donc $z_{i,j}=z_{j,i}$ pour $i\neq j$.

Sur la figure A.4, nous donnons une représentation schématique en dimension 2 d'un découpage de l'espace des phases en domaines métastables ainsi que des points $(x_j)_{j\in\{1,\dots,N\}}$ et des différents points selles $(z_{i,j})_{(i,j)\in\{1,\dots,N\}^2,i\neq j}$.
Le taux de transition de l'état i vers l'état j est calculé en utilisant la formule d'Eyring-Kramers:

$$k_{i,j}=A_{i,j}^{-1}\,e^{-\frac{2}{h}(f(z_{i,j})-f(x_i))}. \tag{A.17}$$

Le préfacteur $A_{i,j}^{-1}$ est:

$$A_{i,j}^{-1}=\frac{|\lambda(z_{i,j})|}{2\pi}\frac{\sqrt{\det\mathrm{Hess}f(x_i)}}{\sqrt{|\det\mathrm{Hess}f(z_{i,j})|}}. \tag{A.18}$$

La modélisation de la dynamique d'état à état en utilisant ce modèle kinetic Monte Carlo, avec les formules (A.17) et (A.18) pour les taux de transition s'appelle la théorie de l'état de transition harmonique dans la littérature physique.

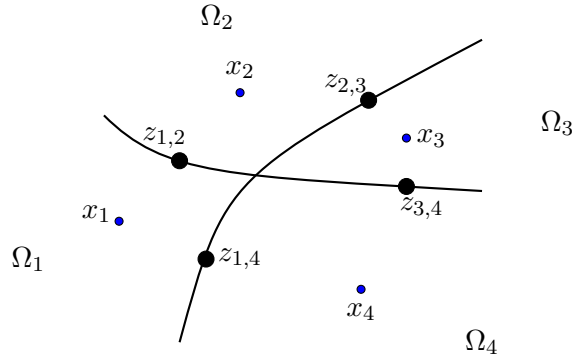

Figure A.4: Représentation schématique d'un système dont la décomposition de l'espace des phases $\mathbb{R}^2$ est composée de 4 domaines métastables $\{\Omega_1, \Omega_2, \Omega_3, \Omega_4\}$. Chaque point x_j représente l'unique minimum global de f dans Ω_j et le point $z_{i,j}$ est l'unique point selle de plus basse énergie sur $\partial\Omega_j \cap \partial\Omega_i$.

A.2.1.4 Justification de l'utilisation des méthodes de Monte-Carlo cinétique

Dans cette section, nous allons expliquer pourquoi les méthodes de Monte-Carlo cinétique peuvent être utilisées pour simuler correctement l'événement de sortie d'un domaine métastable. Ces méthodes peuvent ainsi permettre d'échantillonner efficacement la dynamique d'état à état $\big(S(X_t)\big)_{t\geq 0}$ en simulant les parties de la trajectoire de $\big(S(X_t)\big)_{t\geq 0}$ lorsque le processus est bloqué dans un état métastable.

Soit $(X_t)_{t\geq 0}$ le processus (1) modélisant l'évolution du système et $\Omega \in \{\Omega_1, ..., \Omega_N\}$ un domaine de l'espace des phases correspondant à un état E du système (cf. (A.14) et (A.15)). Définissons le premier temps de sortie du domaine Ω:

$$\tau_\Omega := \inf\{t \geq 0, X_t \notin \Omega\}. \tag{A.19}$$

Voici la définition d'une distribution quasi stationnaire:

Definition A.1. *Une mesure de probabilité ν_h sur Ω est une distribution quasi stationnaire pour le processus $(X_t)_{t\geq 0}$ sur Ω si pour $t \geq 0$ et pour tout ensemble mesurable A de Ω,*

$$\mathbb{P}^{\nu_h}\big[X_t \in A \big| t < \tau_\Omega\big] = \nu_h(A).$$

La notation $\mathbb{P}_\mu$ désigne la probabilité d'un événement sachant que le processus $(X_t)_{t\geq 0}$ est initialement distribué suivant la mesure de probabilité μ i.e. $X_0 \sim \mu$.
Comme le montrent la proposition et le corollaire suivant, sous des propriétés de régularité du domaine Ω et du potentiel f, il existe une unique distribution quasi-stationnaire et la loi du processus $(X_t)_{t\geq 0}$ conditionné à ne pas être sorti de Ω converge en temps long vers cette distribution quasi-stationnaire (cf. [13, 50]).

Proposition A.1. *Supposons que le domaine Ω est un ouvert borné C^∞ et que le potentiel $f : \mathbb{R}^d \to \mathbb{R}$ est C^∞. Alors, il existe une mesure de probabilité ν_h sur Ω et $c > 0$ telle que pour toute mesure de probabilité μ sur Ω, il existe $C(\mu) > 0$ et $t(\mu) > 0$*

tels que pour tout $t \geq t(\mu)$ et tout ensemble mesurable A de Ω:

$$\left|\mathbb{P}^{\mu}\left[X_t \in A \middle| t < \tau_\Omega\right] - \nu_h(A)\right| \leq C(\mu)e^{-ct}. \tag{A.20}$$

Nous déduisons immédiatement le corollaire suivant:

Corollaire A.2. *Supposons que le domaine Ω est un ouvert borné C^∞ et que le potentiel $f : \mathbb{R}^d \to \mathbb{R}$ est C^∞. Alors la mesure ν_h définie pour tout mesurable A de Ω par*

$$\nu_h(A) = \lim_{t\to\infty} \mathbb{P}\left[X_t \in A \middle| t < \tau_\Omega\right],$$

est indépendante de la condition initiale: c'est l'unique distribution quasi stationnaire pour le processus $(X_t)_{t\geq 0}$ sur Ω.

La constante c dans la Proposition A.1 donne, en temps long, le taux de convergence vers la distribution quasi stationnaire.

Remarque A.8. *La distribution quasi stationnaire joue un rôle fondamentale en dynamique des populations pour l'étude des processus conditionnés à la non-extinction comme les dynamiques modélisant l'évolution de populations, cf. par exemple les livres [1] et [15].*

Remarque A.9. *Dans la littérature, on appelle limite de Yaglom la limite en temps long du processus $(X_t)_{t\geq 0}$ conditionné à ne pas être sorti de Ω lorsque cette limite est indépendante de la condition initiale déterministe X_0. En d'autres termes, supposons que la mesure définie pour tout mesurable A de Ω par*

$$\mathcal{Y}(A) := \lim_{t\to\infty} \mathbb{P}_x\left[X_t \in A \middle| t < \tau_\Omega\right],$$

existe et est indépendante de $x \in \Omega$, alors $\mathcal{Y}$ est appelée limite de Yaglom du processus $(X_t)_{t\geq 0}$ associée au temps d'arrêt τ_Ω. Cette appellation a été donnée en référence à A.M Yaglom qui fut le premier à établir l'existence de lois limites pour des processus de branchement conditionnés dans son article [75]. Un résultat standard affirme que la limite de Yaglom est une distribution quasi stationnaire (cf. [15]). C'est pourquoi, il arrive dans la littérature que l'on rencontre l'appellation limite de Yaglom pour désigner une distribution quasi stationnaire.

A l'aide de la distribution quasi stationnaire, on peut donner une définition de la métastabilité d'un domaine:

Définition A.1. *De manière informelle, un domaine Ω est dit métastable si la convergence vers la distribution quasi stationnaire (cf.* (A.20)*) est bien plus rapide que le temps moyen de sortie du domaine Ω.*

Remarquons toutefois que la définition de la métastabilité d'un domaine introduite en Définition A.1 dépend de la condition initiale du processus $(X_t)_{t\geq 0}$ et que selon la Définition A.1, un domaine peut être métastable pour certaines conditions initiales mais pas pour d'autres. Ce point est discuté en Section A.5.3, cf. Remarque A.20.
Une des propriétés importantes de la distribution quasi stationnaire qui sera fondamentale afin de répondre au problème posé en début de cette section est la suivante:

Proposition A.3. *Supposons que le domaine Ω est un ouvert borné C^∞ et que le potentiel $f : \mathbb{R}^d \to \mathbb{R}$ est C^∞. Soit ν_h la distribution quasi stationnaire associée au processus $(X_t)_{t\geq 0}$ et au domaine Ω, introduite par la Proposition A.1. Supposons que $X_0 \sim \nu_h$. Alors, le temps de sortie τ_Ω et le point de sortie X_{τ_Ω} sont indépendants. De plus, il existe une constante $\lambda > 0$ telle que $\tau_\Omega \sim \mathcal{E}(\lambda)$.*

D'après la définition A.1, si le domaine Ω est métastable, le processus $(X_t)_{t\geq 0}$ est, une fois entré dans Ω, très vite distribué suivant la distribution quasi stationnaire ν et d'après la Proposition A.3, le temps passé dans Ω est donc (presque) exponentiellement distribué et (presque) indépendant du prochain état visité. Ces deux points sont les propriétés fondamentales des processus markoviens générés par les algorithmes de Monte-Carlo cinétique (cf. Section A.2.1.2). Cela justifie physiquement l'utilisation des méthodes de Monte-Carlo cinétique pour simuler efficacement les événements de sortie d'un domaine métastable.

Dans la suite, nous allons présenter une méthode permettant d'accélérer l'échantillonnage de la dynamique $\big(S(X_t)\big)_{t\geq 0}$ reposant sur le formalisme des méthodes de Monte-Carlo cinétique et qui ne nécessite pas de calculer les taux de transition entre les états.

A.2.2 Algorithme *temperature accelerated dynamics* et la formule d'Eyring-Kramers

L'algorithme *temperature accelerated dynamics* a été proposé par M.R. Sørensen et A.F Voter [67]. Cet algorithme a pour objectif de simuler de manière efficace la dynamique d'état à état $S(X_t)_{t\geq 0}$ (cf. Section A.2.1.1).

A.2.2.1 Présentation de l'algorithme *temperature accelerated dynamics*

L'idée de départ de l'algorithme provient du constat suivant: le temps de sortie d'un domaine métastable est d'autant plus grand que la température est petite, comme le montre par exemple la formule d'Eyring-Kramers (A.4).

Afin de simuler de manière efficace la dynamique d'état à état $S(X_t)_{t\geq 0}$, l'algorithme *temperature accelerated dynamics* procède comme suit. Considérons le processus $(X_t)_{t\geq 0}$ évoluant à la température h_{low}. On laisse évoluer la dynamique d'état à état $S(X_t)_{t\geq 0}$ jusqu'au premier moment t_j où le processus se retrouve piégé dans un domaine métastable $\Omega_j \subset \mathbb{R}^d$, où $j \in \{1, ..., N\}$. On arrête la dynamique $S(X_t)_{t\geq 0}$ à cet instant t_j. On accélère l'événement de sortie de Ω_j en augmentant la température du processus. Pour cela, on lance dans le domaine Ω_j un autre processus $(Y_t)_{t\geq 0}$ évoluant suivant la même équation d'évolution que $(X_t)_{t\geq 0}$ (ici (1)) mais à une température $h_{high} > h_{low}$ afin d'observer plus vite des sorties du domaine Ω_j. Ce qui aurait dû être l'événement de sortie à la température h_{low}, c'est-à-dire le prochain état k ($k \neq j$) et le temps T_j passé dans Ω_j pour le processus $(X_t)_{t\geq 0}$, se déduit par extrapolation d'un nombre suffisant d'événements de sortie de Ω_j du processus $(Y_t)_{t\geq 0}$ à la température h_{high} (cette étape est expliquée dans la section suivante). On approche ensuite la dynamique d'état à état $S(X_t)_{t\geq 0}$ en lui donnant la valeur j entre les instants t_j et $t_j + T_j$. On laisse ensuite évoluer $S(X_t)_{t\geq t_j+T_j}$ en faisant démarrer le processus $(X_t)_{t\geq t_j+T_j}$ dans le domaine Ω_k. On répète cette procédure à chaque fois que le processus est piégé dans un domaine

métastable. Pour une explication plus détaillée du procédé, le lecteur peut se référer à [67] ou [2] où une version modifiée de l'algorithme originel a aussi été proposée.

A.2.2.2 Loi d'Eyring-Kramers et l'algorithme *temperature accelerated dynamics*

Dans cette section, nous décrivons comment la loi d'Eyring-Kramers est utilisée pour extrapoler un événement de sortie à la température h_{low} à partir d'événements de sortie enregistrés à une température $h_{high} > h_{low}$. Soit $j \in \{1, ..., N\}$ et considérons un domaine Ω_ℓ voisin de Ω_j (i.e. tel que $\partial\Omega_j \cap \partial\Omega_\ell \neq \emptyset$). Supposons que le minimum de f dans $\overline{\Omega}_j$ est atteint en un seul point $x_j \in \Omega_j$ et que f atteint son minimum sur $\partial\Omega_j \cap \partial\Omega_\ell$ en un seul point selle $z_{j,\ell}$. Notons $\tau_{j,\ell}(h)$ la variable aléatoire égale au temps mis par le processus pour sortir de Ω_j à la température h par le point selle $z_{j,\ell}$. Dans l'algorithme *temperature accelerated dynamics*, la formule qui permet de calculer $\tau_{j,\ell}(h_{low})$ à partir $\tau_{j,\ell}(h_{high})$ est (on justifiera cette formule ci-dessous):

$$\tau_{j,\ell}(h_{low}) = \tau_{j,\ell}(h_{high})\, e^{2\left(\frac{1}{h_{low}} - \frac{1}{h_{high}}\right)(f(z_{j,\ell}) - f(x_j))}. \tag{A.21}$$

Expliquons comment, en utilisant (A.21), l'événement de sortie de Ω_j du processus $(X_t)_{t\geq 0}$ à la température h_{low} se déduit par extrapolation d'un nombre suffisant d'événements de sortie de Ω_j du processus $(Y_t)_{t\geq 0}$ à la température h_{high}. Considérons une sortie de $(Y_t)_{t\geq 0}$ vers un état Ω_ℓ voisin de Ω_j. Si c'est la première fois que l'on observe une sortie du processus $(Y_t)_{t\geq 0}$ vers Ω_ℓ, on extrapole le temps de sortie à la température h_{low} en utilisant la formule (A.21) puis on met à jour le plus petit des temps extrapolés et enregistrés jusqu'ici, que l'on note $\tau_{j,min}(h_{low})$. L'algorithme s'arrête lorsque suffisamment d'événements de sortie de $(Y_t)_{t\geq 0}$ ont été observés et que plus aucun autre événement de sortie de $(Y_t)_{t\geq 0}$ ne modifiera la valeur de $\tau_{j,min}(h_{low})$. Le prochain état visité par le processus $(X_t)_{t\geq 0}$ est l'état k pour lequel $\tau_{j,min}(h_{low}) = \tau_{j,k}(h_{low})$ et le temps passé par $(X_t)_{t\geq 0}$ dans l'état j est $T_j = \tau_{j,min}(h_{low})$.

Le formalisme qui permet de justifier ce procédé est celui des algorithmes de Monte-Carlo cinétique où les temps de transition entre les états sont exponentiellement distribués (cf. Section A.2.1.2 et plus particulièrement la Remarque A.7) et où les paramètres des lois exponentielles se calculent avec la loi d'Eyring Kramers (cf. (A.17) et (A.18)). Dans l'algorithme *temperature accelerated dynamics*, ce formalisme est utilisé. Il est en effet supposé qu'à la température h:

$$\tau_{j,\ell}(h) \sim \mathcal{E}\big(k_{j,\ell}\big) \quad \text{où} \quad k_{j,\ell} = A_{j,\ell}^{-1}\, e^{-\frac{2}{h}(f(z_{j,\ell}) - f(x_j))}$$

avec, pour la dynamique de Langevin suramortie (1):

$$A_{j,\ell} = \frac{2\pi}{|\lambda(z_{j,\ell})|} \frac{|\sqrt{\det \mathrm{Hess} f(z_{j,\ell})}|}{\sqrt{\det \mathrm{Hess} f(x_j)}}.$$

Le calcul du paramètre $k_{j,\ell}(h)$ de la loi exponentielle de $\tau_{j,\ell}(h)$ se fait donc en utilisant la formule d'Eyring-Kramers. Ainsi, en loi, nous avons l'égalité

$$\tau_{j,\ell}(h_{low}) = \tau_{j,\ell}(h_{high})\, e^{2\left(\frac{1}{h_{low}} - \frac{1}{h_{high}}\right)(f(z_{j,\ell}) - f(x_j))}.$$

Ce qui justifie (A.21).

En conclusion, la formule d'Eyring-Kramers est utilisée pour calculer les taux de transition entre les états dans un algorithme de Monte-Carlo cinétique lorsque l'on souhaite générer efficacement la dynamique d'état à état $\big(S(X_t)\big)_{t\geq 0}$. Elle est aussi utilisée pour extrapoler les temps de sortie à des températures plus basses dans l'algorithme *temperature accelerated dynamics*. **Nous allons désormais nous concentrer sur la question suivante: comment justifier rigoureusement l'utilisation d'un modèle de Monte-Carlo cinétique pour décrire l'événement de sortie d'un domaine métastable pour la dynamique de Langevin suramortie** (1)**?**

A.3 Stratégie pour prouver la formule d'Eyring-Kramers

Cette section a pour objectif d'expliquer l'approche que nous avons adoptée pour prouver la formule d'Eyring-Kramers. Notre stratégie est la suivante. La première étape consiste à trouver une expression des taux de transition compatible avec l'utilisation d'un algorithme de Monte-Carlo cinétique pour modéliser l'évènement de sortie d'un état métastable. La seconde étape est d'étudier le comportement asymptotique précis de ces expressions dans la limite d'une petite température.
La section est organisée comme suit. En Section A.3.1, nous proposons d'abord une expression pour les taux de transition, puis nous expliquons pourquoi ils sont compatibles avec l'utilisation d'une méthode de Monte-Carlo cinétique et enfin nous expliquons notre stratégie pour étudier le comportement asymptotique des taux de transition proposés. Enfin, en Section A.3.2, nous rappelons les approches qui ont été proposées jusqu'à aujourd'hui dans la littérature mathématique pour obtenir la loi d'Eyring-Kramers.

A.3.1 Expression des taux de transition entre les états

En Section A.3.1.1, nous donnons l'expression des taux de transition et nous expliquons pourquoi ces expressions sont compatibles avec une méthode Monte-Carlo cinétique. En Section A.3.1.2, nous expliquons notre stratégie de preuve pour obtenir un équivalent précis à basse température des taux de transition.

A.3.1.1 Expression des taux de transition

Soit $(X_t)_{t\geq 0}$ le processus (1). Considérons la collection de domaines $\{\Omega_1, ..., \Omega_N\}$ introduite en (A.14) qui forme une partition de l'espace des phases $\mathbb{R}^d$ en domaines métastables où chaque domaine Ω_j correspond à un état j du système (cf. (A.15)). Pour chaque $i \in \{1, ..., N\}$, τ_{Ω_i} désigne le premier temps de sortie du domaine Ω_i (cf. Définition A.19).

Considérons désormais un entier $i \in \{1, ..., N\}$. Pour $j \in \{1, ..., N\}$, $j \neq i$, nous définissons le taux de transition de l'état i vers l'état j par

$$k_{i,j}^L := \frac{1}{\mathbb{E}_{\nu_{h,\Omega_i}}\big[\tau_{\Omega_i}\big]} \mathbb{P}^{\nu_{h,\Omega_i}}\big[X_{\tau_{\Omega_i}} \in \partial\Omega_i \cap \partial\Omega_j\big], \tag{A.22}$$

où ν_{h,Ω_i}désigne la distribution quasi stationnaire associée au processus $(X_t)_{t\geq 0}$ et au domaine Ω_i (cf. Définition A.1). L'exposant L dans la notation $k_{i,j}^L$ indique que

nous considérons un système dont l'évolution est modélisée par l'équation de Langevin suramortie (1). Remarquons que lorsque l'état i n'est pas voisin de l'état j nous avons $\partial\Omega_i \cap \partial\Omega_j = \emptyset$ et ainsi on a bien $k^L_{i,j} = 0$.

Remarque A.10. *Si l'on veut retrouver la formule d'Eyring-Kramers* (A.17)-(A.18)*, il faut multiplier l'expression* (A.22) *par un facteur* $\frac{1}{2}$*. Ceci est dû au fait suivant: une fois que le processus* (1) *est sur* $\partial\Omega_i \cap \partial\Omega_j$*, il a, dans la limite* $h \to 0$*, une chance sur deux de revenir dans* Ω_i *et une chance sur deux d'aller dans* Ω_j*. En effet, en dimension un, ce résultat se montre en utilisant un calcul similaire à celui permettant de prouver* (A.6)*. En dimension supérieure, on peut se ramener au cas de la dimension un en utilisant un système de coordonnées adapté autour de* z_j*. Des méthodes similaires à celles utilisées pour prouver [4, Lemma B.1] permettent aussi de montrer ce résultat.*

Nous allons maintenant expliquer pourquoi l'expression des taux de transition (A.22) est compatible avec un algorithme de Monte-Carlo cinétique pour modéliser l'événement de sortie de l'état i. Pour cela, supposons que le domaine Ω_i est un ouvert borné C^∞ et que le potentiel $f : \mathbb{R}^d \to \mathbb{R}$ du système est C^∞; ceci nous permettra d'utiliser les propositions A.1 et A.3 pour la justification qui suit. Dans ce cas, et comme nous l'avons vu en fin de Section A.2.1.4, puisque le domaine Ω_i est métastable, le processus $(X_t)_{t\geq 0}$ est rapidement (en comparaison du temps moyen de sortie $\mathbb{E}\big[\tau_{\Omega_i}\big]$) distribué suivant la distribution quasi stationnaire ν_{h,Ω_i} (cf. Définition A.1 et Proposition A.1). Il est donc raisonnable d'étudier l'événement de sortie de Ω_i en supposant que le processus est initialement distribué suivant la distribution quasi stationnaire ν_{h,Ω_i}. De plus, lorsque $X_0 \sim \nu_{h,\Omega_i}$, d'après la Proposition A.3, il existe λ_i telle que $\tau_{\Omega_i} \sim \mathcal{E}(\lambda_i)$ et donc d'après (A.22), nous avons:

$$\sum_{j=1, j\neq i}^{N} k^L_{i,j} = \frac{1}{\mathbb{E}_{\nu_{h,\Omega_i}}\big[\tau_{\Omega_i}\big]} \mathbb{P}_{\nu_{h,\Omega_i}}\big[X_{\tau_{\Omega_i}} \in \partial\Omega_i\big] = \frac{1}{\mathbb{E}_{\nu_{h,\Omega_i}}\big[\tau_{\Omega_i}\big]} = \lambda_i. \tag{A.23}$$

Le choix d'avoir distribué initialement le processus $(X_t)_{t\geq 0}$ suivant ν_{h,Ω_i} dans la définition des taux de transition (A.22) est donc compatible avec la première étape de la récurrence d'un algorithme de Monte-Carlo cinétique qui permet d'échantillonner le temps passé dans chaque état, cf. Section A.2.1.2. De plus, lorsque $X_0 \sim \nu_{h,\Omega_i}$, d'après la Proposition A.3, le temps de sortie et le point de sortie sont indépendants. Enfin, d'après (A.22) et (A.23), nous avons pour tout $\ell \in \{1, ..., N\}$, $\ell \neq i$:

$$\mathbb{P}^{\nu_{h,\Omega_i}}\big[X_{\tau_{\Omega_i}} \in \partial\Omega_i \cap \partial\Omega_\ell\big] = \frac{k_{i,\ell}}{\sum_{j=1,\, j\neq i}^{N} k_{i,j}},$$

et donc la probabilité de passer de l'état i à l'état ℓ est $\frac{k_{i,\ell}}{\sum_{j=1,\, j\neq i}^{N} k_{i,j}}$. Ainsi, l'expression des taux de transition (A.22) est compatible avec la deuxième étape de la récurrence d'un algorithme de Monte-Carlo cinétique qui permet d'échantillonner le prochain état visité, cf. Section A.2.1.2.

A.3.1.2 Stratégie pour étudier la limite à basse température des taux de transition

Dans la suite, nous abandonnons l'indice $i \in \{1, ..., N\}$ et notons

$$\Omega = \Omega_i \in \{\Omega_1, ..., \Omega_N\}$$

un domaine métastable du processus (1) (cf. (A.14)). Afin d'expliquer notre stratégie pour étudier dans la limite d'une petite température les taux de transition (A.22) entre les états du système, nous allons montrer que les taux de transition (A.22) peuvent s'exprimer à l'aide des éléments spectraux de l'opérateur infinitésimal de la diffusion (1) avec conditions homogènes de Dirichlet sur $\partial\Omega$. Rappelons d'abord quelques résultats standards sur le générateur infinitésimal de la diffusion (1).

Dans toute cette section, le domaine Ω est un ouvert borné C^∞ et le potentiel $f : \mathbb{R}^d \to \mathbb{R}$ est C^∞.

<u>Un problème aux valeurs propres relié à la distribution quasi stationnaire sur Ω.</u>

Considérons l'opérateur $L^{(0)}_{f,h}$ défini par:

$$\phi \in C^\infty_c(\mathbb{R}^d, \mathbb{R}) \mapsto L^{(0)}_{f,h}\phi = \frac{h}{2}\Delta\phi - \nabla f \cdot \nabla\phi, \tag{A.24}$$

où $C^\infty_c(\mathbb{R}^d, \mathbb{R})$ désigne l'espace vectoriel des fonctions infiniment dérivables de $\mathbb{R}^d$ dans $\mathbb{R}$ et à support compact. L'exposant (0) dans la notation $L^{(0)}_{f,h}$ fait référence au fait que l'on travaille avec un opérateur agissant sur des fonctions (c'est-à-dire des 0-formes). Pour justifier les conditions aux limites associées à l'opérateur $L^{(0)}_{f,h}$ sur $\partial\Omega$, il faut comprendre quelles sont les conditions aux limites satisfaites par la loi du processus (1) conditionné à rester dans Ω. Pour cela, considérons le semi groupe (sous-markovien) du processus (1) absorbé au bord de Ω: il est défini pour tout $\phi \in C^\infty(\mathbb{R}^d, \mathbb{R})$, $x \in \overline{\Omega}$ et $t \geq 0$ par:

$$\big(P_t\phi\big)(x) = \mathbb{E}_x\big[\phi(X_t)\, 1_{\{t \leq \tau_\Omega\}}\big].$$

Un calcul d'Ito, montre que (au moins formellement):

$$\partial_t P_t\phi = L^{(0)}_{f,h}\, P_t\phi.$$

Un candidat naturel pour être le générateur infinitésimal du semi groupe de diffusion $(P_t)_{t\geq 0}$ est donc l'opérateur $L^{(0)}_{f,h}$. Il faut désormais identifier les conditions aux limites sur $\partial\Omega$ du générateur infinitésimal du semi groupe de diffusion $(P_t)_{t\geq 0}$. Par un résultat classique sur les semi groupes fortement continus, pour tout $t > 0$, $P_t\phi$ appartient au domaine de son générateur infinitésimal. Or, pour tout $t > 0$ et $x \in \partial\Omega$, nous avons:

$$\big(P_t\phi\big)(x) = 0.$$

Les conditions aux limites à associer à $L^{(0)}_{f,h}$ sont donc des conditions de Dirichlet sur $\partial\Omega$. Afin d'introduire un cadre fonctionnel adapté à l'opérateur $L^{(0)}_{f,h}$ avec des conditions de Dirichlet sur $\partial\Omega$, remarquons que pour tout $\phi \in C^\infty_c(\Omega)$ et $\psi \in C^\infty_c(\Omega)$,

$$\int_\Omega \phi\, \big(L^{(0)}_{f,h}\psi\big)\, e^{-\frac{2}{h}f} = -\frac{h}{2}\int_\Omega \nabla\phi \cdot \nabla\psi\, e^{-\frac{2}{h}f}.$$

Introduisons alors les espaces de Hibert suivants:

$$L^2_w(\Omega) = \left\{ u : \Omega \to \mathbb{R},\ \int_\Omega u^2(x) e^{-\frac{2}{h} f(x)}\, dx < \infty \right\}$$

et

$$H^1_w(\Omega) := \left\{ u : \Omega \to \mathbb{R},\ u \in L^2_w(\Omega) \text{ et pour tout } i = 1, ..., d : \partial_i u \in L^2_w(\Omega) \right\}. \tag{A.25}$$

Nous avons le résultat suivant qui permet de définir l'opérateur $L^{(0)}_{f,h}$ avec des conditions de Dirichlet sur $\partial\Omega$.

Proposition A.4. *L'extension de Friedrichs associée à la forme quadratique*

$$\phi \in C^\infty_c(\Omega) \mapsto \frac{h}{2} \int_\Omega |\nabla \phi|^2\, e^{-\frac{2}{h} f},$$

sur $L^2_w(\Omega)$, est notée $-L^{D,(0)}_{f,h}(\Omega)$. C'est un opérateur non borné, auto-adjoint et strictement positif sur $L^2_w(\Omega)$ dont le domaine est

$$D\left(L^{D,(0)}_{f,h}(\Omega)\right) = H^1_{w,0}(\Omega) \cap H^2_w(\Omega)$$

où $H^1_{w,0}(\Omega) = \{u \in H^1_w(\Omega),\ u = 0 \text{ sur } \partial\Omega\}$.

Preuve. La forme quadratique

$$\phi \in C^\infty_c(\Omega) \mapsto \frac{h}{2} \int_\Omega |\nabla \phi|^2\, e^{-\frac{2}{h} f}$$

est symétrique, positive et fermable et sa fermeture est la forme quadratique

$$Q :\ w \in H^1_{w,0}(\Omega) \mapsto \frac{h}{2} \int_\Omega |\nabla w|^2\, e^{-\frac{2}{h} f}.$$

Soit $-L^{D,(0)}_{f,h}(\Omega)$ l'opérateur auto-adjoint associé à Q. Il est défini sur le domaine

$$D\left(-L^{D,(0)}_{f,h}(\Omega)\right) = \left\{ u \in H^1_{w,0}(\Omega),\ \exists b \in L^2_w(\Omega),\ \forall v \in H^1_{w,0}(\Omega),\ Q(u,v) = \langle b, v \rangle_{L^2_w} \right\},$$

par

$$-L^{D,(0)}_{f,h}(\Omega) u = b.$$

Soit $u \in D\left(-L^{D,(0)}_{f,h}(\Omega)\right)$. Au sens des distributions, nous avons donc

$$-\frac{h}{2} \mathrm{div}\left(e^{-\frac{2}{h} f} \nabla u\right) = b$$

pour une fonction $b \in L^2_w(\Omega)$. D'après un résultat standard de régularité elliptique, la fonction u appartient à $H^2_w(\Omega)$. Ainsi, nous avons $D\left(-L^{D,(0)}_{f,h}(\Omega)\right) \subset H^1_{w,0}(\Omega) \cap H^2_w(\Omega)$. Une intégration par parties montre que $H^1_{w,0}(\Omega) \cap H^2_w(\Omega) \subset D\left(-L^{D,(0)}_{f,h}(\Omega)\right)$. Ce qui conclut la preuve de la proposition.

∎

Le domaine Ω étant borné et C^∞, l'espace $H^1_w(\Omega)$ s'injecte de manière compacte dans $L^2_w(\Omega)$ et ainsi l'opérateur $-L^{D,(0)}_{f,h}(\Omega)$ est à résolvante compacte: son spectre est donc discret. Dans la suite nous notons $\lambda_h > 0$ sa plus petite valeur propre. Nous avons alors le résultat suivant (c'est un résultat standard sur la première valeur propre d'un opérateur elliptique, cf. par exemple [28, Théorème 2]):

Proposition A.5. *La plus petite valeur propre λ_h de $-L^{D,(0)}_{f,h}(\Omega)$ est simple et son vecteur propre associé, noté u_h, a un signe sur Ω. De plus, $u_h \in C^\infty(\overline{\Omega})$.*

Preuve. Par un résultat standard de régularité elliptique, tous les vecteurs propres de $-L^{D,(0)}_{f,h}(\Omega)$ sont dans $C^\infty(\overline{\Omega})$. L'opérateur $-L^{D,(0)}_{f,h}(\Omega)$ est auto-adjoint et donc par le principe du min-max:

$$\lambda_h = \min_{v \in H^1_{w,0}(\Omega)} \frac{h}{2} \frac{\displaystyle\int_\Omega |\nabla v|^2 \, e^{-\frac{2}{h}f}}{\displaystyle\int_\Omega v^2 e^{-\frac{2}{h}f}}, \tag{A.26}$$

et toute fonction u est un vecteur propre associé à λ_h si et seulement si u est un minimiseur de (A.26). Soit u un vecteur propre associé à λ_h. Puisque nous avons

$$\big|\nabla |u|\big|^2 = \big|\nabla u\big|^2,$$

nous en déduisons que la fonction $|u|$ est aussi un minimiseur de (A.26) et donc est un vecteur propre associé à λ_h. En utilisant l'inégalité de Harnack, nous obtenons que $|u| > 0$ sur Ω. Supposons par l'absurde que λ_h est une valeur propre dégénérée de $-L^{D,(0)}_{f,h}(\Omega)$. Soient alors v_1 et v_2 deux vecteurs propres libres associés à λ_h. Les deux fonctions v_1 et v_2 étant continues, il existe $x_0 \in \Omega$ tel que $v_1(x_0) \neq v_2(x_0)$. Ainsi la fonction

$$w = v_2(x_0)v_1 - v_1(x_0)v_2$$

est non identiquement nulle sur Ω: c'est donc un vecteur propre associé à λ_h. On en déduit de ce qui précède que $|w| > 0$ sur Ω, ce qui est absurde car $w(x_0) = 0$. Ainsi λ_h est non dégénérée. ∎

Dans la suite et sans perte de généralité, nous supposons que

$$u_h > 0 \text{ sur } \Omega \quad \text{et} \quad \int_\Omega u_h^2(x) \; e^{-\frac{2}{h}f(x)} dx = 1. \tag{A.27}$$

Le lien entre la distribution quasi stationnaire ν_h (cf. Définition A.1) et u_h est donné par la proposition suivante (cf. par exemple [50]):

Proposition A.6. *L'unique distribution quasi stationnaire associée au processus* (1) *et au domaine Ω est:*

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

où u_h est le vecteur propre associé à la plus petite valeur propre de $-L^{D,(0)}_{f,h}(\Omega)$ (cf. Proposition A.5) qui satisfait (A.27).

Nous pouvons ensuite énoncer un résultat sur l'événement de sortie plus précis que la Proposition A.3:

Proposition A.7. *Considérons la dynamique* (1) *et la distribution quasi stationnaire* ν_h *associée au domaine* Ω. *Si* X_0 *est distribué selon* ν_h, *les variables aléatoires* τ_Ω *et* X_{τ_Ω} *sont indépendantes. De plus,* τ_Ω *est exponentiellement distribuée de paramètre* λ_h *et la loi de* X_{τ_Ω} *a une densité par rapport à la mesure de Lebesgue sur* $\partial\Omega$ *donnée par:*

$$z \in \partial\Omega \mapsto -\frac{h}{2\lambda_h} \frac{\partial_n u_h(z) e^{-\frac{2}{h} f(z)}}{\int_\Omega u_h(y) e^{-\frac{2}{h} f(y)} dy}, \tag{A.28}$$

où u_h *est le vecteur propre associé à la plus petite valeur propre de* $-L_{f,h}^{D,(0)}(\Omega)$ *(cf. Proposition A.5).*

La notation $\partial_n = n \cdot \nabla$ désigne la dérivée normale et n le vecteur normal sortant de Ω.

Stratégie générale pour étudier la limite à basse température des taux de transition (A.22).

Rappelons que $\Omega = \Omega_i \in \{\Omega_1, ..., \Omega_N\}$ désigne un domaine métastable du processus (1) (cf. (A.14)) correspondant à un état i du système (cf. (A.15)). Dans la suite, pour tout $j \in \{1, ...N\}$, $j \neq i$, nous notons simplement

$$k_j^L = k_{i,j}^L$$

le taux de transition de l'état i vers l'état j défini en (A.22). Nous pouvons désormais donner une autre expression des taux de transition définis en (A.22) à l'aide du premier vecteur u_h associé à la plus petite valeur propre λ_h de $-L_{f,h}^{D,(0)}(\Omega)$. D'après la Proposition A.7, le taux de transition k_j^L, pour $j \in \{1, ..., N\}$ telle que $\Omega_j \neq \Omega$, a pour expression:

$$k_j^L = -\frac{h}{2} \frac{\int_{\partial\Omega \cap \partial\Omega_j} \partial_n u_h(z) e^{-\frac{2}{h} f(z)} \sigma(dz)}{\int_\Omega u_h(y) e^{-\frac{2}{h} f(y)} dy} \tag{A.29}$$

où σ désigne la mesure de Lebesgue sur $\partial\Omega$. De plus, toujours d'après la Proposition A.7, lorsque le processus (1) est initialement distribué suivant la distribution quasi stationnaire ν_h, le temps moyen passé dans le domaine Ω est:

$$\mathbb{E}_{\nu_h}\left[\tau_\Omega\right] = \frac{1}{\lambda_h} \tag{A.30}$$

et la loi de sortie du domaine Ω est donnée par :

$$\mathbb{P}^{\nu_h}\left[X_{\tau_\Omega} \in \Sigma\right] = -\frac{h}{2\lambda_h} \frac{\int_\Sigma \partial_n u_h(z) e^{-\frac{2}{h} f(z)} \sigma(dz)}{\int_\Omega u_h(y) e^{-\frac{2}{h} f(y)} dy}, \tag{A.31}$$

où $\Sigma \subset \partial\Omega$ est un ensemble mesurable.

Remarque A.11. *Bien que λ_h n'apparaisse pas dans l'expression des taux de transition* (A.29)*, son comportement asymptotique peut suffir à obtenir la formule d'Eyring-Kramers pour certains taux de transition. En effet, supposons que le domaine Ω_j soit tel que*

$$\lim_{h\to 0} \mathbb{P}^{\nu_h}\left[X_{\tau_\Omega} \in \partial\Omega \cap \partial\Omega_j\right] = 1.$$

Il vient alors d'après (A.22) *et d'après* (A.30)*:*

$$\lim_{h\to 0} \lambda_h \, k_j^L = 1.$$

Toutefois, l'étude du comportement asymptotique de λ_h quand $h \to 0$ ne suffit pas a priori à obtenir le comportement asymptotique de tous les taux de transition comme le montre aussi l'expression (A.29)*.*

Au vu des expressions (A.29), (A.30) et (A.31), notre stratégie est d'étudier le comportement précis dans la limite d'une petite température ($h \to 0$) de:

1. la première valeur propre λ_h de l'opérateur $-L_{f,h}^{D,(0)}(\Omega)$,
2. de la dérivée normale du vecteur propre u_h associé à λ_h,
3. et de la quantité $\int_\Omega u_h(y) e^{-\frac{2}{h}f(y)} dy$.

Notre analyse nous permet d'expliciter les taux d'erreur lors du passage à la limite $h \to 0$. Enfin, nous avons étendu nos résultats sur la distribution de sortie (i.e. sur la loi de X_{τ_Ω}) à des conditions déterministes dans le domaine Ω.

A.3.2 Littérature mathématique sur la loi d'Eyring-Kramers

Cette section a pour but de rappeler les contributions mathématiques obtenues jusqu'ici concernant la loi d'Eyring-Kramers. Le lecteur peut se référer à l'article [3] pour une revue sur le sujet ainsi que pour une explication des différentes techniques utilisées. Il y a deux approches qui se détachent dans la littérature: les approches globales et les approches locales.

A.3.2.1 Les approches globales

Les approches globales reposent sur l'étude à basse température ($h \to 0$) des valeurs propres du générateur infinitésimal $L_{f,h}^{(0)}$ de la diffusion (1) sur tout l'espace $\mathbb{R}^d$. Il est possible de montrer, que si le potentiel f a m minima locaux notés $\{x_1, ..., x_m\}$, alors l'opérateur (A.24) a exactement m valeurs propres exponentiellement petites dans la limite $h \to 0$ que l'on note $\{\lambda_1, \lambda_2, ..., \lambda_m\}$ avec $\lambda_1 = 0 < \lambda_2 \leq .... \leq \lambda_m$. De plus, les $m-1$ valeurs propres $\{\lambda_2, ..., \lambda_m\}$ satisfont une loi d'Eyring-Kramers. En effet, on peut montrer que si l'on suppose que pour chaque $k \in \{2, ..., m\}$ il existe un unique point z_k tel que

$$f(z_k) = \inf_{\gamma \in \mathcal{P}(x_k, B_k)} \sup_{t\in[0,1]} f(\gamma(t))$$

où B_k est une réunion de petites boules centrées en chacun des minima locaux de f plus bas en énergie que x_k et $\mathcal{P}(x_k, B_k)$ est l'ensemble des courbes $\gamma \in C^0([0,1], \mathbb{R}^d)$ telles

que $\gamma(0) = x_k$ et $\gamma(1) \in B_k$. , alors dans la limite $h \to 0$

$$\lambda_k = \frac{|\lambda(z_k)|}{2\pi} \frac{\sqrt{\det \mathrm{Hess} f(x_k)}}{|\sqrt{\det \mathrm{Hess} f(z_k)}|} e^{-\frac{2}{h}(f(z_k)-f(x_k))}(1+o(h)), \tag{A.32}$$

où $\lambda(z_k)$ est la valeur propre négative de la matrice hessienne de f en z_k. Pour faire le lien avec la Section A.1.2.1 et plus précisément avec la formule (A.4), le point z_k est le point selle de plus basse énergie qui connecte x_k à tous les autres minima locaux de f qui sont plus bas en énergie que x_k. Dans les articles [6,7,27], chacune des valeurs propres λ_k (pour $k \in \{2, ..., m\}$) a été reliée au temps moyen mis par le processus (1) pour aller d'un minimum local x_k à un autre minimum plus bas en énergie et une approche basée sur la théorie du potentiel a permis d'obtenir la formule (A.32). Dans [36], l'utilisation de techniques d'analyse semi-classique a aussi permis d'obtenir (A.32).

Citons par ailleurs le travail récent [58] qui généralise les résultats obtenus dans [36]. Le lecteur peut aussi se référer aux travaux plus anciens [59], [44], [17], [18], [16]. Les résultats qui découlent d'une approche globale permettent d'avoir accès aux comportements asymptotiques à basse température des temps moyens successifs pour aller d'un minimum local vers le minimum global. Ils ne permettent pas d'obtenir la formule d'Eyring-Kramers pour tous les taux de transition.
Ces approches globales sont utilisées pour construire une dynamique markovienne en projetant à l'aide d'une méthode de Galerkine le générateur infinitésimal de la diffusion (1) sur l'espace propre associé aux m petites valeurs propres $\{\lambda_1, ..., \lambda_m\}$. Cette projection permet d'avoir une très bonne approximation du générateur infinitésimal à basse température. Ceci a été largement étudié par Schütte et ses collaborateurs [66] en partant du travail [65]

A.3.2.2 Les approches locales

Dans cette thèse nous adoptons une approche locale: nous étudions l'événement de sortie d'un domaine $\Omega \subset \mathbb{R}^d$ (le point sortie et le temps de sortie) à basse température.

La théorie des grandes déviations.

L'approche la plus connue pour étudier l'événement de sortie à basse température est sans doute la théorie des grandes déviations développée par Freidlin et Wentzell dans les années 1970 et dont le livre [30] résume les principaux travaux. Cette théorie repose principalement sur l'étude de petits bouts de processus définis à l'aide d'une suite croissante de temps d'arrêt. La notion de fonction de taux y est fondamentale: elle donne le coût d'une déviation du processus par rapport à une trajectoire déterministe (la première utilisation de la fonction de taux est due à Schilder [62] pour un mouvement Brownien).
Voici quelques résultats typiques dus à Freidlin et Wentzell (cf. [30, Théorème 2.1, Théorème 4.1, Théorème 5.1]). Soit Ω un domaine ouvert borné C^∞. Rappelons que τ_Ω désigne le premier temps de sortie de Ω, cf. (A.19). Supposons que $\partial_n f > 0$ sur $\partial\Omega$ et que f a un unique point critique x_0 dans Ω qui est non dégénéré et tel que $f(x_0) = \min_{\overline{\Omega}} f$. Alors pour tout $x \in \Omega$:

$$\lim_{h\to 0} h \ln \mathbb{E}^x\left[\tau_\Omega\right] = 2(\inf_{\partial\Omega} f - f(x_0)).$$

De plus, pour tout $x \in \Omega$ tel que $f(x) < \inf_{\partial\Omega} f$ et pour tout $\delta > 0$, il existe $\delta_0 \in (0, \delta]$ tel que pour tout $y \in \partial\Omega$:

$$\lim_{h\to 0} h \ln \mathbb{P}^x \big[|X_{\tau_\Omega} - y| < \delta_0\big] = 2(f(y) - \inf_{\partial\Omega} f).$$

Enfin, si l'infimum de f sur $\partial\Omega$ est atteint en un seul point $y_0 \in \partial\Omega$, alors pour tout $\delta > 0$:

$$\lim_{h\to 0} \mathbb{P}^x \big[|X_{\tau_\Omega} - y_0| < \delta\big] = 1.$$

En d'autres termes, quand la température tend vers 0, le processus sort de Ω autour y_0. Un autre résultat dû à Day [19] affirme que sous les hypothèses énoncées ci-dessus, lorsque $h \to 0$, le temps de sortie τ_Ω converge en loi vers une variable exponentiellement distribuée de paramètre λ_h et pour tout $x \in \Omega$

$$\lim_{h\to 0} \lambda_h \mathbb{E}_x \big[\tau_\Omega\big] = 1,$$

où λ_h est la plus petite valeur propre de $-L^{D,(0)}_{f,h}(\Omega)$ (cf. Proposition A.5). Les résultats issus des grandes déviations s'appliquent dans des situations bien plus générales que celles que que l'on utilise dans cette thèse (par exemple à des fonctions f ayant plusieurs points critiques dans Ω ou à des processus non réversibles [5]...). Toutefois, trois problèmes se posent si l'on veut prouver la formule d'Eyring-Kramers à l'aide des résultats issus de la théorie des grandes déviations: le premier est qu'il est souvent bien difficile de calculer explicitement l'énergie d'activation, le second est que les résultats ne permettent pas de determiner le préfacteur $A_{i,j}$ dans (A.17) et le troisième est que les résultats obtenus ne donnent pas d'estimées d'erreur.

Approche par des équations aux dérivées partielles.

Un des résultats les plus connus concernant le comportement à basse température de la loi du point de sortie X_{τ_Ω}, obtenu dans [60] à l'aide de calculs formels, est le suivant: soit $F \in C^\infty(\partial\Omega, \mathbb{R})$ et $x \in \Omega$, alors quand $h \to 0$:

$$\mathbb{E}_x\big[F\big(X_{\tau_\Omega}\big)\big] = \frac{\int_{\partial\Omega} F(z)\partial_n f(z)\, e^{-\frac{2}{h}f(z)}\, dz}{\int_{\partial\Omega} \partial_n f\, e^{-\frac{2}{h}f}\, d\sigma} + o(h), \tag{A.33}$$

Ainsi, quand la température est petite, le processus sort presque sûrement autour des minima globaux de $f|_{\partial\Omega}$: la loi de X_{τ_Ω} se concentre sur $\arg\min_{\partial\Omega} f$. De plus, un équivalent asymptotique de l'espérance de τ_Ω quand $h \to 0$ a aussi été formulé dans [60]. Ces limites ont été obtenues en étudiant les équations aux dérivées partielles satisfaites par les fonctions $x \in \Omega \mapsto \mathbb{E}_x\big[F\big(X_{\tau_\Omega}\big)\big]$ et $x \in \Omega \mapsto \mathbb{E}_x\big[\tau_\Omega\big]$ et en y injectant des développements formels. Le lecteur peut aussi se référer aux articles [60,63,64] et [53,54] pour des études similaires à [60]. La formule (A.33) a été prouvée rigoureusement par Kamin dans [47]. Cette formule a été ensuite étendue aux dynamiques non réversibles par Kamin dans [46] et par Perthame dans [61]. Les résultats obtenus dans [46, 47, 61] ne permettent toutefois pas d'obtenir un équivalent précis de la probabilité de sortir par un point qui n'est pas un minimum global de f sur le bord de Ω.

Enfin, nous mentionnons [22, 23, 37, 44, 51, 56, 57] pour une étude du comportement asymptotique de λ_h et u_h (cf. Proposition A.5) dans la limite d'une petite température. Le lecteur peut aussi se référer à l'article [20] pour une revue de la littérature sur le comportement à basse température de l'événement de sortie d'un domaine.

Remarque A.12. *Certains auteurs ont prouvé la convergence vers un processus markovien de sauts en utilisant un changement d'échelle en temps. On renvoie par exemple à [49] pour une diffusion unidimensionnelle dans un double puits et à [31, 57] pour un problème similaire en dimension supérieure. Dans [68], il est montré qu'un changement d'échelle temporelle permet d'obtenir une convergence de la diffusion vers un processus markovien à sauts entre les minima globaux du potentiel f en supposant que ces derniers sont séparés par des points selles à la même hauteur.*

Dans cette thèse et comme nous l'avons expliqué en Section A.3.1.2, nous adoptons une approche locale pour étudier l'événement de sortie à basse température afin de montrer que l'on peut modéliser l'événement de sortie par un modèle markovien de sauts paramétré par les formules d'Eyring-Kramers.

A.4 Résultats du Chapitre B

Les résultats que nous allons présenter dans cette section sont ceux du Chapitre B dont les articles supports sont [25] et [26]. Dans le Chapitre B, nous obtenons des estimées précises sur la loi de X_{τ_Ω} et sur l'espérance de τ_Ω afin notamment d'obtenir un équivalent précis des taux de transition (A.22) dans la limite $h \to 0$.

Dans toute cette section le domaine Ω est un sous domaine ouvert C^∞ connexe et borné de $\mathbb{R}^d$. Précisons toutefois que nos résultats (du Chapitre B et du Chapitre C) ont été prouvés dans le cadre géométrique plus général où $\overline{\Omega}$ est une variété compacte, C^∞, riemannienne, connexe, orientée, de dimension d et de bord $\partial\Omega$, et dans ce cas Ω est l'intérieur de $\overline{\Omega}$. Nous rappelons que le processus étudié est le processus de Langevin suramorti (1):

$$dX_t = -\nabla f(X_t) + \sqrt{h}\, dB_t, \tag{A.34}$$

où $f : \mathbb{R}^d \to \mathbb{R}$ est l'énergie potentielle du système considéré ($d \in \mathbb{N}^*$), $h > 0$ est sa température et $(B_t)_{t\geq 0}$ un mouvement brownien standard dans $\mathbb{R}^d$. Afin d'étudier l'événement de sortie du domaine Ω, nous rappelons que τ_Ω désigne le premier temps de sortie de Ω:

$$\tau_\Omega := \inf\{t \geq 0, X_t \notin \Omega\}.$$

Dans toute la suite, la fonction f est supposée de classe C^∞. Rappelons enfin que nous cherchons à obtenir des estimées précises sur l'événement de sortie de Ω, c'est-à-dire sur le couple $(X_{\tau_\Omega}, \tau_\Omega)$. Dans la suite nous aurons besoin des définitions suivantes.

Definition A.2. *Soit $F \in C^\infty(\mathbb{R}^d)$. On dit que $x \in \mathbb{R}^d$ est un point critique non dégénéré de F si $\nabla F(x) = 0$ et si la hessienne de F en x est inversible. Soit x un point critique non dégénéré de F, on dit que x est un point selle de F si la matrice hessienne de f a exactement une seule valeur propre négative. Enfin, F est une fonction de Morse si elle est C^∞ et si tous ses points critiques sont non dégénérés.*

Remarque A.13. *Remarquons qu'une fonction de Morse a un nombre fini de points critiques dans tout compact de $\mathbb{R}^d$. En effet, les points critiques d'une fonction de Morse sont isolés.*

A.4.1 Les hypothèses sur la fonction f

Introduisons les hypothèses suivantes sur f (la numérotation des hypothèses est la même que dans le Chapitre B).

- **[H1]** La fonction f est C^∞. Les fonctions $f : \overline{\Omega} \to \mathbb{R}$ et la restriction de f au bord de Ω, notée $f|_{\partial\Omega}$, sont des fonctions de Morse (cf. Définition A.2). De plus, $|\nabla f|(x) \neq 0$ pour tout $x \in \partial\Omega$.

- **[H2]** La fonction f a un unique minimum global x_0 dans $\overline{\Omega}$ et

$$\min_{\partial\Omega} f > \min_{\overline{\Omega}} f = \min_{\Omega} f = f(x_0).$$

  Le point x_0 est l'unique point critique de f dans $\overline{\Omega}$. La fonction $f|_{\partial\Omega}$ a exactement $n \geq 1$ minima locaux notés $(z_i)_{i=1,...,n}$. Ils sont ordonnés tels que $f(z_1) \leq .... \leq f(z_n)$.

- **[H3]** $\partial_n f(x) > 0$ pour tout $x \in \partial\Omega$ (où ∂_n désigne la dérivée extérieure à Ω).

Sous l'hypothèse **[H2]**, l'entier $n_0 \in \{1, ..., n\}$ est défini comme le nombre de minima globaux de $f|_{\partial\Omega}$, i.e.:

$$f(z_1) = ... = f(z_{n_0}) < f(n_{n_0+1}) \leq ... \leq f(z_n).$$

Sur la Figure A.5, nous représentons sur un exemple en dimension 2 les points $(z_i)_{i=1,...,n}$ dans un cas où $n = 4$ et $n_0 = 2$. L'hypothèse **[H1]** implique que la fonction f ne peut pas avoir de point selle au bord de Ω. En réalité, sous les hypothèses **[H1]**, **[H2]** et **[H3]**, ce sont les points $(z_i)_{i=1,...,n}$ qui jouent le rôle de points selles. Ils sont appelés des points selles généralisés d'indice 1 pour $-L^{D,(0)}_{f,h}$, d'après [37, Section 5.2]. Cette dénomination est liée au fait que sous **[H1]**, **[H2]**, **[H3]** et lorsque l'on prolonge la fonction f par $-\infty$ en dehors de $\overline{\Omega}$, les points $(z_i)_{i=1,...,n}$ sont géométriquement des points selles (le prolongement de f par $-\infty$ est consistant avec les conditions aux limites de Dirichlet utilisées pour définir l'opérateur $-L^{D,(0)}_{f,h}$).

Nous définissons ensuite la fonction $g : \overline{\Omega} \to \mathbb{R}^+$ par

$$g(x) = \left|\nabla f(x)\right| \text{ pour } x \in \Omega \text{ et } g(x) = \left|\nabla_T f(x)\right| \text{ pour } x \in \partial\Omega, \tag{A.35}$$

où $\nabla_T f$ désigne le gradient tangentiel de f dans le bord de Ω. Les hypothèses dont nous aurons besoin dans cette section reposent sur la distance dans $\overline{\Omega}$ entre les points $(z_i)_{i=1,...,n}$ en terme de distance géodésique pour la métrique g définie en (A.35). Cette distance est appelée distance d'Agmon et elle est définie comme suit. Pour deux points $x \in \overline{\Omega}$ et $y \in \overline{\Omega}$, la distance d'Agmon entre x et y est définie par:

$$d_a(x, y) := \inf_{\gamma \in \mathrm{Lip}(x,y)} L(\gamma, (0, 1)), \tag{A.36}$$

où $\mathrm{Lip}(x, y)$ est l'ensemble des courbes Lipschitz $\gamma : [0, 1] \to \overline{\Omega}$ telles que $\gamma(0) = 1$ et $\gamma(1) = y$, et pour $\gamma \in \mathrm{Lip}(x, y)$,

$$L(\gamma, (0, 1)) = \int_0^1 g(\gamma(t))|\gamma'(t)|dt.$$

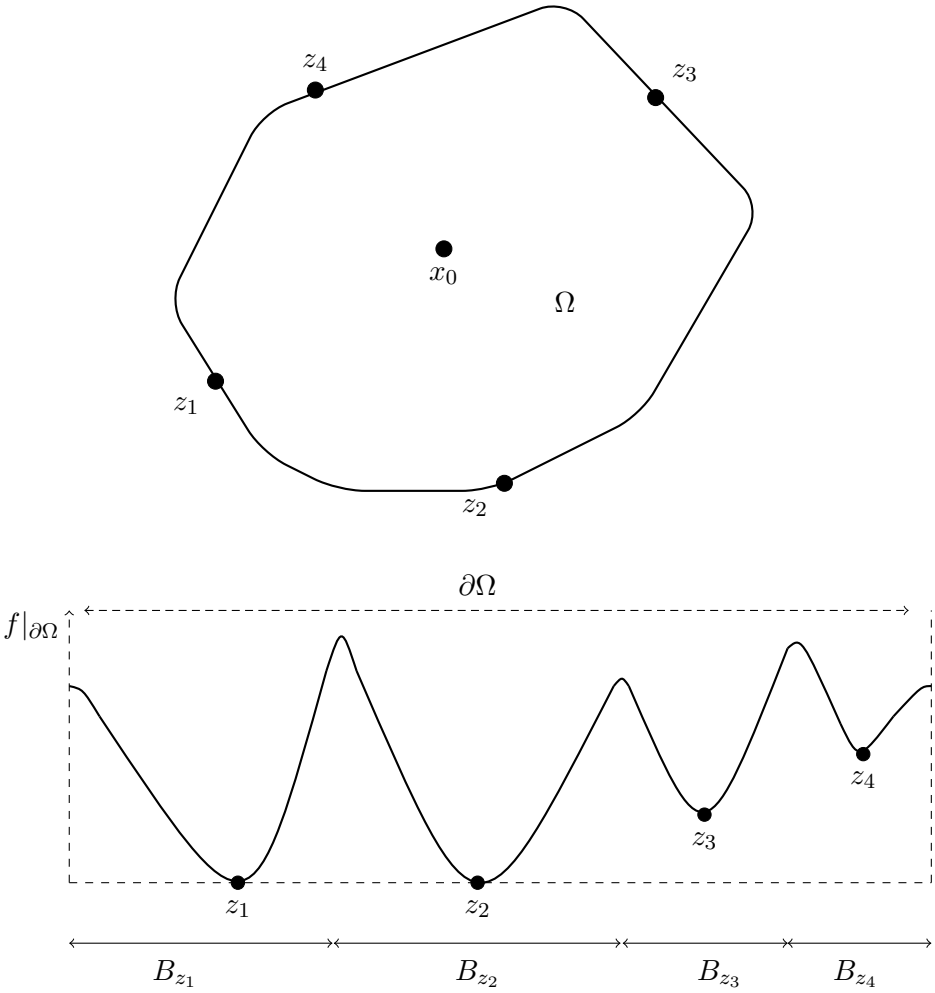

Figure A.5: Représentation schématique en dimension deux d'une fonction f satisfaisant les hypothèses **[H1]**, **[H2]** et **[H3]**, ainsi que sa restriction au bord de Ω, $f|_{\partial\Omega}$. Sur ce dessin, $n = 4$ et $n_0 = 2$.

Remarque A.14. *Dans la cas où $\Omega = \mathbb{R}^d$, la distance d'Agmon est un outil standard pour étudier la concentration des vecteurs propres des opérateurs de Schrödinger semi-classique (cf. par exemple [34, 35, 38–42]). Dans cette thèse, nous adaptons la définition classique de la distance d'Agmon afin de prendre en compte le bord de Ω, cf.* (A.35) *et* (A.36)*: on considère une métrique définie par la norme du gradient tangentiel de f sur le bord de Ω.*

Enfin, nous définissons les ensembles suivants. Pour $i \in \{1, ..., n\}$, B_{z_i} désigne le bassin d'attraction de z_i pour la dynamique de gradient

$$\frac{d}{dt}x(t) = -\nabla_T f\big(x(t)\big)$$

dans $\partial\Omega$. Autrement dit pour $i \in \{1, ..., n\}$:

$$B_{z_i} = \{y \in \partial\Omega,\ \lim_{t\to\infty} x(t) = z_i \text{ si } x(0) = y\}.$$

De plus, on définit pour tout $i \in \{1, ..., n\}$

$$B^c_{z_i} := \partial\Omega \setminus B_{z_i}.$$

Sur la Figure A.5, nous représentons sur un exemple en dimension 2 les ensembles $(B_{z_i})_{i=1,...,n}$ dans un cas où $n = 4$ et $n_0 = 2$.

A.4.2 Enoncés des résultats du Chapitre B

Comme expliqué en toute fin de Section A.3.1.2, nous cherchons à obtenir des équivalents précis lorsque $h \to 0$ des quantités suivantes: λ_h, $\partial_n u_h$ et $\int_\Omega u_h e^{-\frac{2}{h}f}$, où u_h est le vecteur propre associé à la plus petite valeur propre λ_h de $-L^{D,(0)}_{f,h}$ qui satisfait (A.27). Ceci permet ensuite d'obtenir des équivalents précis de la loi de X_{τ_Ω} (cf. (A.31)) et des taux de transition entre états définis en (A.22) (cf. aussi (A.29)).

Voici les résultats que nous avons obtenus.

Proposition A.8. *Soit u_h le vecteur propre associé à la plus petite valeur propre λ_h de $-L^{D,(0)}_{f,h}$ (cf. Propositions A.4 et A.5) qui satisfait* (A.27)*. Sous les hypothèses **[H1]**, **[H2]**, **[H3]** et si*

$$f(z_1) - f(x_0) > f(z_n) - f(z_1) \tag{A.37}$$

et pour tout $i \in \{1, ..., n\}$,

$$d_a(z_i, B^c_{z_i}) > \max[f(z_n) - f(z_i),\, f(z_i) - f(z_1)], \tag{A.38}$$

alors,

1. *Dans la limite $h \to 0$:*

$$\lambda_h = \frac{\sqrt{\det \text{ Hess} f(x_0)}}{\sqrt{\pi h}} \sum_{i=1}^{n_0} \frac{\partial_n f(z_i)}{\sqrt{\det \text{ Hess} f|_{\partial\Omega}(z_i)}}\; e^{-\frac{2}{h}(f(z_1)-f(x_0))}\,(1 + O(h))\,. \tag{A.39}$$

2. *Dans la limite $h \to 0$*

$$\int_\Omega u_h(x)\; e^{-\frac{2}{h}f(x)} dx = \frac{\pi^{\frac{d}{4}}}{(\det \text{ Hess} f(x_0))^{1/4}}\; h^{\frac{d}{4}}\; e^{-\frac{1}{h}f(x_0)}(1 + O(h)). \tag{A.40}$$

De plus, nous avons obtenu le théorème suivant sur le comportement asymptotique de $\partial_n u_h$; c'est un des résultats principaux du Chapitre B.

Théorème A.1. *Supposons que les hypothèses de la Proposition A.8 soient satisfaites. Soient $i \in \{1, ..., n\}$ et $\Sigma_i \subset \partial\Omega$ un ouvert contenant z_i et tels que $\overline{\Sigma_i} \subset B_{z_i}$. Alors, dans la limite $h \to 0$:*

$$\int_{\Sigma_i} (\partial_n u_h)\, e^{-\frac{2}{h}f} = A_i(h)\, e^{-\frac{2f(z_i)-f(x_0)}{h}}\,(1 + O(h))\,, \tag{A.41}$$

où

$$A_i(h) = -\frac{(\det \text{ Hess} f(x_0))^{1/4} \partial_n f(z_i) 2\pi^{\frac{d-2}{4}}}{\sqrt{\det \text{ Hess} f|_{\partial\Omega}(z_i)}} h^{\frac{d-6}{4}}.$$

Ces résultas ont les conséquences suivantes.

Corollaire A.9. *Supposons que les hypothèses de la Proposition A.8 soient satisfaites. Soient $i \in \{1, ..., n\}$ et $\Sigma_i \subset \partial\Omega$ un ouvert contenant z_i et tels que $\overline{\Sigma_i} \subset B_{z_i}$. Alors, dans la limite $h \to 0$:*

$$\mathbb{P}^{\nu_h}\left[X_{\tau_\Omega} \in \Sigma_i\right] = \frac{\partial_n f(z_i)}{\sqrt{\det \text{ Hess} f_{|\partial\Omega}(z_i)}} \left(\sum_{k=1}^{n_0} \frac{\partial_n f(z_k)}{\sqrt{\det \text{ Hess} f_{|\partial\Omega}(z_k)}} \right)^{-1} e^{-\frac{2}{h}(f(z_i)-f(z_1))}(1+O(h)), \tag{A.42}$$

où ν_h est la distribution quasi stationnaire associée au processus (A.34) *et au domaine Ω (cf. Proposition* (A.6)*). De plus, si Σ_i est la frontière commune entre l'état Ω et un état Ω_i, alors dans la limite $h \to 0$*

$$k_i^L = \frac{1}{\sqrt{\pi h}} \partial_n f(z_i) \frac{\sqrt{\det \text{ Hess} f(x_0)}}{\sqrt{\det \text{ Hess} f_{|\partial\Omega}(z_i)}} e^{-\frac{2}{h}(f(z_i)-f(x_0))}(1 + O(h)), \tag{A.43}$$

où k_i^L est le taux de transition défini par (A.22) *pour aller de Ω vers Ω_i.*

Remarquons que (A.42) est une consequence de (A.39), (A.40) et (A.41) (cf. (A.31)) et que (A.43) est une conséquence de (A.40) et (A.41) d'après (A.29).

Remarque A.15. *La nouveauté de nos travaux réside dans les résultats* (A.41), (A.42) *et* (A.43)*. La principale difficulté est de prouver* (A.41) *ce qui nécessite un équivalent précis de $\int_{\Sigma_i} (\partial_n u_h)\, e^{-\frac{2}{h}f}$ lorsque z_i n'est pas un minimum global de f sur $\partial\Omega$, c'est-à-dire lorsque $i \in \{n_0 + 1, ..., n\}$.*

En Chapitre B, les résultats (A.41) et (A.42) ont été généralisés à d'autres domaines $\Sigma \subset \partial\Omega$ (ne contenant pas forcément un point $z \in \{z_1, ..., z_n\}$), c'est l'autre résultat principal du Chapitre B et que nous ne présentons pas dans cette section. De plus, à l'aide de résultats dit de "leveling" très précis sur la fonction $x \mapsto \mathbb{E}^x[F(X_{\tau_\Omega})]$, nous avons généralisé l'équivalent (A.42) à des conditions initiales déterministes dans Ω c'est-à-dire quand $X_0 = x \in \Omega$.

Remarque A.16. *Le préfacteur dans* (A.43) *n'est pas* (A.18)*. En voici l'explication. D'une part, la présence du terme $\frac{\partial_n f(z_i)}{\sqrt{h}}$ dans* (A.43) *est due au fait que les points $(z_i)_{i=1,...,n}$ ne sont pas des points selles pour f sur $\mathbb{R}^d$ (car $\partial_n f > 0$ sur $\partial\Omega$ d'après* ***[H2]****). D'autre part, il manque un facteur* 2 *dans* (A.43) *par rapport à* (A.18) *qui s'explique par le fait que dans l'expression des taux de transition* (A.22)*, on considère en réalité le taux de transition vers l'état $\partial\Omega \cap \partial\Omega_i$ et que le processus* (A.34) *a dans la limite $h \to 0$, lorsqu'il atteint $\partial\Omega \cap \partial\Omega_i$, une chance sur deux de revenir dans Ω et une chance sur deux d'aller dans Ω_i (cf. Remarque A.10).*

Nous avons aussi cherché à savoir si l'hypothèse sur la distance d'Agmon (A.38) était nécessaire pour obtenir nos résultats et plus particulièrement pour obtenir (A.42). Pour cela, nous avons construit un exemple en dimension deux pour lequel l'hypothèse (A.38) n'était pas vérifiée et nous avons constaté que le préfacteur obtenu numériquement n'était pas celui obtenu dans (A.42). Nous renvoyons au Chapitre B pour plus de détails sur ce point.

Les outils utilisés dans la preuve de la Proposition A.8 et du Théorème A.1 sont principalement issus du domaine de l'analyse semi-classique et plus précisément des travaux [37, 51].

A.4.3 Explication des preuves de la Proposition A.8 et du Théorème A.1

Dans cette section, nous expliquons comment prouver la Proposition A.8 et le Théorème A.1.

A.4.3.1 Point de départ de la preuve de la Proposition A.8 et du Théorème A.1

Soit u_h le vecteur propre associé à la plus petite valeur propre λ_h de $-L_{f,h}^{D,(0)}$ (cf. Propositions A.4 et A.5) qui satisfait (A.27). Au vu de (A.31) et pour obtenir (A.42), nous voulons étudier le comportement asymptotique du gradient de u_h sur $\partial\Omega$. Le premier point à observer est que le gradient de u_h est aussi solution d'un problème aux valeurs propres pour la même valeur propre λ_h. Précisons un peu les choses. Rappelons que u_h satisfait

$$\begin{cases} -L_{f,h}^{(0)} u_h = \lambda_h u_h \text{ dans } \Omega, \\ u_h = 0 \text{ sur } \partial\Omega. \end{cases}$$

Si l'on dérive cette expression, nous obtenons que le gradient de u_h est solution du problème aux valeurs propres suivant

$$\begin{cases} -L_{f,h}^{(1)} \nabla u_h = \lambda_h \nabla u_h \text{ dans } \Omega, \\ \nabla_T u_h = 0 \text{ sur } \partial\Omega, \\ \left(\frac{h}{2}\mathrm{div} - \nabla f \cdot\right) \nabla u_h = 0 \text{ sur } \partial\Omega, \end{cases} \tag{A.44}$$

où

$$L_{f,h}^{(1)} = \frac{h}{2}\Delta - \nabla f \cdot \nabla - \mathrm{Hess}\, f \tag{A.45}$$

est un opérateur agissant que les 1-formes (c'est-à-dire les champs de vecteurs). Ainsi, $(\nabla u_h, \lambda_h)$ est un couple vecteur propre-valeur propre de $-L_{f,h}^{D,(1)}$ qui est l'opérateur $-L_{f,h}^{(1)}$ associé à des conditions au bord de type tangentiel Dirichlet, cf. (A.44).
Le deuxième point clé (cf. [37, Chapter 3]) est que, sous les hypothèses **[H1]**, **[H2]** et **[H3]** et dans la limite $h \to 0$, l'opérateur $-L_{f,h}^{D,(0)}$ a exactement une valeur propre inférieure à $\frac{\sqrt{h}}{2}$ (c'est λ_h) et l'opérateur $-L_{f,h}^{D,(1)}$ a exactement n valeurs propres inférieures $\frac{\sqrt{h}}{2}$. En fait, toutes ces petites valeurs propres sont exponentiellement petites et les autres sont minorées par une constante dans la limite $h \to 0$. En particulier λ_h est une valeur propre exponentiellement petite des opérateurs $-L_{f,h}^{D,(0)}$ et $-L_{f,h}^{D,(1)}$, c'est-à-dire que pour h assez petit

$$\lambda_h \leq Ce^{-\frac{c}{h}},$$

pour $c > 0$ et $C > 0$ indépendants de h. Dans la suite, on appelle $\pi_h^{(0)}$ le projecteur spectral orthogonal dans $L_w^2(\Omega)$ associé à λ_h pour l'opérateur $-L_{f,h}^{D,(0)}$ et $\pi_h^{(1)}$ le projecteur spectral orthogonal dans $L_w^2(\Omega)$ associé aux n plus petites valeurs propres de l'opérateur $-L_{f,h}^{D,(1)}$. D'après ce qui précède, nous avons:

$$\mathrm{Ran}\, \pi_h^{(0)} = \mathrm{vect}\, u_h, \quad \dim \mathrm{Ran}\, \pi_h^{(1)} = n \tag{A.46}$$

et

$$\nabla u_h \in \operatorname{Ran} \pi_h^{(1)}. \tag{A.47}$$

Remarquons en plus, d'après la Proposition A.4, que

$$\lambda_h = \frac{h}{2} \|\nabla u_h\|^2_{L^2_w}. \tag{A.48}$$

Pour étudier λ_h et ∇u_h, l'objectif a donc été de construire une base de $\operatorname{Ran} \pi_h^{(1)}$ adaptée à la preuve de la Proposition A.8 et du Théorème A.1. Cette base a été construite en utilisant des quasi-modes.

A.4.3.2 Schéma de la preuve de (A.42)

Ici, nous présentons un schéma de la preuve de (A.42). Rappelons que d'après la Proposition A.4, nous travaillons dans l'espace

$$L^2_w(\Omega) = \Big\{ u : \Omega \to \mathbb{R},\ \int_\Omega u^2(x) e^{-\frac{2}{h} f(x)}\, dx < \infty \Big\}.$$

Rappelons que (cf. (A.25))

$$H^1_w(\Omega) = \big\{ u : \Omega \to \mathbb{R},\ u \in L^2_w(\Omega) \text{ et pour tout } i = 1, ..., d : \partial_i u \in L^2_w(\Omega) \big\}.$$

Ces normes s'étendent de manière naturelle sur les 1-formes (c'est-à-dire sur les champs de vecteur) comme suit

$$\Lambda^1 L^2_w(\Omega) := \Big\{ u = {}^t(u_1, ..., u_d) : \Omega \to \mathbb{R}^d,\ \forall k \in \{1, ..., d\},\ \int_\Omega u_k^2(x) e^{-\frac{2}{h} f(x)}\, dx < \infty \Big\},$$

et

$$\Lambda^1 H^1_w(\Omega) := \big\{ u = {}^t(u_1, ..., u_d) : \Omega \to \mathbb{R}^d,\ \forall (i,k) \in \{1, ..., d\}^2,\ \partial_i u_k \in L^2_w(\Omega) \big\}.$$

Dans la suite on note $\|.\|_{L^2_w}$ (resp. $\|.\|_{H^1_w}$) pour désigner à la fois la norme de $L^2_w(\Omega)$ et $\Lambda^1 L^2_w(\Omega)$ (resp. $H^1_w(\Omega)$ et $\Lambda^1 H^1_w(\Omega)$). Enfin, sans confusion possible, $\langle ., . \rangle_{L^2_w}$ désigne à la fois le produit scalaire associé à la norme de $L^2_w(\Omega)$ et celui associé à la norme de $\Lambda^1 L^2_w(\Omega)$.

D'après (A.31) et pour obtenir (A.42), nous voulons étudier le comportement asymptotique de λ_h et du gradient de u_h sur $\partial\Omega$. Au vu de (A.47) et (A.46), pour toute base orthonormale $(\psi_j)_{j \in \{1,...,n\}}$ de $\operatorname{Ran} \pi_h^{(1)}$, on a dans $L^2_w(\Omega)$

$$\nabla u_h = \sum_{j=1}^n \langle \nabla u_h, \psi_j \rangle_{L^2_w} \psi_j, \tag{A.49}$$

et d'après (A.48), on a

$$\lambda_h = \frac{h}{2} \sum_{j=1}^n \big| \langle \nabla u_h, \psi_j \rangle_{L^2_w} \big|^2. \tag{A.50}$$

En particulier, nous avons pour tout $k \in \{1, ..., n\}$,

$$\int_{\Sigma_k} \partial_n u_h \, e^{-\frac{2}{h}f} = \sum_{j=1}^{n} \langle \nabla u_h, \psi_j \rangle_{L^2_w} \int_{\Sigma_k} \psi_j \cdot n \, e^{-\frac{2}{h}f}, \tag{A.51}$$

où l'on rappelle que Σ_k est un ouvert de $\partial\Omega$ tel que $z_k \in \Sigma_k$ et $\overline{\Sigma_k} \subset B_{z_k}$.

Etape 1. Approximation de u_h.

D'après (A.51), il nous a fallu trouver une approximation de u_h dans $L^2_w(\Omega)$. Sous les hypothèses **[H1]**, **[H2]** et **[H3]**, l'approximation de u_h est assez simple. Considérons

$$\tilde{u} := \frac{\chi}{\|\chi\|_{L^2_w}}, \tag{A.52}$$

où $\chi \in C^\infty_c(\Omega, \mathbb{R}^+)$ et $\chi = 1$ sur $\{x \in \Omega, d(x, \partial\Omega) \geq \varepsilon\}$ où $\varepsilon > 0$. En particulier, pour ε assez petit, $\chi = 1$ au voisinage de x_0 (ce que nous supposons dans la suite).
Expliquons en quoi $\tilde{u}$ est un bon choix pour approcher u_h. Comme $-L^{D,(0)}_{f,h}$ est auto-adjoint sur $L^2_w(\Omega)$, il vient que (d'après la Proposition A.4)

$$\|(1 - \pi^{(0)}_h)\tilde{u}\|^2_{L^2_w} \leq \frac{C}{\sqrt{h}} \langle -L^{D,(0)}_{f,h}\tilde{u}, \tilde{u} \rangle_{L^2_w} = \frac{Ch}{2\sqrt{h}} \frac{\displaystyle\int_\Omega |\nabla\chi|^2 e^{-\frac{2}{h}f}}{\displaystyle\int_\Omega \chi^2 e^{-\frac{2}{h}f}}.$$

Comme $f(x_0) = \min_\Omega f < \min_{\partial\Omega} f$ et x_0 est l'unique minimum global de f sur $\overline{\Omega}$ (d'après **[H2]**), nous obtenons en utilisant une méthode de Laplace (x_0 est un point critique non dégénéré de f et $\chi(x_0) = 1$):

$$\int_\Omega \chi^2 e^{-\frac{2}{h}f} = \frac{(\pi h)^{\frac{d}{2}}}{\sqrt{\mathrm{detHess} f(x_0)}} e^{-\frac{2}{h}f(x_0)}.$$

Ainsi, si ε est assez petit, pour tout $\delta > 0$, nous obtenons quand $h \to 0$

$$\|(1 - \pi^{(0)}_h)\tilde{u}\|^2_{L^2_w} = O(e^{-\frac{2}{h}(f(z_1) - f(x_0) - \delta)}).$$

Et donc dans la limite $h \to 0$, nous avons

$$\pi^{(0)}_h \tilde{u} = \tilde{u} + O(e^{-\frac{1}{h}(f(z_1) - f(x_0) - \delta)}) \text{ dans } L^2_w(\Omega).$$

Comme $\pi^{(0)}_h$ est le projecteur orthogonal dans $L^2_w(\Omega)$ sur u_h et comme $\chi \geq 0$, nous obtenons pour tout $\delta > 0$, quand $h \to 0$

$$u_h = \frac{\pi^{(0)}_h \tilde{u}}{\|\pi^{(0)}_h \tilde{u}\|_{L^2_w}} = \tilde{u} + O(e^{-\frac{1}{h}(f(z_1) - f(x_0) - \delta)}) \text{ dans } L^2_w(\Omega), \tag{A.53}$$

pour $c > 0$ indépendant de h. Ceci justifie que $\tilde{u}$ est une bonne approximation de u_h. Enfin remarquons que (A.53) implique (A.40). En effet, d'après (A.53), nous avons pour tout $\delta > 0$,

$$\int_\Omega u_h \, e^{-\frac{2}{h}f} = \int_\Omega \tilde{u} \, e^{-\frac{2}{h}f} \left(1 + O(e^{-\frac{c}{h}})\right) + \sqrt{\int_\Omega e^{-\frac{2}{h}f}} \, O(e^{-\frac{1}{h}(f(z_1) - f(x_0) - \delta)}).$$

En utilisant le fait que $f(x_0) \leq f(z_1)$ pour tout $x \in \overline{\Omega}$ et (A.52), en prenant $\delta < f(z_1) - f(x_0)$, nous obtenons quand $h \to 0$

$$\int_\Omega u_h \, e^{-\frac{2}{h}f} = \frac{\displaystyle\int_\Omega \chi e^{-\frac{2}{h}f}}{\sqrt{\displaystyle\int_\Omega \chi^2 e^{-\frac{2}{h}f}}} \, (1 + O(e^{-\frac{c}{h}})) + O(e^{-\frac{1}{h}(f(x_0)+c)}),$$

où $c > 0$ est indépendant de h. Une méthode de Laplace implique, quand $h \to 0$:

$$\int_\Omega u_h(x) \; e^{-\frac{2}{h}f(x)} dx = \frac{\pi^{\frac{d}{4}}}{(\det \mathrm{Hess} f(x_0))^{1/4}} \; h^{\frac{d}{4}} \; e^{-\frac{1}{h}f(x_0)}(1 + O(h)).$$

Ce qui prouve (A.40).

<u>Etape 2</u>. Construction d'une base de $\mathrm{Ran}\, \pi_h^{(1)}$ adaptée à l'approximation de $\partial_n u_h$.

Au vu de (A.51), l'idée a été de construire n 1-formes $(\widetilde{\psi}_j)_{j\in\{1,...,n\}}$ telles que projetées sur $\mathrm{Ran}\, \pi_h^{(1)}$, elles forment une base de $\mathrm{Ran}\, \pi_h^{(1)}$ qui permette d'obtenir une estimée précise de $\partial_n u_h$ sur chacun des Σ_j. Chacun des vecteurs $\widetilde{\psi}_j$ pour $j \in \{1, ..., n\}$ est appelé dans la littérature un quasi-mode (sous-entendu ici pour $-L_{f,h}^{D,(1)}$). Un quasi-mode pour $-L_{f,h}^{D,(1)}$ est une 1-forme w suffisamment régulière telle que dans une certaine norme,

$$\pi_h^{(1)} w = w + o(1), \tag{A.54}$$

dans la limite $h \to 0$.

Remarque A.17. *Avec cette appellation, la fonction $\tilde{u}$ définie par* (A.52) *est un quasi-mode pour $\pi_h^{(0)}$.*

Une des difficultés majeures de nos travaux a résidé dans la construction de la famille $(\widetilde{\psi}_j)_{j\in\{1,...,n\}}$ pour que le résidu $o(h)$ dans (A.54) lorsque $w = \widetilde{\psi}_k$ soit de l'ordre (cf. (A.38))

$$\big\|(1 - \pi_h^{(1)})\widetilde{\psi}_k\big\|_{H_w^1} = O\big(e^{-\frac{1}{h}\max[f(z_n)-f(z_k),\, f(z_k)-f(z_1)]}\big). \tag{A.55}$$

Ceci afin d'obtenir dans un premier temps que la famille

$$\big(\pi_h^{(1)}\widetilde{\psi}_j\big)_{j\in\{1,...,n\}}$$

forme une base de $\mathrm{Ran}\, \pi_h^{(1)}$ et afin d'obtenir dans un second temps, après orthonormalisation de la famille $\big(\pi_h^{(1)}\widetilde{\psi}_j\big)_{j\in\{1,...,n\}}$, quand $h \to 0$ (cf. (A.51)):

$$\forall k \in \{1, ..., n\}, \; \int_{\Sigma_k} \partial_n u_h \, e^{-\frac{2}{h}f} = \sum_{j=1}^n \langle \nabla \tilde{u}, \widetilde{\psi}_j \rangle_{L_w^2} \int_{\Sigma_k} \widetilde{\psi}_j \cdot n \, e^{-\frac{2}{h}f} + O\big(e^{-\frac{2f(z_k)-f(x_0)+c}{h}}\big) \tag{A.56}$$

et (cf. (A.50))

$$\lambda_h = \frac{h}{2} \sum_{j=1}^n |\langle \nabla \tilde{u}, \widetilde{\psi}_j \rangle_{L_w^2}|^2 + O\big(e^{-\frac{2}{h}(f(z_1)-f(x_0)+c)}\big) \tag{A.57}$$

où $c > 0$ est indépendante de h et $\tilde{u}$ défini par (A.52) est une approximation de u_h (cf. (A.53)). Dans ce qui suit, nous expliquons comment nous construisons la famille $\big(\widetilde{\psi}_j\big)_{j\in\{1,...,n\}}$ afin d'obtenir (A.56) et (A.57). Puis, nous expliquons comment ont été calculés les termes $\Big(\int_{\Sigma_j} \widetilde{\psi}_j \cdot n\, e^{-\frac{2}{h}f}\Big)_{j\in\{1,...,n\}}$ et $\Big(\langle \nabla\tilde{u}, \widetilde{\psi}_j\rangle_{L^2_w}\Big)_{j\in\{1,...,n\}}$.

Etape 2a. Construction de la famille $(\widetilde{\psi}_j)_{j\in\{1,...,n\}}$.

Pour construire chacune des 1-formes $\widetilde{\psi}_j$, l'idée est de construire des opérateurs $-L^{(1)}_{f,h}$ avec conditions au bord mixtes de Dirichlet et de Neumann sur un domaine $\dot{\Omega}_j \subset \Omega$ tel que $\big(\{z_1, ..., z_n\} \cup \{x_0\}\big) \cap \dot{\Omega}_j = \{z_j\}$. Pour $j \in \{1, ..., n\}$, la 1-forme $\widetilde{\psi}_j$ est dite alors associée au point selle généralisé z_j. Le but des conditions mixtes est d'avoir un opérateur avec une seule valeur propre exponentiellement petite dans la limite $h \to 0$. Nous montrons que cette unique petite valeur propre est en fait égale à 0. Pour construire les opérateurs $-L^{(1)}_{f,h}$ avec conditions au bord mixtes de Dirichlet et de Neumann sur un domaine $\dot{\Omega}_j$, nous utilisons les travaux récents [45] et [32]. La 1-forme $\widetilde{\psi}_j$ associée à z_j est ensuite définie en tronquant chaque vecteur propre $v^{(1)}_{h,j}$ associé à la valeur propre 0 de l'opérateur $-L^{(1)}_{f,h}$ avec conditions mixtes sur $\dot{\Omega}_j$:

$$\widetilde{\psi}_j := \frac{\chi_j\, v^{(1)}_{h,j}}{\|\chi_j\, v^{(1)}_{h,j}\|_{L^2_w}}, \tag{A.58}$$

où χ_j est une fonction de cut-off bien choisie dont le support est inclus dans $\overline{\dot{\Omega}_j}$.

Pour $j \in \{1, ..., n\}$, le quasi-mode $\widetilde{\psi}_j$ n'est pas construit localement autour de z_j, autrement dit $\dot{\Omega}_j$ n'est pas un petit voisinage de z_j dans $\overline{\Omega}$ et doit être aussi grand que souhaité dans Ω. C'est une différence par rapport à la littérature et notamment par rapport à [37]. Ceci est dû au fait que, d'une part, nous regardons la probabilité de sortie du processus (1) sur des domaines Σ_j arbitrairement grands dans B_{z_j} et, d'autre part, que nous avons besoin de suffisamment de décroissance du quasi-mode $\widetilde{\psi}_j$ pour obtenir (A.55), comme expliqué dans l'étape suivante.

Etape 2b. Précision du quasi-mode $\widetilde{\psi}_j$ pour $j \in \{1, ..., n\}$

Pour obtenir un terme d'erreur suffisamment petit dans (A.54) (afin d'obtenir (A.55) puis (A.56)), il faut quantifier la décroissance de $\widetilde{\psi}_j$ en dehors de tout voisinage de z_j. Cette décroissance de $\widetilde{\psi}_j$ est obtenue avec des estimées d'Agmon sur $v^{(1)}_{h,j}$ qui permettent de localiser $\widetilde{\psi}_j$ autour de z_j. Pour $j \in \{1, ..., n\}$, nous prouvons une estimée d'Agmon de la forme

$$\big\|\chi_j\, v^{(1)}_{h,j} e^{\frac{1}{h}d_a(.,z_j)}\big\|_{H^1_w} = O(h^{-N}), \tag{A.59}$$

pour tout $N \in \mathbb{N}$, où d_a est la distance d'Agmon définie en (A.36). Autrement dit, la décroissance de $v^{(1)}_{h,j}$ en dehors de tout voisinage de z_j est caractérisée par la distance d'Agmon (A.36). Afin obtenir (A.59), nous étudions les propriétés de la distance d'Agmon (A.36) et la présence du bord de Ω introduit des difficultés techniques. L'estimée d'Agmon (A.59) est obtenue en adaptant à notre cas des méthodes développées

dans [37, 51].

Pour chaque $j \in \{1, ..., n\}$, en utilisant le fait que

$$\|(1-\pi_h^{(1)})\widetilde{\psi}_j\|_{L^2_w}^2 \leq \frac{C}{\sqrt{h}}\langle -L_{f,h}^{D,(1)}\widetilde{\psi}_j, \widetilde{\psi}_j\rangle_{L^2_w}$$

et (A.59), il est possible de montrer que

$$\|(1-\pi_h^{(1)})\widetilde{\psi}_j\|_{L^2_w}^2 \leq C\, e^{-\frac{2}{h}\inf_{\mathrm{supp}\nabla\chi_j} d_a(.,z_j)}.$$

Ainsi, afin que (A.55) soit satisfaite, le support de $\nabla\chi_j$ doit pouvoir être aussi proche que souhaité de x_0 et $B^c_{z_j}$. Ceci explique les hypothèses (A.37) et (A.38), et le fait que le quasi-mode $\widetilde{\psi}_j$ ne soit pas construit seulement dans un voisinage de z_j mais dans un domaine $\dot{\Omega}_j$ très grand dans Ω, contrairement a ce qui a été fait dans [37].

A la fin de cette étape, nous avons une famille $(\widetilde{\psi}_j)_{j\in\{1,...,n\}}$ qui satisfait les estimées (A.55). Ceci nous a permis d'obtenir quand $h \to 0$ (cf. (A.56)),

$$\forall k \in \{1, ..., n\},\ \int_{\Sigma_k} \partial_n u_h\, e^{-\frac{2}{h}f} = \sum_{j=1}^{n} \langle \nabla\tilde{u}, \widetilde{\psi}_j\rangle_{L^2_w} \int_{\Sigma_k} \widetilde{\psi}_j \cdot n\, e^{-\frac{2}{h}f} + O\big(e^{-\frac{2f(z_k)-f(x_0)+c}{h}}\big),$$

où $c > 0$ est indépendante de h.

<u>Etape 3</u>. Calcul des termes $\Big(\int_{\Sigma_j} \widetilde{\psi}_j \cdot n\, e^{-\frac{2}{h}f}\Big)_{j\in\{1,...,n\}}$ et $\Big(\langle \nabla\tilde{u}, \widetilde{\psi}_j\rangle_{L^2_w}\Big)_{j\in\{1,...,n\}}$.

Au vu de (A.56) et (A.57), pour chaque $j \in \{1, ..., n\}$, il faut calculer explicitement un équivalent précis des quantités

$$\int_{\Sigma_j} \widetilde{\psi}_j \cdot n\, e^{-\frac{2}{h}f} \text{ et } \langle \nabla\tilde{u}, \widetilde{\psi}_j\rangle_{L^2_w}.$$

Pour cela, nous utilisons une approximation WKB de $v^{(1)}_{h,j}$, que l'on note $v^{(1)}_{z_j,wkb}$ pour chaque $j \in \{1, ..., n\}$. Dans la littérature, $v^{(1)}_{z_j,wkb}$ est construit localement autour de z_j (cf. par exemple [37,51]). Nous étendons la construction de $v^{(1)}_{z_j,wkb}$ à des voisinages dans $\overline{\Omega}$ de domaines arbitrairement grands dans B_{z_j} (puisque Σ_j est n'importe quel domaine inclus dans B_{z_j}). La comparaison entre $v^{(1)}_{h,j}$ et $v^{(1)}_{z_j,wkb}$ est aussi étendue à des voisinages dans $\overline{\Omega}$ de domaines arbitrairement grands dans B_{z_j}.

Une fois le calcul des termes $\Big(\int_{\Sigma_j} \widetilde{\psi}_j \cdot n\, e^{-\frac{2}{h}f}\Big)_{j\in\{1,...,n\}}$ et $\Big(\langle \nabla\tilde{u}, \widetilde{\psi}_j\rangle_{L^2_w}\Big)_{j\in\{1,...,n\}}$ terminé, on conclut la preuve de (A.39) en utilisant (A.57) et on conclut la preuve de (A.41) en utilisant (A.56).

Les principales difficultés que nous avons rencontrées lors de ces étapes se situent, d'une part, dans la construction des quasi-modes $(\widetilde{\psi}_j)_{j\in\{1,...,n\}}$ sur des domaines arbitrairement grands dans Ω et, d'autre part, dans l'obtention loin de z_j des estimées (A.59) ainsi que des estimées permettant de comparer $v^{(1)}_{h,j}$ avec son approximation $v^{(1)}_{z_j,wkb}$.

Remarque A.18. *En pratique, pour construire les quasi-modes pour* $-L^{(1)}_{f,h}$*, on travaille en fait plutôt avec l'opérateur de Witten sur les* 1*-formes*

$$\Delta^{(1)}_{f,h} = -h^2\,\Delta + |\nabla f|^2 - h\Delta f + 2h\,\mathrm{Hess}\,f,$$

ce qui nous permet de nous appuyer sur des résultats obtenus dans la littérature. Pour $j \in \{1, ..., n\}$*, nous construisons dans le Chapitre B le quasi-mode* $v^{(1)}_{h,j}$ *en utilisant le vecteur propre* $u^{(1)}_{h,j}$ *associé à la valeur propre* 0 *d'un Laplacien de Witten* $\Delta^{(1)}_{f,h}$ *avec conditions au bord mixtes de Dirichlet et de Neumann sur un domaine* $\dot{\Omega}_j \subset \Omega$ *tel que* $\big(\{z_1, ..., z_n\} \cup \{x_0\}\big) \cap \dot{\Omega}_j = \{z_j\}$*. Nous définissons ensuite* $v^{(1)}_{h,j}$ *par*

$$v^{(1)}_{h,j} = e^{\frac{1}{h}f} u^{(1)}_{h,j}.$$

Cette définition s'explique par le fait que les opérateurs $\Delta^{(1)}_{f,h}$ *et* $-L^{(1)}_{f,h}$ *(cf.* (C.34)*) sont liés par la relation*

$$\Delta^{(1)}_{f,h} = -2h\, e^{-\frac{1}{h}f} L^{(1)}_{f,h} e^{\frac{1}{h}f}.$$

A.5 Résultats du Chapitre C

Les résultats que nous allons présenter dans cette section sont ceux du Chapitre C dont l'article support [24] est en cours de rédaction.

Dans toute cette section le domaine Ω est un sous domaine ouvert C^∞ connexe et borné de $\mathbb{R}^d$. Nous rappelons que le processus étudié est le processus de Langevin suramorti (1):

$$dX_t = -\nabla f(X_t) + \sqrt{h}\, dB_t, \tag{A.60}$$

où $f : \mathbb{R}^d \to \mathbb{R}$ est l'énergie potentielle du système considéré ($d \in \mathbb{N}^*$), $h > 0$ est sa température et $(B_t)_{t\geq 0}$ un mouvement brownien standard dans $\mathbb{R}^d$. Afin d'étudier l'événement de sortie du domaine Ω, nous rappelons que τ_Ω désigne le premier temps de sortie de Ω:

$$\tau_\Omega := \inf\{t \geq 0, X_t \notin \Omega\}.$$

Dans toute la suite, la fonction f est supposée de classe C^∞.

A.5.1 Motivation

La motivation première du Chapitre C est de justifier les résultats obtenus de manière formelle dans [60] concernant la concentration de la loi de X_{τ_Ω} sur $\arg\min_{\partial\Omega} f = \{z \in \partial\Omega,\ f(z) = \min_{\partial\Omega} f\}$. Avant de rappeler les résultats obtenus dans [60], donnons une définition précise de la concentration de la loi de X_{τ_Ω} sur un ensemble de points de $\partial\Omega$. Soit $\mathcal{Y} \subset \partial\Omega$. La loi de X_{τ_Ω} se concentre sur $\mathcal{Y}$, si pour tout voisinage $\mathcal{V}_\mathcal{Y}$ de $\mathcal{Y}$ dans $\partial\Omega$, on a

$$\lim_{h\to 0} \mathbb{P}\left[X_{\tau_\Omega} \in \mathcal{V}_\mathcal{Y}\right] = 1,$$

et si pour tout $x \in \mathcal{Y}$ et pour tout voisinage $\mathcal{V}_x$ de x dans $\partial\Omega$

$$\lim_{h\to 0} \mathbb{P}\left[X_{\tau_\Omega} \in \mathcal{V}_x\right] > 0.$$

De manière intuitive, on s'attend à ce que la loi de X_{τ_Ω} se concentre sur les points où f atteint son minimum sur $\partial\Omega$. Ce résultat a été obtenu de manière formelle dans [60] dans le cas de frontière caractéristique (i.e. $\partial_n f(x) = 0$ pour tout $x \in \partial\Omega$) et de frontière non caractéristique (i.e. $\partial_n f(x) > 0$ pour tout $x \in \partial\Omega$).

Remarque A.19. *Remarquons que le Corollaire B.10 donne des informations encore plus précises que la concentration de la loi de X_{τ_Ω}. Il permet de donner un résultat asymptotique précis de la la loi de X_{τ_Ω} autour des points selles généralisés de f qui ne sont pas des minimas globaux de f au bord (cf. Remarque A.15). Ceci dit, dans cette section, nous travaillons dans un cadre géométrique beaucoup plus général que dans la Section A.4.*

A.5.2 Position du problème

Les formules obtenues dans [60] ont été prouvées rigoureusement dans [46, 47, 61] dans le cas où $\partial_n f > 0$ sur $\partial\Omega$ et f a un seul point critique dans Ω (qui est alors son unique minimum global dans $\overline{\Omega}$). Les techniques utilisées en analyse semi-classique nous permettent de généraliser considérablement ce cadre géométrique. Par exemple, les résultats du Chapitre C permettent de considérer une situation avec plusieurs points critiques dans Ω et de s'affranchir de l'hypothèse $\partial_n f > 0$ sur $\partial\Omega$ (ceci dit, nous n'avons pas considéré le cas où f a des points selles sur $\partial\Omega$). En supposant toujours que f et $f|_{\partial\Omega}$ sont des fonctions de Morse, et $|\nabla f| \neq 0$ sur $\partial\Omega$, les questions que nous nous sommes posées sont les suivantes:

- Quelles sont les conditions géométriques pour que, lorsque $X_0 \sim \nu_h$, la loi de X_{τ_Ω} se concentre à basse température sur les points où f atteint son minimum sur $\partial\Omega$ (ou sur un sous ensemble de ces points)?
- Sous quelles conditions ces résultats se généralisent à une condition initiale déterministe dans Ω ?

Les résultats du Chapitre C ont pour objectif de répondre à ces questions.

Terminons cette section par la remarque suivante déjà utilisée dans la Section A.4.1. Lorsque f et $f|_{\partial\Omega}$ sont des fonctions de Morse, et $|\nabla f| \neq 0$ sur $\partial\Omega$, c'est l'ensemble

$$\{z \text{ est un minimum local de } f|_{\partial\Omega}\} \cap \{z \in \partial\Omega,\, \partial_n f(z) > 0\} \tag{A.61}$$

qui joue le rôle des points selles de f au bord. Lorsque l'on prolonge la fonction f par $-\infty$ en dehors de $\overline{\Omega}$, les points $(z_i)_{i=1,\dots,n}$ sont en effet géométriquement des points selles. L'ensemble (A.61) est appelé points selles généralisés d'indice 1 de $-L_{f,h}^{D,(0)}$ au bord, d'après [37, Section 5.2].

A.5.3 Des exemples en dimension un

Dans cette section, nous allons apporter des débuts de réponses aux questions posées en Section A.5.2 avec des exemples en dimension un. Rappelons un petit résultat qui nous permettra de faire des calculs dans cette cette section. Soit $z_1 < z_2$ et $f \in C^\infty([z_1, z_2], \mathbb{R})$. En utilisant la formule de Dynkin, l'unique solution v du problème elliptique

$$\frac{h}{2}v'' - v'f' = 0 \text{ et } v(z_1) = 0,\, v(z_2) = 1,$$

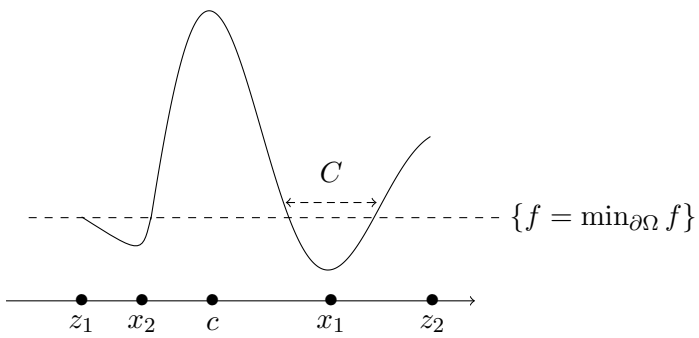

Figure A.6: Exemple d'une fonction, où partant de la distribution quasi stationnaire ou du minimum global x_1 de f dans Ω, la loi de X_{τ_Ω} ne se concentre pas sur des points où f atteint son minimum sur $\partial\Omega$

satisfait

$$\forall x \in [z_1, z_2],\ v(x) = \mathbb{P}^x\big[X_{\tau_{(z_1,z_2)}} = z_2\big].$$

Ainsi, pour tout $x \in [z_1, z_2]$:

$$\mathbb{P}^x[X_{\tau_{(z_1,z_2)}} = z_2] = \frac{\displaystyle\int_{z_1}^{x} e^{\frac{2}{h}f}}{\displaystyle\int_{z_1}^{z_2} e^{\frac{2}{h}f}},$$

et donc, pour tout $x \in [z_1, z_2]$:

$$\mathbb{P}^x[X_{\tau_{(z_1,z_2)}} = z_1] = \frac{\displaystyle\int_{x}^{z_2} e^{\frac{2}{h}f}}{\displaystyle\int_{z_1}^{z_2} e^{\frac{2}{h}f}}. \tag{A.62}$$

A.5.3.1 Exemple 1

L'objectif ici est de construire un exemple en dimension un pour lequel partant du minimum global de f dans Ω ou de la distribution quasi stationnaire ν_h, la loi de X_{τ_Ω} ne se concentre pas sur des points où f atteint son minimum sur $\partial\Omega$. Pour cela on considère l'exemple de la Figure A.6 pour lequel nous avons le résultat suivant.

Proposition A.10. *Soient $z_1 < z_2$ et $f \in C^\infty([z_1, z_2], \mathbb{R})$ une fonction de Morse. Supposons que $f(z_1) < f(z_2)$, $\{x \in [z_1, z_2], f'(x) = 0\} = \{x_2, c, x_1\}$ avec $z_1 < x_2 < c < x_1 < z_2$ et $f(x_1) < f(x_2) < f(z_1) < f(z_2) < f(d) < f(c)$ (cf. Figure A.6). Alors, pour tout $x \in (c, z_2]$, il existe $c > 0$ telle que dans la limite $h \to 0$:*

$$\mathbb{P}^x[X_{\tau_{(z_1,z_2)}} = z_1] = O(e^{-\frac{c}{h}}) \text{ et donc } \mathbb{P}^x[X_{\tau_{(z_1,z_2)}} = z_2] = 1 + O(e^{-\frac{c}{h}}). \tag{A.63}$$

De plus il existe $c > 0$ telle que dans la limite $h \to 0$:

$$\mathbb{P}^{\nu_h}[X_{\tau_{(z_1,z_2)}} = z_1] = O(e^{-\frac{c}{h}}) \quad \text{et donc} \quad \mathbb{P}^{\nu_h}[X_{\tau_{(z_1,z_2)}} = z_2] = 1 + O(e^{-\frac{c}{h}}), \tag{A.64}$$

où ν_h est la distribution quasi stationnaire associé au processus (A.60) *sur* (z_1, z_2).

Preuve. Prouvons d'abord (A.63). En utilisant (A.62) et une méthode de Laplace, pour tout $x \in (c, z_2]$, il existe $c > 0$ telle que dans la limite $h \to 0$:

$$\mathbb{P}^x[X_{\tau_{(z_1,z_2)}} = z_1] = O(e^{-\frac{c}{h}}).$$

Ainsi, pour tout $x \in (c, z_2]$, il existe $c > 0$ telle que dans la limite $h \to 0$:

$$\mathbb{P}^x[X_{\tau_{(z_1,z_2)}} = z_2] = 1 + O(e^{-\frac{c}{h}}).$$

Prouvons ensuite (A.64). Pour cela, nous allons d'abord montrer qu'il existe une fonction $\chi \in C_c^\infty((c, z_2), [0, 1])$ telle que $\chi = 1$ dans un voisinage de x_1 et

$$u_h = \frac{\chi}{\|\chi\|_{L^2_w}}\big(1 + O(e^{-\frac{c}{h}})\big) + r, \tag{A.65}$$

où $r \in L^2_w(z_1, z_2)$ satisfait $\|r\|_{L^2_w} = O(e^{-\frac{c}{h}})$ et $c > 0$ est indépendante de h. Soit

$$\tilde{u} := \frac{\chi}{\|\chi\|_{L^2_w}}.$$

Soit $\beta > 0$ et $\widetilde{\pi}_h^{(0)}$ le projecteur associé aux valeurs propres de $-L_{f,h}^{D,(0)}$ inférieures à $e^{-\frac{2}{h}(f(z_2)-f(x_1))}e^{\frac{\beta}{h}}$. D'après [37, Théorème 1], il existe $\beta > 0$ telle que pour h assez petit,

$$\operatorname{Ran} \widetilde{\pi}_h^{(0)} = 1.$$

Ainsi,

$$\operatorname{Ran} \widetilde{\pi}_h^{(0)} = \operatorname{Vect}\,(u_h).$$

En utilisant une méthode de Laplace, pour tout $\delta > 0$, en choisissant χ telle que $\sup_{\operatorname{supp}\,\chi'} f \leq f(z_2) - \delta$, nous obtenons

$$\begin{aligned}
\Big\|(1 - \widetilde{\pi}_h^{(0)})\tilde{u}\Big\|^2_{L^2_w} &\leq e^{\frac{2}{h}(f(z_2)-f(x_1))}e^{-\frac{\beta}{h}}\Big\langle -L_{f,h}^{D,(0)}\frac{\chi}{\|\chi\|_{L^2_w}}, \frac{\chi}{\|\chi\|_{L^2_w}}\Big\rangle_{L^2_w} \\
&= \frac{h\, e^{\frac{2}{h}(f(z_2)-f(x_1))}e^{-\frac{\beta}{h}}}{2}\frac{\displaystyle\int_{z_1}^{z_2} |\nabla\chi|^2 e^{-\frac{2}{h}f}}{\displaystyle\int_{z_1}^{z_2} \chi^2 e^{-\frac{2}{h}f}} \\
&\leq Ce^{-\frac{\beta-\delta}{h}}.
\end{aligned}$$

Ainsi, en prenant $\delta < \beta$, il existe $c > 0$ telle que dans la limite $h \to 0$,

$$\Big\|(1 - \widetilde{\pi}_h^{(0)})\tilde{u}\Big\|_{L^2_w} = O(e^{-\frac{c}{h}}).$$

Dès lors, pour h assez petit

$$u_h = \frac{\widetilde{\pi}_h^{(0)}\tilde{u}}{\|\widetilde{\pi}_h^{(0)}\tilde{u}\|_{L^2_w}},$$

ce qui prouve (A.65). En utilisant (A.65), nous avons à l'aide d'une méthode de Laplace, quand $h \to 0$:

$$\int_{z_1}^{z_2} u_h\, e^{-\frac{2}{h}f} = f''(x_1)^{-\frac{1}{4}}(\pi h)^{\frac{1}{4}}e^{-\frac{1}{h}f(x_1)}(1 + O(h)).$$

De plus, si on note $g(x) = \mathbb{P}^x[X_{\tau_{(z_1,z_2)}} = z_1]$ pour $x \in [z_1, z_2]$, d'après la Proposition A.6 et comme $\chi \in C_c^\infty((c,d),[0,1])$ et $\|g\|_{L^\infty} \leq 1$, nous avons dans la limite $h \to 0$ (en utilisant (A.65) dans la troisième égalité):

$$\begin{aligned}
\mathbb{P}^{\nu_h}[X_{\tau_{(z_1,z_2)}} = z_1] &= \frac{\displaystyle\int_{z_1}^{z_2} g(x)\, u_h\, e^{-\frac{2}{h}f}}{\displaystyle\int_{z_1}^{z_2} u_h\, e^{-\frac{2}{h}f}} = \frac{1}{\displaystyle\int_{z_1}^{z_2} u_h\, e^{-\frac{2}{h}f}} \left[\int_{z_1}^{c} u_h g e^{-\frac{2}{h}f} + \int_{c}^{z_2} u_h g e^{-\frac{2}{h}f}\right] \\
&= \frac{1}{\displaystyle\int_{z_1}^{z_2} u_h\, e^{-\frac{2}{h}f}} \left[\int_{z_1}^{c} r g e^{-\frac{2}{h}f} + \int_{c}^{z_2} \frac{\chi g e^{-\frac{2}{h}f}}{\|\chi\|_{L^2_w}} + \int_{c}^{z_2} r g e^{-\frac{2}{h}f}\right] \\
&= \frac{1}{\displaystyle\int_{z_1}^{z_2} u_h\, e^{-\frac{2}{h}f}} \left[\frac{\displaystyle\int_{c}^{z_2} \chi(x) \int_{x}^{z_2} e^{\frac{2}{h}(f(y)-f(x))} dy dx}{\|\chi\|_{L^2_w} \displaystyle\int_{z_1}^{z_2} e^{\frac{2}{h}f}} + O(e^{-\frac{1}{h}(f(x_1)+c)})\right] \\
&= \frac{1}{\displaystyle\int_{z_1}^{z_2} u_h\, e^{-\frac{2}{h}f}} \left[\frac{O(e^{\frac{2}{h}(f(z_2)-f(x_1))})}{\|\chi\|_{L^2_w} \displaystyle\int_{z_1}^{z_2} e^{\frac{2}{h}f}} + O(e^{-\frac{1}{h}(f(x_1)+c)})\right] = O(e^{-\frac{c}{h}}),
\end{aligned}$$

où nous avons utilisé (A.62) dans la quatrième inégalité. Ce qui conclut la preuve de (A.64).

∎

Ainsi, dans le régime petite température et lorsque $X_0 = x \in (c, z_2)$ ou $X_0 \sim \nu_h$ le processus (A.60) sort de $\Omega = (z_1, z_2)$ par le point z_2. Pourtant, le point selle généralisé z_2 (cf. (A.61)) n'est pas le minimum de f sur le bord de Ω. Ceci peut s'expliquer de la manière suivante. La métastabilité la plus importante dans Ω est causée par la barrière de potentiel $f(z_2) - f(x_1)$ et ce à cause de la présence du point selle $c \in \Omega$ d'énergie $f(c) > f(z_2)$. La loi de X_{τ_Ω} lorsque $X_0 = x \in (c, z_2)$ ne peut alors se concentrer que sur z_2 puisque qu'il est moins coûteux pour le processus de sortir par z_2 que de franchir la barrière de potentiel $f(c) - f(x_1)$ pour sortir par z_1. De plus, on peut montrer que distribution quasi stationnaire ν_h se concentre autour du point x_1 ce qui explique que loi de X_{τ_Ω} lorsque $X_0 \sim \nu_h$ se concentre sur z_2. Concernant les deux questions soulevées en Section A.5.2, ceci indique qu'à basse température, il existe des cas où le processus (A.34), partant d'un minimum global de f dans Ω ou de la distribution quasi stationnaire, sort par un point de la frontière qui n'est pas un minimum global de $f_{|\partial\Omega}$.

Cet exemple suggère aussi la chose suivante. Si l'on veut montrer que la loi de X_{τ_Ω} se concentre en des points où f atteint son minimum sur le bord, il convient d'exclure les cas où la métastabilité la plus forte dans Ω n'est pas exclusivement causée par des barrières d'énergies impliquant des points où f atteint son minimum sur le bord. Une solution pour empêcher que la loi de X_{τ_Ω} se concentre en des points où f n'atteint pas son minimum sur le bord, est de supposer que la fermeture de la composante connexe C de $\{f < \min_{\partial\Omega} f\}$ qui contient le minimum global x_1 de f intersecte le bord de Ω. Cette hypothèse a été le point de départ de nos travaux au Chapitre C.

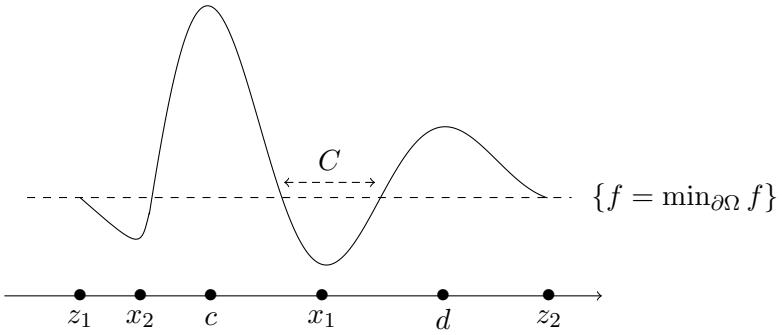

Figure A.7: Exemple d'une fonction, où partant de la distribution quasi stationnaire ou du minimum global x_1 de f dans Ω, la loi de X_{τ_Ω} se concentre sur z_2 qui est un point où f atteint son minimum sur $\partial\Omega$ mais qui n'est pas un point selle généralisé pour $-L_{f,h}^{D,(0)}$.

A.5.3.2 Exemple 2

L'objectif ici est de construire un exemple en dimension un pour lequel partant du minimum global de f dans Ω ou de la distribution quasi stationnaire ν_h (cf. Proposition A.6), la loi de X_{τ_Ω} se concentre en un point où f atteint son minimum sur $\partial\Omega$ mais qui n'est pas un point selle généralisé pour $-L_{f,h}^{D,(0)}$ (rappelons qu'un point selle généralisé pour $-L_{f,h}^{D,(0)}$ est un point du bord qui géométriquement est un point selle de f lorsque elle est prolongée par $-\infty$ en dehors de $\overline{\Omega}$, cf. (A.61)). Pour cela on considère l'exemple de la figure C.12 pour lequel nous avons le résultat suivant.

Proposition A.11. *Soient $z_1 < z_2$ et $f \in C^\infty([z_1, z_2], \mathbb{R})$ une fonction de Morse. Supposons que $f(z_1) = f(z_2)$, $\{x \in [z_1, z_2], f'(x) = 0\} = \{x_2, c, x_1, d\}$ avec $z_1 < x_2 < c < x_1 < d < z_2$ et $f(x_1) < f(x_2) < f(z_1) < f(d) < f(c)$ (cf. Figure C.12). Alors, pour tout $x \in (c, z_2]$, il existe $c > 0$ telle que dans la limite $h \to 0$:*

$$\mathbb{P}^x[X_{\tau_{(z_1,z_2)}} = z_1] = O(e^{-\frac{c}{h}}) \text{ et donc } \mathbb{P}^x[X_{\tau_{(z_1,z_2)}} = z_2] = 1 + O(e^{-\frac{c}{h}}).$$

De plus il existe $c > 0$ telle que dans la limite $h \to 0$:

$$\mathbb{P}^{\nu_h}[X_{\tau_{(z_1,z_2)}} = z_1] = O(e^{-\frac{c}{h}}) \quad \text{et donc} \quad \mathbb{P}^{\nu_h}[X_{\tau_{(z_1,z_2)}} = z_2] = 1 + O(e^{-\frac{c}{h}}), \tag{A.66}$$

où ν_h est la distribution quasi stationnaire associé au processus (A.60) *sur* (z_1, z_2) *(cf. Proposition A.6).*

La Proposition A.11 se prouve exactement comme la Proposition A.10.

Dans cet exemple représenté en Figure C.12, la métastabilité associée à la barrière $f(d) - f(x_1)$ est plus forte que la métastabilité associée au bord de Ω. Là encore, cette situation est exclue si on suppose que la fermeture de la composante connexe de $\{f < \min_{\partial\Omega} f\}$ qui contient le minimum global x_1 de f intersecte le bord de Ω.

Remarque A.20. *Les deux exemples de cette section indiquent que la métastabilité (cf. Définition A.1) dépend de la condition initiale $x \in \Omega$. En effet, on a montré avec ces*

deux exemples, que l'événement de sortie de Ω n'est pas toujours le même partant de la distribution quasi stationnaire ν_h et partant d'un point $x \in \Omega$.

A.5.4 Enoncés des résultats du Chapitre C

Dans cette section, nous ne présentons qu'une version simplifiée des résultats du Chapitre C. L'objectif est d'exhiber un cadre géométrique simple qui assure, d'une part, que la loi de X_{τ_Ω} se concentre sur les mêmes points du bord lorsque $X_0 \sim \nu_h$ ou $X_0 \sim x \in \Omega$ pour $x \in \{f < \min_{\partial\Omega} f\}$ et, d'autre part, que cette concentration se fait sur des points selles généralisés de f appartenant à $\arg\min_{\partial\Omega} f$. On définit les deux hypothèses suivantes:

- **[H-Morse]** La fonction f est C^∞. Les fonctions $f : \overline{\Omega} \to \mathbb{R}$ et la restriction de f au bord de Ω, notée $f|_{\partial\Omega}$, sont des fonctions de Morse (cf. Définition A.2). De plus, $|\nabla f|(x) \neq 0$ pour tout $x \in \partial\Omega$.
- **[H-Min]** L'ensemble $\{f < \min_{\partial\Omega} f\}$ est non vide, connexe et satisfait

$$\arg\min_{\Omega} f \subset \{f < \min_{\partial\Omega} f\} \quad \text{et} \quad \overline{\{f < \min_{\partial\Omega} f\}} \cap \partial\Omega \neq \emptyset.$$

Remarquez que sous les hypothèses **[H-Morse]** et **[H-Min]** nous avons

$$\min_{\partial\Omega} f > \min_{\overline{\Omega}} f = \min_{\Omega} f.$$

Sous les hypothèses **[H-Morse]** et **[H-Min]**, nous notons

$$\overline{\{f < \min_{\partial\Omega} f\}} \cap \partial\Omega = \{z_1, ..., z_{k_0}\}, \tag{A.67}$$

où $\overline{\{f < \min_{\partial\Omega} f\}}$ désigne la fermeture de l'ensemble $\{f < \min_{\partial\Omega} f\}$ dans $\overline{\Omega}$.

Remarque A.21. *Les points $\{z_1, ..., z_{k_0}\}$ sont des points selles généralisés de f sur $\partial\Omega$ (cf.* (A.61)*), i.e. qui satisfont*

$$\{z_1, ..., z_{k_0}\} = \{z \in \partial\Omega,\, \partial_n f(z) > 0\} \cap \arg\min_{\partial\Omega} f \tag{A.68}$$

*En effet, d'une part, pour tout $i \in \{1, ..., k_0\}$, $\partial_n f(z_i) \neq 0$ puisque $\nabla f(z_i) \neq 0$ (d'après **[H-Morse]**) et comme z_i n'est pas un minimum local de f dans $\overline{\Omega}$ (car $z_i \in \overline{\{f < \min_{\partial\Omega} f\}}$), nous avons nécessairement $\partial_n f(z_i) > 0$. Ce qui montre une première inclusion dans* (A.68)*. L'inclusion inverse est triviale.*

Remarque A.22. *Sous l'hypothèse **[H-Min]**, la dérivée normale de f peut changer de signe et la fonction peut avoir des points selles dans Ω plus haut que $\min_{\partial\Omega} f$ comme sur l'exemple en dimension 1 représenté par la Figure A.8.*

L'hypothèse **[H-Min]** a pour but d'assurer que la distribution quasi stationnaire ν_h se concentre dans $\{f < \min_{\partial\Omega} f\}$ et que partant d'un point $x \in \{f < \min_{\partial\Omega} f\}$ ou de ν_h, la concentration de la loi de X_{τ_Ω} se fait sur les points selles généralisés de f au bord $\{z_1, ..., z_{k_0}\}$ (cf. (A.67)). Remarquez que l'hypothèse **[H-Min]** n'est vérifiée dans aucun des deux exemples donnés en Section A.5.3. Le théorème suivant (qui est une conséquence des résultats du Chapitre C) montre, d'une part, que ν_h se concentre sur $\{f < \min_{\partial\Omega} f\}$ et, d'autre part, que partant d'un point $x \in \{f < \min_{\partial\Omega} f\}$ ou de ν_h, la concentration de la loi de X_{τ_Ω} se fait sur $\{z_1, ..., z_{k_0}\}$.

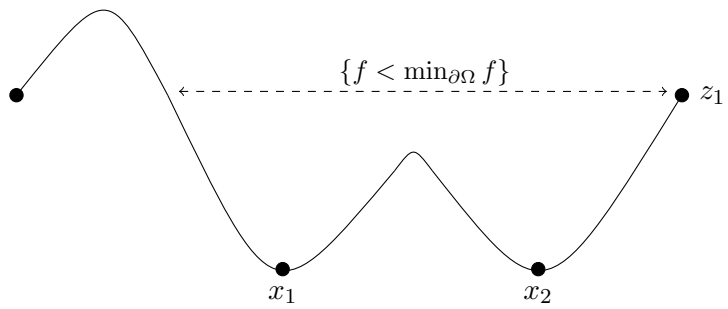

Figure A.8: Un exemple en dimension 1 dans lequel l'hypothèse **[H-Min]** est satisfaite, la dérivée normale de f sur $\partial\Omega$ change de signe et la fonction f a un point selle dans Ω plus haut que $\min_{\partial\Omega} f$.

Théorème A.2. *Supposons que les hypothèses **[H-Morse]** et **[H-Min]** sont satisfaites. Soit ν_h la distribution quasi-stationnaire associée au processus* (A.60) *sur Ω. Alors, dans la limite $h \to 0$*

$$\nu_h\big(\{f < \min_{\partial\Omega} f\}\big) = 1 + O(h).$$

Soit $F \in C^\infty(\partial\Omega, \mathbb{R})$. Nous avons dans la limite $h \to 0$:

$$\mathbb{E}^{\nu_h}\left[F\left(X_{\tau_\Omega}\right)\right] = \sum_{i=1}^{k_0} F(z_i)\, a_i + O(h), \tag{A.69}$$

où pour $i \in \{1, ..., k_0\}$,

$$a_i = \frac{\partial_n f(z_i)}{\sqrt{\det\ \mathrm{Hess} f\big|_{\partial\Omega}(z_i)}} \left(\sum_{j=1}^{k_0} \frac{\partial_n f(z_j)}{\sqrt{\det\ \mathrm{Hess} f\big|_{\partial\Omega}(z_j)}} \right)^{-1}.$$

De plus, si $\mathrm{supp} F \cap \{z_1, ..., z_{k_0}\} = \emptyset$, il existe $c > 0$ telle que dans la limite $h \to 0$:

$$\mathbb{E}^{\nu_h}\left[F\left(X_{\tau_\Omega}\right)\right] = O(e^{-\frac{c}{h}}). \tag{A.70}$$

Enfin, (A.69) *et* (A.70) *sont aussi vraies lorsque $X_0 = x \in \{f < \min_{\partial\Omega} f\}$.*

Dans le Chapitre C nous obtenons des résultats similaires sous des hypothèses plus faibles sur f. De plus, nous donnons des équivalents précis quand $h \to 0$ de λ_h et du comportement asymptotique de $\partial_n u_h$. Nous renvoyons pour cela au Chapitre C.

A.5.5 Schéma de la preuve du Théorème A.2

Dans cette section, nous allons donner le schéma de la preuve de (A.69) qui constitue le résultat principal du Théorème A.2. Rappelons tout d'abord que d'après (A.31), pour $F \in C^\infty(\partial\Omega, \mathbb{R})$

$$\mathbb{E}^{\nu_h}\big[F(X_{\tau_\Omega})\big] = -\frac{h}{2\lambda_h} \frac{\displaystyle\int_\Sigma F\, \partial_n u_h e^{-\frac{2}{h} f}}{\displaystyle\int_\Omega u_h e^{-\frac{2}{h} f}},$$

où u_h est le vecteur propre associé à la plus petite valeur propre λ_h de $-L_{f,h}^{D,(0)}$. Ainsi, afin de prouver (A.69), nous étudions le comportement asymptotique quand $h \to 0$ des quantités

$$\lambda_h,\ \partial_n u_h \text{ et } \int_\Omega u_h e^{-\frac{2}{h}f}. \tag{A.71}$$

Sous les hypothèses [**H-Morse**] et [**H-Min**], nous définissons les entiers suivants

$$m_0 := \text{Card}\left(\arg\min_\Omega f\right)$$

et

$$\begin{aligned} m_1 :&= \text{Card}\Big(\{z \text{ est un minimum local de } f|_{\partial\Omega}\} \cap \{z \in \partial\Omega,\ \partial_n f(z) > 0\}\Big) \\ &+ \text{Card}\Big(\{z \text{ est un point selle de } f\}\Big), \end{aligned} \tag{A.72}$$

où nous rappelons qu'un point selle est par définition un point critique x de f tel que la matrice hessienne de f en x a une seule valeur propre négative (cf. Définition A.2). L'entier m_1 est le nombre de points selles généralisés de f dans $\overline{\Omega}$ (cf. [37, Section 5.2]).

Pour étudier le comportement asymptotique des quantités (A.71), le point de départ est d'observer que le gradient de u_h est aussi solution d'un problème aux valeurs propres pour la même valeur propre λ_h (comme en Section A.4.3). Rappelons ce point. La fonction u_h satisfait

$$\begin{cases} -L_{f,h}^{(0)} u_h = \lambda_h u_h \text{ dans } \Omega, \\ u_h = 0 \text{ sur } \partial\Omega. \end{cases}$$

Si l'on dérive cette expression, nous obtenons que le gradient de u_h est solution du problème aux valeurs propres suivant

$$\begin{cases} -L_{f,h}^{(1)} \nabla u_h = \lambda_h \nabla u_h \text{ dans } \Omega, \\ \nabla_T u_h = 0 \text{ sur } \partial\Omega, \\ \left(\dfrac{h}{2}\text{div} - \nabla f \cdot\right) \nabla u_h = 0 \text{ sur } \partial\Omega, \end{cases} \tag{A.73}$$

où

$$L_{f,h}^{(1)} = \frac{h}{2}\Delta - \nabla f \cdot \nabla - \text{Hess}\, f \tag{A.74}$$

est un opérateur agissant que les 1-formes (c'est-à-dire les champs de vecteur). Ainsi, $(\nabla u_h, \lambda_h)$ est un couple vecteur propre-valeur propre de $-L_{f,h}^{D,(1)}$ qui est l'opérateur $-L_{f,h}^{(1)}$ associé à des conditions au bord de type tangentiel Dirichlet, cf. (A.73).
Pour poursuivre le raisonnement, rappelons que, sous les hypothèses [**H-Morse**] et [**H-Min**] et dans la limite $h \to 0$, l'opérateur $-L_{f,h}^{D,(0)}$ a exactement m_0 valeurs propres inférieures à $\frac{\sqrt{h}}{2}$ et l'opérateur $-L_{f,h}^{D,(1)}$ a exactement m_1 valeurs propres inférieures à $\frac{\sqrt{h}}{2}$ (cf. [37, Chapter 3]). En fait, toutes ces petites valeurs propres sont exponentiellement petites et les autres sont minorées par une constante dans la limite $h \to 0$. En particulier λ_h est une valeur propre exponentiellement petite des opérateurs $-L_{f,h}^{D,(0)}$

et $-L_{f,h}^{D,(1)}$. Dans la suite, on appelle $\pi_h^{(0)}$ (respectivement $\pi_h^{(1)}$) le projecteur orthogonal dans $L_w^2(\Omega)$ sur les m_0 (respectivement m_1) petites valeurs propres de l'opérateur $-L_{f,h}^{D,(0)}$ (respectivement $-L_{f,h}^{D,(1)}$). D'après ce qui précède, nous avons:

$$\dim \operatorname{Ran} \pi_h^{(0)} = m_0, \quad \dim \operatorname{Ran} \pi_h^{(1)} = m_1$$

et

$$\nabla u_h \in \operatorname{Ran} \pi_h^{(1)}.$$

Nous allons maintenant expliquer la procédure adoptée pour prouver le Théorème A.2. Pour cela, introduisons l'ensemble des minima locaux de f

$$\mathcal{U}_0^{\Omega} := \{x \in \Omega,\, x \text{ est un minimum local de } f\},$$

et l'ensemble des points selles généralisés de f dans $\overline{\Omega}$

$$\mathcal{U}_1^{\overline{\Omega}} = \Big(\{z \text{ est un minimum local de } f|_{\partial\Omega}\} \cap \{z \in \partial\Omega,\, \partial_n f(z) > 0\}\Big) \bigcup \{z \text{ est un point selle de } f\}.$$

Rappelons que d'après (A.72), $m_1 = \operatorname{Card}\Big(\mathcal{U}_1^{\overline{\Omega}}\Big)$. La première étape de la preuve consiste à définir deux fonctions $\widetilde{\mathbf{j}}$ et $\mathbf{j}$. La fonction $\widetilde{\mathbf{j}}$ associe à chaque minimum local x de f la composante connexe de l'ensemble $\{f < \lambda\}$ qui contient x où $\lambda - f(x)$ est la barrière d'énergie minimale que le processus (A.60) doit franchir pour aller vers un autre minimum local de f plus bas en énergie que x ou pour sortir de Ω. La fonction

$$\mathbf{j} : U_0^{\overline{\Omega}} \to \mathcal{P}(\mathcal{U}_1^{\overline{\Omega}})$$

associe à chaque minimum local x de f les points selles généralisés de f dans $\overline{\Omega}$ qui appartiennent au bord de $\widetilde{\mathbf{j}}(x)$.

La deuxième étape consiste à construire une base de $\operatorname{Ran} \pi_h^{(0)}$ et de $\operatorname{Ran} \pi_h^{(1)}$. Pour cela, on construit deux familles de quasi-modes, notées $(\widetilde{u}_k)_{k\in\{1,\dots,m_0\}}$ et $(\widetilde{\psi}_j)_{j\in\{1,\dots,m_1\}}$, que l'on projette ensuite respectivement sur $\operatorname{Ran} \pi_h^{(0)}$ et $\operatorname{Ran} \pi_h^{(1)}$. Pour construire la famille de 1-formes $(\widetilde{\psi}_j)_{j\in\{1,\dots,m_1\}}$, nous procédons comme suit. Pour chaque point selle z de f dans Ω, en suivant la procédure de [36], nous construisons une 1-forme dont le support est un petit voisinage de z dans Ω. Pour un minimum local z de $f_{|\partial\Omega}$ pour lequel $\partial_n f(z) > 0$, nous construisons une 1-forme dans un petit voisinage de z dans $\overline{\Omega}$ comme proposé dans [37]. Pour construire la famille de fonction $(\widetilde{u}_k)_{k\in\{1,\dots,m_0\}}$, nous construisons pour chaque minimum local x de f une fonction dont le support est quasiment tout l'ensemble $\widetilde{\mathbf{j}}(x)$ (cette procédure s'inspire de [36, 37, 43]).

La troisième étape consiste à obtenir un équivalent précis de λ_h quand $h \to 0$. La valeur propre λ_h est égale au carré de la plus petite valeur singulière non nulle de l'opérateur

$$\nabla : \operatorname{Ran} \pi_h^{(0)} \to \operatorname{Ran} \pi_h^{(1)}.$$

Pour étudier le comportement asymptotique quand $h \to 0$ de cette valeur singulière, nous utilisons les bases construites à l'étape précédente pour $\operatorname{Ran} \pi_h^{(0)}$ et $\operatorname{Ran} \pi_h^{(1)}$. L'analyse de ce problème de dimension finie s'inspire de techniques utilisées dans [43].

Nous étudions ensuite le comportement asymptotique de la dérivée normale de u_h au bord de Ω pour en déduire que la loi de X_{τ_Ω} se concentre sur des points de $\arg\min_{\partial\Omega} f$ lorsque $X_0 \sim \nu_h$. Enfin, nous démontrons des résultats dit de "leveling" sur la fonction

$$x \mapsto \mathbb{E}_x[F(X_{\tau_\Omega})]$$

pour obtenir, lorsque $X_0 = x \in \{f < \min_{\partial\Omega} f\}$, la concentration de la loi de X_{τ_Ω} sur les même points de $\arg\min_{\partial\Omega} f$ que lorsque $X_0 \sim \nu_h$.

En conclusion les résultats principaux du Chapitre C sont les suivants:

1. Nous utilisons des techniques développées dans [36,37,43] pour étudier d'une part le comportement asymptotique précis de λ_h et $\partial_n u_h$, et d'autre part la concentration de la loi de X_{τ_Ω} sur des points de $\arg\min_{\partial\Omega} f$ lorsque $X_0 \sim \nu_h$.

2. Nous identifions les points de $\arg\min_{\partial\Omega} f$ où la loi de X_{τ_Ω} se concentre lorsque $X_0 \sim \nu_h$ en explicitant les probabilités de sortie par chacun de ces points.

3. Nous étendons les résultats précédents sur la loi de X_{τ_Ω} pour une condition déterministe: $X_0 = x$ avec $f(x) < \min_{\partial\Omega} f$.

4. Les résultats sont obtenus sous des hypothèses géométriques assez faibles sur la fonction f et nous illustrons sur des exemples en quoi ces hypothèses sont nécessaires pour obtenir les résultats obtenus.

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Chapter B

Sharp asymptotics of the first exit point density

Abstract

We consider the exit event from a metastable state for the overdamped Langevin dynamics $dX_t = -\nabla f(X_t)dt + \sqrt{h}dB_t$. Using tools from semiclassical analysis, we prove that, starting from the quasi stationary distribution within the state, the exit event can be modeled using a jump Markov process parametrized with the Eyring-Kramers formula, in the small temperature regime $h \to 0$. We provide in particular sharp asymptotic estimates on the exit distribution which demonstrate the importance of the prefactors in the Eyring-Kramers formula. Numerical experiments indicate that the geometric assumptions we need to perform our analysis are likely to be necessary. These results also hold starting from deterministic initial conditions within the well which are sufficiently small in energy. From a modelling viewpoint, this gives a rigorous justification of the transition state theory and the Eyring-Kramers formula, which are used to relate the overdamped Langevin dynamics (a continuous state space Markov dynamics) to kinetic Monte Carlo or Markov state models (discrete state space Markov dynamics). From a theoretical viewpoint, our analysis paves a new route to study the exit event from a metastable state for a stochastic process.

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B.1 Motivation and presentation of the results

In materials science, biology and chemistry, atomistic models are now used on a daily basis in order to predict the macroscopic properties from a microscopic description of matter. The basic ingredient is a potential energy function $f : \mathbb{R}^d \to \mathbb{R}$ which associates to a set of coordinates of particles the energy of the system. In practice, d is very large, since the system contains many particles (from tens of thousands to millions).

Using this function f, two types of models are built: continuous state space Markov models (stochastic differential equations), such as the Langevin or overdamped Langevin dynamics, and discrete state space Markov models (jump Markov processes). The objective of the analysis presented in this work is to make a rigorous link between these two types of approaches, and in particular to provide a justification of the use of Eyring-Kramers laws to parameterize jump Markov models, by studying the exit event from a metastable state for the overdamped Langevin dynamics.

Jump Markov models are used by practitioners for many reasons. From a modelling viewpoint, new insights can be gained by building such coarse-grained models, that are easier to handle than a large-dimensional stochastic differential equation. From a numerical viewpoint, it is possible to simulate a jump Markov model over timescales which are much larger than the original Langevin dynamics. Moreover, there are many algorithms which use the underlying jump Markov model in order to accelerate the sampling of the original dynamics [67, 70, 71].

The section is organized as follows. First, the two models under consideration are introduced, namely the overdamped Langevin dynamics in Section B.1.1, and the underlying jump Markov process in Section B.1.2. Next, Section B.1.3 is devoted to a review of the mathematical literature dealing with metastable processes and the exit event from a metastable state. In Section B.1.4, the notion of quasi stationary distribution is reviewed. This is a crucial tool in our analysis, in order to connect the overdamped Langevin dynamics to a jump Markov process. Then, in Section B.1.5, our main result (Theorem B.1) is stated. In Section B.1.6, we generalize Theorem B.1 in various directions and discuss the geometric assumptions used to state Theorem B.1. Finally, in Section B.1.7, we give an outline of the proof of Theorem B.1, together with the general organization of the paper.

B.1.1 Overdamped Langevin dynamics and metastability

The continuous state space Markov model we consider in this work is the so-called overdamped Langevin dynamics in $\mathbb{R}^d$

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

driven by the potential function $f : \mathbb{R}^d \to \mathbb{R}$. We assume in the following that f is a C^∞ Morse function (all the critical points are non degenerate). The parameter $h = 2k_BT > 0$ is proportional to the temperature T and $(B_t)_{t\geq 0}$ is a standard d-dimensional Brownian motion. One henceforth assumes that

$$\exists h_0,\, \forall h < h_0,\, \int_{\mathbb{R}^d} e^{-\frac{2}{h}f(x)}dx < \infty.$$

The invariant probability measure of (B.1) is

$$\frac{e^{-\frac{2}{h}f(x)}\,dx}{\displaystyle\int_{\mathbb{R}^d} e^{-\frac{2}{h}f(y)}dy}. \tag{B.2}$$

The basic observation which motivates the use of a jump Markov model to obtain a reduced description of the dynamics (B.1) is the following. In many practical cases of interest in biology, physics or chemistry, the dynamics (B.1) is metastable, meaning that the process $(X_t)_{t\geq 0}$ remains trapped for very long times in some regions (called metastable states). It is thus tempting to introduce an underlying jump process among these metastable states.

Let us consider a region $\Omega \subset \mathbb{R}^d$ and the associated exit event from Ω. More precisely, let us introduce

$$\tau_\Omega = \inf\{t \geq 0 | X_t \notin \Omega\} \tag{B.3}$$

the first exit time from Ω. The exit event from Ω is fully characterized by the couple of random variables $(\tau_\Omega, X_{\tau_\Omega})$. The focus of this work is the justification of a jump Markov process to model the exit event from the region Ω, in the small temperature regime $h \to 0$.

B.1.2 From the potential function to a jump Markov process

The potential function f can also be used to build a jump Markov process to describe the evolution of the system. Jump Markov models are continuous-time Markov processes with values in a discrete state space. In molecular dynamics such processes are known as kinetic Monte Carlo models [72] or Markov state models [7, 63, 64].

Kinetic Monte Carlo models The basic requirement to build a kinetic Monte Carlo model is a discrete collection of states $D \subset \mathbb{N}$, with associated rates $k_{i,j} \geq 0$ for transitions from state i to state j, where $(i,j) \in D \times D$ and $i \neq j$. The neighboring states of state i are those states j such that $k_{i,j} > 0$. The dynamics is then given by a jump Markov process $(Z_t)_{t\geq 0}$ with infinitesimal generator $L \in \mathbb{R}^{D\times D}$, where $L_{i,j} = k_{i,j}$ for $i \neq j$.

To be more precise, let us describe how to build the jump process $(Z_t)_{t\geq 0}$ by defining the residence times $(T_n)_{n\geq 0}$ and the subordinated Markov chain $(Y_n)_{n\geq 0}$. Starting at time 0 from a state $Y_0 \in D$, the model consists in iterating the following two steps over $n \geq 0$: given Y_n,

- first sample the residence time T_n in Y_n as an exponential random variable with parameter $\sum_{j\neq Y_n} k_{Y_n,j}$: $\forall i \in D$, $\forall t > 0$,

$$\mathbb{P}(T_n > t | Y_n = i) = \exp\left(-\sum_{j\neq i} k_{i,j}\, t\right), \tag{B.4}$$

- and then sample *independently from* T_n the next visited state Y_{n+1} using the following law:

$$\forall j \neq i,\ \mathbb{P}(Y_{n+1} = j | Y_n = i) = \frac{k_{i,j}}{\sum_{j\neq i} k_{i,j}}. \tag{B.5}$$

The continuous time Markov process $(Z_t)_{t\geq 0}$ is then defined as:

$$\forall n \geq 0,\, \forall t \in \left[\sum_{m=0}^{n-1} T_m, \sum_{m=0}^{n} T_m\right),\; Z_t = Y_n$$

with the convention $\sum_{m=0}^{-1} T_m = 0$.

Transition rates and Eyring Kramers law Starting from the potential function $f : \mathbb{R}^d \to \mathbb{R}$, one approach to build a kinetic Monte Carlo model is to consider a collection of disjoint subsets $(\Omega_k)_{k\in D}$ which form a partition of the space $\mathbb{R}^d$ and to set the transition rates $k_{i,j}$ by considering transitions between these subsets, see for example [9, 24, 72, 73].

The concept of jump rate between two states is one of the fundamental notions in the modelling of materials. Many papers have been devoted to the rigorous evaluation of jump rates from a full-atom description. The most famous formula is probably the rate derived in the harmonic transition state theory [52, 69], which gives an explicit expression for the rate in terms of the underlying potential energy function: this is the Eyring-Kramers formula, that we now introduce.

Let us consider a subset Ω of $\mathbb{R}^d$, which should be thought as one of the subsets $(\Omega_k)_{k\in D}$ introduced above, say the state $k = 0$. If Ω is metastable (in a sense which will be made precise below), it seems sensible to model the exit event from Ω using a jump Markov model, as introduced in the previous paragraph. As explained above, this requires to define jump rates $(k_{0,j})$ from the state 0 to the neighboring states j. The aim of this paper is to prove that the rates associated with the dynamics (B.1) can be approximated using the Eyring-Kramers formula which writes:

$$k_{0,j} = A_{0,j}\, e^{-\frac{2}{h}(f(z_j)-f(x_0))} \tag{B.6}$$

where $A_{0,j} > 0$ is a prefactor, $x_0 = \arg\min_{x\in\Omega} f(x)$ is the global minimum of f on Ω which is assumed to be unique and $z_j = \arg\min_{z\in\partial\Omega_j} f(z)$ where $\partial\Omega_j$ denotes the part of the boundary $\partial\Omega$ which connects the region Ω (numbered 0) with the neighboring region numbered j (see Figure B.1 for a schematic representation when Ω has 4 neighboring states).

The prefactors $A_{0,j}$ depend on the dynamics under consideration and on the potential function f around x_0 and z_j. If Ω is the basin of attraction of x_0 for the gradient dynamics $\dot{x} = -\nabla f(x)$ so that the points z_j are order one saddle points, the prefactor writes for the overdamped Langevin dynamics (B.1)

$$A_{0,j} = \frac{1}{2\pi}|\lambda^-(z_j)|\sqrt{\frac{\det(\mathrm{Hess} f)(x_0)}{|\det(\mathrm{Hess} f)(z_j)|}}, \tag{B.7}$$

where $\lambda^-(z_j)$ is the negative eigenvalue of the Hessian of f at z_j. The formulas (B.6)–(B.7) have been obtained by Kramers [44], but also by many authors previously, see the exhaustive review of the literature reported in [29]. We also refer to [29] for generalizations to the Langevin dynamics.

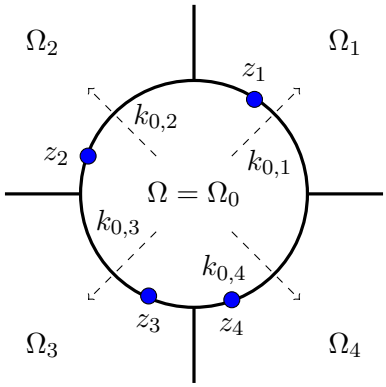

Figure B.1: The domain $\Omega = \Omega_0$ is associated with state 0. The neighboring domains $(\Omega_i)_{i=1,\dots,4}$ correspond to the four possible next visited states, with associated rates $(k_{0,i})_{i=1,\dots,4}$. For $i = 1, \dots, 4$, the point z_i represent the lowest energy point on $\partial\Omega \cap \partial\Omega_i$.

B.1.3 Review of the mathematical literature on the Eyring-Kramers formula

Let us give the main mathematical approaches to the study of the exit event from a domain for stochastic process in $\mathbb{R}^d$. See also [2] for a nice review.

Global approaches. Some authors adopt a global approach: they look at the spectrum of the infinitesimal generator of the continuous space dynamics in the small temperature regime $h \to 0$. It can be shown that there are exactly m small eigenvalues, m being the number of local minima of f, and that these eigenvalues satisfy the Eyring-Kramers law (B.6), with an energy barrier $f(z_i) - f(x_i)$, $i = 1, \dots, m$. Here, the saddle point z_i attached to the local minimum x_i is defined by (it is here implicitly assumed that the inf sup value is attained at a single saddle point z_i)

$$f(z_i) = \inf_{\gamma \in \mathcal{P}(x_i, B_i)} \sup_{t \in [0,1]} f(\gamma(t))$$

where $\mathcal{P}(x_i, B_i)$ denotes the set of continuous paths from $[0, 1]$ to $\mathbb{R}^d$ such that $\gamma(0) = x_i$ and $\gamma(1) \in B_i$ with B_i the union of small balls around local minima lower in energy than x_i. For the dynamics (B.1), we refer for example to the work [33] based on semi-classical analysis results for Witten Laplacian and the articles [5, 6, 20] where a potential theoretic approach is adopted. In the latter results, a connection is made between the small eigenvalues and mean transition times between metastable states. Let us also mention the earlier results [40, 56]. These spectral approaches give the cascade of relevant time scales to reach from a local minimum an other local minimum which is lower in energy. They do not give any information about the typical time scale to go from one local minimum to any other local minimum (say from the global minimum to the second lower minimum for example). These global approaches can be used to build jump Markov models using a Galerkin projection of the infinitesimal generator of $(X_t)_{t \geq 0}$ onto the first m eigenmodes, which gives an excellent approximation of the infinitesimal generator. This has been extensively investigated by Schütte and his collaborators [64], starting with the seminal work [63].

Local approaches. In this work, we are interested in a local approach, namely the study of the exit event (exit time and exit point) from a fixed given metastable state Ω. The most famous approach to study the exit event is the large deviation theory [25]. It relies essentially on the study of slices of the process defined with a suitable sequence of increasing stopping times. In the theory of large deviations, the notion of rate functional is fundamental and gives the cost of deviating from a deterministic trajectory.

In the small temperature regime, large deviation results provide the exponential rates (B.6), but without the prefactors and without precise error bounds. It can also be proven that the exit time is exponentially distributed in this regime, see [13]. For the dynamics (B.1), a typical result on the exit point distribution is the following (see [25, Theorem 5.1]): for all Ω' compactly embedded in Ω, for any $\gamma > 0$, for any $\delta > 0$, there exists $\delta_0 \in (0, \delta]$ and $h_0 > 0$ such that for all $h < h_0$, for all $x \in \Omega'$ such that $f(x) < \min_{\partial\Omega} f$, and for all $y \in \partial\Omega$,

$$\mathrm{e}^{-\frac{h}{2}(f(y)-\min_{\partial\Omega} f+\gamma)} \leq \mathbb{P}^x(X_{\tau_\Omega} \in \mathcal{V}_{\delta_0}(y)) \leq \mathrm{e}^{-\frac{h}{2}(f(y)-\min_{\partial\Omega} f-\gamma)} \tag{B.8}$$

where $\mathcal{V}_{\delta_0}(y)$ is a δ_0-neighborhood of y in $\partial\Omega$.
The strength of large deviation theory is that it is very general: it applies to any dynamics (reversible or non reversible) and in a very general geometric setting, even though it may be difficult in such general cases to make explicit the rate functional, and thus to determine the exit rates. See for example [4] for a recent contribution to the non reversible case.

Many authors have developed partial differential approach to the same problem. We refer to [14] for a comprehensive review. In particular, formal approaches to study the exit time and the exit point distribution have been developed by Matkowsky, Schuss and collaborators in [55,57,61,62] and by Maier and Stein in [50,51], using formal expansions for singularly perturbed elliptic equations. Some of the results cited above actually consider more general dynamics than (B.1). Rigorous version of these derivations have been obtained in [15, 16, 21, 40, 42, 53, 54, 59].

Rescaling in time and convergence to a jump process. Finally, some authors prove the convergence to a jump Markov process using a rescaling in time. See for example [43] for a one-dimensional diffusion in a double well, and [26, 54] for a similar problem in larger dimension. In [68], a rescaled in time diffusion process converges to a jump Markov process living on the global minima of the potential f, assuming they are separated by saddle points having the same heights.

In this work, we are interested in precise asymptotics of the distribution of X_{τ_Ω}. Our approach is local, justifies the Eyring-Kramers formula (6) with the prefactors and provides sharp error estimates (see (B.25)). It uses techniques developed in particular in the previous works [33, 34, 47, 48]. Our analysis requires to combine various tools from semiclassical analysis to address new questions: sharp estimates on quasimodes far from the critical points for Witten Laplacians on manifolds with boundary, a precise analysis of the normal derivative on the boundary of the first eigenfunction of Witten Laplacians, and fine properties of the Agmon distance on manifolds with boundary.

Let us finally mention that a summary of the results of this work appeared in [18].

B.1.4 Quasi stationary distribution

The quasi stationary distribution is the cornerstone of our analysis. The quasi stationary distribution can be seen as a local equilibrium for a metastable stochastic process when it is trapped in a metastable region. It is actually useful in order to make precise quantitatively what a metastable domain is. In all what follows, we focus on the overdamped Langevin dynamics (B.1) and a domain $\Omega \subset \mathbb{R}^d$. For generalizations to other processes, we refer to [11] and in particular to [58] for the existence of the quasi stationary distribution for the Langevin dynamics.

B.1.4.1 Definition and a first property of quasi stationary distributions

Let us first define the quasi stationary distribution.

Definition B.1. *Let $\Omega \subset \mathbb{R}^d$ and consider the dynamics (B.1). A quasi stationary distribution is a probability measure ν_h supported in Ω such that*

$$\forall t \geq 0,\, \nu_h(A) = \frac{\displaystyle\int_\Omega \mathbb{P}^x\left[X_t \in A, t < \tau_\Omega\right] \nu_h(dx)}{\displaystyle\int_\Omega \mathbb{P}^x\left[t < \tau_\Omega\right] \nu_h(dx)}.$$

Here and in the following, the superscript x indicates that the stochastic process starts from $x \in \mathbb{R}^d$: $X_0 = x$. In words, if X_0 is distributed according to ν_h, then $\forall t > 0$, X_t is still distributed according to ν_h conditionally on $X_s \in \Omega$ for all $s \in (0, t)$. It is important to notice that ν_h is not the invariant measure (B.2) of the original process restricted to Ω.

In all the following, we will consider that Ω is a bounded domain in $\mathbb{R}^d$. In this context, we have the following results from [46].

Proposition B.1. *Let $\Omega \subset \mathbb{R}^d$ be a bounded domain and consider the dynamics* (B.1)*. Then, there exists a probability measure ν_h with support in Ω such that, whatever the law of the initial condition X_0 with support in Ω,*

$$\lim_{t\to\infty} \|\mathrm{Law}(X_t | t < \tau_\Omega) - \nu_h\|_{TV} = 0. \tag{B.9}$$

Here and in the following, $\mathrm{Law}(X_t | t < \tau_\Omega)$ denotes the law of X_t conditional to the event $\{t < \tau_\Omega\}$. A corollary of this proposition is that the quasi stationary distribution ν_h exists and is unique.

This proposition also explains why it is relevant to consider the quasi stationary distribution for a metastable domain. The domain Ω is metastable if the convergence in (B.9) is much quicker than the exit from Ω. In the following of this paper, we will assume that Ω is a metastable domain, and we will thus consider the exit event from Ω, assuming that X_0 is distributed according to the quasi stationary distribution ν_h.

B.1.4.2 An eigenvalue problem related to the quasi stationary distribution

In this section, a connection is made between the quasi stationary distribution and an eigenvalue problem for the infinitesimal generator of the dynamics (B.1)

$$L^{(0)}_{f,h} = -\nabla f \cdot \nabla + \frac{h}{2}\,\Delta \tag{B.10}$$

with Dirichlet boundary conditions on $\partial\Omega$. In the notation $L^{(0)}_{f,h}$, the superscript (0) indicates that we consider an operator on functions, namely 0-forms. Here and in the following, we assume that the domain Ω is a connected open bounded C^∞ domain in $\mathbb{R}^d$. The basic observation to define our functional framework is that the operator $L^{(0)}_{f,h}$ is self-adjoint on the weighted L^2 space

$$L^2_w(\Omega) = \left\{ u : \Omega \to \mathbb{R},\ \int_\Omega u^2(x) e^{-\frac{2}{h}f(x)}\, dx < \infty \right\}$$

(the weighted Sobolev spaces $H^k_w(\Omega)$ are defined similarly). Indeed, for any smooth test functions u and v with compact supports in Ω, one has

$$\int_\Omega (L^{(0)}_{f,h} u) v e^{-\frac{2}{h}f} = \int_\Omega (L^{(0)}_{f,h} v) u e^{-\frac{2}{h}f} = -\frac{h}{2} \int_\Omega \nabla u \cdot \nabla v\, e^{-\frac{2}{h}f}.$$

This gives a proper framework to introduce the Dirichlet realization $L^{D,(0)}_{f,h}(\Omega)$ on Ω of the operator $L^{(0)}_{f,h}$:

Proposition B.2. *The Friedrichs extension associated with the quadratic form*

$$\phi \in C^\infty_c(\Omega) \mapsto \frac{h}{2} \int_\Omega |\nabla \phi|^2\, e^{-\frac{2}{h}f(x)} dx,$$

on $L^2_w(\Omega)$, is denoted $-L^{D,(0)}_{f,h}(\Omega)$. It is a non negative unbounded self adjoint operator on $L^2_w(\Omega)$ with domain

$$D\left(L^{D,(0)}_{f,h}(\Omega)\right) = H^1_{w,0}(\Omega) \cap H^2_w(\Omega)$$

where $H^1_{w,0}(\Omega) = \{u \in H^1_w(\Omega),\ u = 0 \text{ on } \partial\Omega\}$.

Proof. The quadratic form $\phi \in C^\infty_c(\Omega) \mapsto \frac{h}{2}\int_\Omega |\nabla\phi|^2\, e^{-\frac{2}{h}f(x)} dx$ is symmetric, non negative and closable and its closure is the quadratic form $Q : w \in H^1_{w,0}(\Omega) \mapsto \frac{h}{2}\int_\Omega |\nabla w|^2\, e^{-\frac{2}{h}f(x)} dx$. Let $-L^{D,(0)}_{f,h}(\Omega)$ be the self adjoint operator associated with Q, which domains is

$$D\left(-L^{D,(0)}_{f,h}(\Omega)\right) = \left\{ u \in H^1_{w,0}(\Omega),\ \exists b \in L^2_w(\Omega),\ \forall v \in H^1_{w,0}(\Omega),\ Q(u,v) = \langle b, v\rangle_{L^2_w} \right\},$$

and $-L^{D,(0)}_{f,h}(\Omega) u = b$. Let $u \in D\left(-L^{D,(0)}_{f,h}(\Omega)\right)$. Then, in the sense of distribution, it holds $-\frac{h}{2}\mathrm{div}\left(e^{-\frac{2}{h}f}\nabla u\right) = b$ and from standard regularity results for elliptic operators, we get $u \in H^2_w(\Omega)$. Therefore $D\left(-L^{D,(0)}_{f,h}(\Omega)\right) = H^1_{w,0}(\Omega) \cap H^2_w(\Omega)$.

∎

The compact injection $H^1_w(\Omega) \subset L^2_w(\Omega)$ implies that the operator $L^{D,(0)}_{f,h}(\Omega)$ has a compact resolvent. Consequently, its spectrum is purely discrete. Let us introduce $\lambda_h > 0$ the smallest eigenvalue of $-L^{D,(0)}_{f,h}(\Omega)$. One has the following proposition (see also [46]), which follows from standard results for the first eigenfunction of an elliptic operator, see for example [27].

Proposition B.3. *The smallest eigenvalue λ_h of $-L_{f,h}^{D,(0)}(\Omega)$ is non degenerate and its associated eigenfunction u_h has a sign on Ω. Moreover $u_h \in C^\infty(\overline{\Omega})$.*

Without loss of generality, one can assume that:

$$u_h > 0 \text{ on } \Omega \quad \text{and} \quad \int_\Omega u_h^2(x)\, e^{-\frac{2}{h}f(x)} dx = 1. \tag{B.11}$$

The eigenvalue-eigenfunction couple (λ_h, u_h) satisfies:

$$\begin{cases} -L_{f,h}^{(0)} u_h = \lambda_h u_h \text{ on } \Omega, \\ \qquad u_h = 0 \text{ on } \partial\Omega. \end{cases} \tag{B.12}$$

The link between the quasi stationary distribution ν_h (see Definition C.1) and u_h is given by the following proposition (see for example [46]):

Proposition B.4. *The unique quasi stationary distribution ν_h associated with the dynamics* (B.1) *and the domain Ω is given by:*

$$\nu_h(dx) = \frac{u_h(x) e^{-\frac{2}{h}f(x)}}{\displaystyle\int_\Omega u_h(y) e^{-\frac{2}{h}f(y)} dy} dx, \tag{B.13}$$

where u_h is the eigenfunction associated with the smallest eigenvalue of $-L_{f,h}^{D,(0)}(\Omega)$ (see Proposition B.3) which satisfies (B.11).

B.1.4.3 Back to the jump Markov process

As explained in Section B.1.4.1, if the process remains for a sufficiently long time in the domain Ω, it is natural to consider the exit event starting from the quasi stationary distribution attached to Ω. The next proposition characterizes the law of this exit event.

Proposition B.5. *Let us consider the dynamics* (B.1) *and the quasi stationary distribution ν_h associated with the domain Ω. If X_0 is distributed according to ν_h, the random variables τ_Ω and X_{τ_Ω} are independent. Furthermore τ_Ω is exponentially distributed with parameter λ_h and the law of X_{τ_Ω} has a density with respect to the Lebesgue measure on $\partial\Omega$ given by*

$$z \in \partial\Omega \mapsto -\frac{h}{2\lambda_h} \frac{\partial_n u_h(z) e^{-\frac{2}{h}f(z)}}{\displaystyle\int_\Omega u_h(y) e^{-\frac{2}{h}f(y)} dy}, \tag{B.14}$$

where u_h is the eigenfunction associated with the smallest eigenvalue of $-L_{f,h}^{D,(0)}(\Omega)$ (see Proposition B.3) which satisfies (B.11).

Here and in the following, $\partial_n = n \cdot \nabla$ stands for the normal derivative and n is the unit outward normal on $\partial\Omega$.

This proposition shows that, starting from the quasi-stationary distribution in the domain Ω, the exit event can be modeled by a jump Markov process *without any approximation*. Indeed, using the notation of Section B.1.2, let us consider that $\Omega \subset \mathbb{R}^d$ is associated with the state 0. Let us assume that Ω is surrounded be n neighbourding

states, associated with domains $(\Omega_i)_{i=1,\dots,n}$ (see Figure B.1 for a schematic representation when $n = 4$). Let us define the transition rates:

$$\forall i \in \{1, \dots n\},\ k_{0,i} = \frac{\mathbb{P}^{\nu_h}\left(X_{\tau_\Omega} \in \partial\Omega \cap \Omega_i\right)}{\mathbb{E}^{\nu_h}(\tau_\Omega)}. \tag{B.15}$$

Then, by Proposition C.4, the exit event is such that:

- The residence time τ_Ω is exponentially distributed with parameters $\sum_{i=1}^n k_{0,i}$.
- The next visited state is independent of the residence time and is i with probability $\frac{k_{0,i}}{\sum_{j=1}^n k_{0,j}}$.

This is exactly the two properties (B.4) and (B.5) which are required to define a transition using a jump Markov process. The quasi stationary distribution can thus be used to parameterize the underlying jump Markov process if the domains are metastable.

The question we would like to address in this work is now the following: what is the error introduced when one approximates the exact rates (B.15) using the Eyring-Kramers formula (B.6)–(B.7). From Proposition C.4, since $\mathbb{E}^{\nu_h}(\tau_\Omega) = 1/\lambda_h$, one has the following formula for the exact rates:

$$k_{0,i} = -\frac{h}{2} \frac{\displaystyle\int_{\partial\Omega\cap\partial\Omega_i} (\partial_n u_h)(z)\, e^{-\frac{2}{h}f(z)}\, \sigma(dz)}{\displaystyle\int_\Omega u_h(y)\, e^{-\frac{2}{h}f(y)}\, dy} \tag{B.16}$$

where σ denotes the Lebesgue measure on $\partial\Omega$. We will be able to prove that in the small temperature regime $h \to 0$, the exact rates (B.16) can indeed be accurately approximated by the Eyring-Kramers formula (B.6) with explicit error bounds. The asymptotic analysis is done directly on the rates, and not only on the logarithm of the rates (which is the typical result obtained with the large deviation theory for example, see Section B.1.3).

B.1.5 Statement of the main result

We state in this section the main result of this work (Theorem B.1) on the asymptotic behavior of the normal derivative $\partial_n u_h$ in the regime $h \to 0$, as well as its corollary on the exit point density and the accuracy of the approximation of the exit rates by the Eyring-Kramers formula.

This section is organized as follows. We introduce in Section B.1.5.1 a crucial tool in our analysis, the Agmon distance. Then, in Section B.1.5.2, we give the set of hypotheses which will be needed throughout this work. Finally, Section B.1.5.3 is dedicated to the statement of our main result.

B.1.5.1 Agmon distance

Our results hold under some geometric assumptions which require to introduce the so-called Agmon distance. The objective of this section is to introduce this distance, which is particularly useful to quantify the decay of eigenfunctions away from critical points [35, 66]. We introduce the Agmon distance in a general setting, namely for Ω a Riemannian manifold, but one could think of Ω as a C^∞ connected open bounded subset of $\mathbb{R}^d$.

Definition B.2. *Let $\overline{\Omega}$ be a C^∞ oriented connected compact Riemannian manifold of dimension d with boundary $\partial\Omega$ and $f : \overline{\Omega} \to \mathbb{R}$ be C^∞. Define $g : \overline{\Omega} \to \mathbb{R}$ by*

$$\forall x \in \Omega,\ g(x) = |\nabla f(x)| \ \text{ and } \ \forall x \in \partial\Omega,\ g(x) = |\nabla_T f(x)|\,, \tag{B.17}$$

where for any $x \in \partial\Omega$, $\nabla_T f(x)$ denotes the tangential gradient of the function f on $\partial\Omega$. One defines the length L of a Lipschitz curve $\gamma : I \to \overline{\Omega}$, where $I \subset \mathbb{R}$ is an interval, by

$$L(\gamma, I) := \int_I g\left(\gamma(t)\right) \left|\gamma'(t)\right| dt \in [0, +\infty].$$

Let us recall that the Rademacher theorem (see for example [23]) states that every Lipschitz function admits almost everywhere a derivative (which is then bounded by the Lipschitz constant). Therefore, if I is bounded, then $L(\gamma, I) < \infty$. Let us now define the Agmon distance.

Definition B.3. *Let g be the function introduced in Definition B.2. The Agmon distance between $x \in \overline{\Omega}$ and $y \in \overline{\Omega}$ is defined by*

$$d_a\left(x, y\right) = \inf_{\gamma \in \mathrm{Lip}(x,y)} L\left(\gamma, (0,1)\right), \tag{B.18}$$

where $\mathrm{Lip}\left(x, y\right)$ *is the set of curves $\gamma : [0,1] \to \overline{\Omega}$ which are Lipschitz with $\gamma(0) = x$, $\gamma(1) = y$.*

The Agmon distance is obviously symmetric, non negative and satisfies the triangular inequality. It is a distance if the critical points of f and $f_{\big|\partial\Omega}$ are isolated (see Proposition B.31 below). Let us mention that in the case when Ω is a manifold without boundary, the Agmon distance introduced in Definition B.3 coincides with the Agmon distance defined in [38, Appendix 2].

We will give in Section B.3 more details about the Agmon distance we consider. In particular, it will be shown that the Agmon distance to the critical points of $f|_{\partial\Omega}$ coincides with the solution to the eikonal equation $|\nabla\Phi|^2 = |\nabla f|^2$ in neighborhoods of the critical points. This requires to use the tangential gradient of f on $\partial\Omega$ in the definition of the Agmon distance (see (B.17)).

B.1.5.2 Notations and hypotheses

As already stated above, we assume that Ω is a connected open bounded C^∞ domain of $\mathbb{R}^d$ and $f : \mathbb{R}^d \to \mathbb{R}$ is a C^∞ function.[1] We will need the following set of assumptions:
[H1] The function $f : \overline{\Omega} \to \mathbb{R}$ is a Morse function on Ω and the restriction of f to the boundary of Ω denoted by $f_{\big|\partial\Omega}$, is a Morse function. The function f does not have any critical point on $\partial\Omega$.
[H2] The function f has a unique global minimum $x_0 \in \Omega$ in $\overline{\Omega}$:

$$\min_{\partial\Omega} f > \min_{\overline{\Omega}} f = \min_{\Omega} f = f(x_0).$$

[1] Actually, as explained in Section B.2, we will perform the analysis in a more general setting, namely when $\overline{\Omega}$ is a C^∞ oriented connected compact Riemannian manifold. In this introductory section, we stick to a simpler presentation, with Ω a subset of $\mathbb{R}^d$.

The point x_0 is the unique critical point of f in $\overline{\Omega}$. The function $f|_{\partial\Omega}$ has exactly $n \geq 1$ local minima denoted by $(z_i)_{i=1,\ldots,n}$ such that $f(z_1) \leq f(z_2) \leq \ldots \leq f(z_n)$.
[H3] $\partial_n f > 0$ on $\partial\Omega$.

In the following, $n_0 \in \{1, \ldots, n\}$ denotes the number of points in $\arg\min f|_{\partial\Omega}$:

$$f(z_1) = \ldots = f(z_{n_0}) < f(z_{n_0+1}) \leq \ldots \leq f(z_n).$$

We will need to define the basins of attraction of the local minima z_i for the dynamics $\dot{x} = -\nabla_T f(x)$ in $\partial\Omega$, where, we recall, for any $x \in \partial\Omega$, $\nabla_T f(x)$ denotes the tangential gradient of f on $\partial\Omega$.

Definition B.4. *Assume that **[H1]** holds. For each local minimum $z \in \partial\Omega$, one denotes by $B_z \subset \partial\Omega$ the open basin of attraction in $\partial\Omega$ of z for the dynamics $\dot{x} = -\nabla_T f(x)$ in $\partial\Omega$. Additionally define $B_z^c := \partial\Omega \setminus B_z$.*

From this definition, one obviously has that for each local minimum $z \in \partial\Omega$, for any $x \in B_z$, $f(x) \geq f(z)$.

As a consequence of the assumption **[H1]**, the determinants of the Hessians of f (resp. of $f|_{\partial\Omega}$) at the critical points of f (resp. of $f|_{\partial\Omega}$) are non zero. These quantities appear in the prefactors of the Eyring-Kramers law (see Equation (B.25) below).

Remark B.1. *Let us recall how the Hessians are defined. Let $\phi : N \to \mathbb{R}$ be a C^∞ function defined on a Riemannian C^∞ manifold N of dimension d. By standard results of Riemannian geometry, the Hessian* Hess $\phi(x)$ *of ϕ at a point $x \in N$ is defined as a bilinear symmetric form acting on vectors in the tangent space $T_x N$ as:*

$$\forall X, Y \in \Gamma(TN), \text{ Hess } \phi(X, Y) = \nabla_X d\phi(Y) \tag{B.19}$$

where ∇ is the covariant derivative (Levi-Civita connection) and $d\phi$ is the differential of ϕ. Then, det Hess $\phi(x)$ *is defined as the determinant of the bilinear form* Hess $\phi(x)$ *in any orthonormal basis of $T_x N$.*

In practice, det Hess $\phi(x)$ *can be computed using a local chart as follows. Let us assume that x_0 is a critical point of ϕ: $d_{x_0}\phi = 0$. Let us introduce $\psi : y \in U \mapsto \psi(y) \in V$ a local chart around x_0, where $U \subset \mathbb{R}^d$ is a neighborhood of 0, $V \subset N$ is a neighborhood of x_0 and $\psi(0) = x_0$. Let us assume in addition that the vectors $(e_i)_{i=1,\ldots,d} := \left(\frac{\partial\psi}{\partial y_i}(0)\right)_{i=1,\ldots,d}$ are orthonormal (thus defining an orthonormal basis of $T_{x_0}N$). Let us introduce the symmetric matrix H associated with the second order differential of $\phi \circ \psi$ at point 0: $\forall (u, v) \in \mathbb{R}^d \times \mathbb{R}^d$*

$$D_0^2(\phi \circ \psi)\left(\sum_{i=1}^d u_i e_i, \sum_{i=1}^d v_i e_i\right) = u^T H v.$$

Then

$$\text{det Hess } \phi(x_0) = \det H.$$

This formula is only valid at a critical point and is a direct consequence of the definition (B.19) *of the Hessian and the explicit expression of the Levi Civita connection in*

the local chart ψ:

$$\nabla_X d\phi(Y)|_x = \sum_{i,j=1}^{d} \left(\frac{\partial^2(\phi\circ\psi)}{\partial y_i \partial y_j}(y) - \sum_{k=1}^{d} \Gamma_{i,j}^k(\psi(y)) \frac{\partial(\phi\circ\psi)}{\partial y_k}(y) \right) Y_i X_j$$

where $x = \psi(y) \in V$, $\Gamma_{i,j}^k(x)$ are the Christoffel symbols of the connection ∇ associated with the basis $\left((\partial_{y_j}\psi)(\psi^{-1}(x))\right)_{j=1,\dots,n}$ of T_xN and $(X_j)_{j=1,\dots,n}$ (respectively $(Y_j)_{j=1,\dots,n}$) are the coordinates of X (respectively Y) in this basis.

B.1.5.3 Main result

In view of equations (B.14) and (B.16), we need to give an estimate of three quantities in order to analyze the exit point density and the asymptotics of the transition rates in the regime $h \to 0$: $\int_\Sigma (\partial_n u_h)\, e^{-\frac{2}{h}f}$ for a subset Σ of $\partial\Omega$, $\int_\Omega u_h\, e^{-\frac{2}{h}f}$ and λ_h, where, we recall (λ_h, u_h) is defined by (B.12). We will consider a subset Σ such that $\Sigma \subset B_{z_i}$ for a local minimum z_i (see Definition B.4 for the definition of B_{z_i}). This is the objective of the next three results.

Theorem B.1. *Assume that **[H1]**, **[H2]** and **[H3]** hold. Moreover assume that*

- $\forall i \in \{1,\dots,n\}$,

$$\inf_{z\in B_{z_i}^c} d_a(z, z_i) > \max[f(z_n) - f(z_i), f(z_i) - f(z_1)], \tag{B.20}$$

- *and*

$$f(z_1) - f(x_0) > f(z_n) - f(z_1). \tag{B.21}$$

Then, for all $i \in \{1,\dots,n\}$ and all open set $\Sigma_i \subset \partial\Omega$ containing z_i and such that $\overline{\Sigma}_i \subset B_{z_i}$, in the limit $h \to 0$

$$\int_{\Sigma_i} (\partial_n u_h)\, e^{-\frac{2}{h}f} d\sigma = A_i(h)\, e^{-\frac{2f(z_i)-f(x_0)}{h}} \left(1 + O(h)\right), \tag{B.22}$$

where u_h is the eigenfunction associated with the smallest eigenvalue of $-L_{f,h}^{D,(0)}(\Omega)$ (see Proposition B.3) which satisfies (B.11) *and*

$$A_i(h) = -\frac{(\det \mathrm{Hess} f(x_0))^{1/4} \partial_n f(z_i) 2\pi^{\frac{d-2}{4}}}{\sqrt{\det \mathrm{Hess} f|_{\partial\Omega}(z_i)}} h^{\frac{d-6}{4}}.$$

Remark B.2. *As will become clear in the proof of Theorem B.1, it can actually be proven that for all $i \in \{1,\dots,n\}$, the remainder $r_i(h) = O(h)$ appearing in* (B.22) *admits a full asymptotic expansion in h: there exists a sequence $(b_{k,i})_{k\geq 0} \in \mathbb{R}^{\mathbb{N}}$ such that for all $N \in \mathbb{N}$, in the limit $h \to 0$,*

$$r_i(h) = h \sum_{k=0}^{N} b_{k,i} h^k + O(h^{N+2}).$$

We do not state our main result with this expansion since, for general domains Ω, the explicit computations of the sequence $(b_{k,i})_{k\geq 0}$ is not possible in practice. This remark also holds for all the residuals $O(h)$ in the next results.

Proposition B.6. *Assume that **[H1]**, **[H2]** and **[H3]** hold. Then when $h \to 0$*

$$\int_\Omega u_h(x)\ e^{-\frac{2}{h}f(x)}dx = \frac{\pi^{\frac{d}{4}}}{(\det\ \mathrm{Hess} f(x_0))^{1/4}}\ h^{\frac{d}{4}}\ e^{-\frac{1}{h}f(x_0)}(1+O(h)),$$

where u_h is the eigenfunction associated with the smallest eigenvalue of $-L_{f,h}^{D,(0)}(\Omega)$ (see Proposition B.3) which satisfies (B.11).

Proposition B.7. *Assume that **[H1]**, **[H2]**, and **[H3]** hold. Then, in the limit $h \to 0$,*

$$\lambda_h = \frac{\sqrt{\det\ \mathrm{Hess} f(x_0)}}{\sqrt{\pi h}} \sum_{i=1}^{n_0} \frac{\partial_n f(z_i)}{\sqrt{\det\ \mathrm{Hess} f_{|\partial\Omega}(z_i)}}\ e^{-\frac{2}{h}(f(z_1)-f(x_0))}\,(1+O(h))\,, \tag{B.23}$$

where λ_h is the smallest eigenvalue of $-L_{f,h}^{D,(0)}(\Omega)$ (see Proposition B.3).

Theorem B.1 is the main contribution of this work. Actually Theorem B.1 will be proven in a more general framework: namely when $\overline{\Omega}$ is a C^∞ connected compact oriented Riemannian d-dimensional manifold with boundary $\partial\Omega$. Theorem B.1, Proposition B.6 and Proposition B.7 are respectively proved in Sections B.4.5, B.5.1.1 and B.5.1.2. For the sake of completeness, we provide a proof of Proposition B.7 in our specific setting, but this result actually holds under weaker geometric assumptions, see [17] or [33].

These results have the following consequence on the first exit point distribution and the estimate of the exact rates $(k_{0,i})$ using the Eyring-Kramers formula (see Section B.1.4.3). We recall that $(X_t)_{t\geq 0}$ denotes the solution to (B.1), τ_Ω is the exit time from the domain Ω and ν_h is the quasi stationary distribution associated with $(X_t)_{t\geq 0}$ and Ω.

Corollary B.8. *Under the hypotheses of Theorem B.1, for $i \in \{1,\dots,n\}$ and for all open sets $\Sigma_i \subset \partial\Omega$ containing z_i and such that $\overline{\Sigma}_i \subset B_{z_i}$, in the limit $h \to 0$:*

$$\mathbb{P}^{\nu_h}\left[X_{\tau_\Omega} \in \Sigma_i\right] = \frac{\partial_n f(z_i)}{\sqrt{\det\ \mathrm{Hess} f_{|\partial\Omega}(z_i)}} \left(\sum_{k=1}^{n_0} \frac{\partial_n f(z_k)}{\sqrt{\det\ \mathrm{Hess} f_{|\partial\Omega}(z_k)}}\right)^{-1} e^{-\frac{2}{h}(f(z_i)-f(z_1))}(1+O(h)). \tag{B.24}$$

The hypotheses (B.20) and (B.21) are discussed in Section B.1.6.2.

As a simple consequence of Corollary B.8, we recover the well-known result that $(X_t)_{t\geq 0}$ leaves Ω around the global minima of f on $\partial\Omega$: for any collection of open sets $(\Sigma_j)_{1\leq j\leq n_0}$ such that for all $j \in \{1,...,n_0\}$, $\overline{\Sigma}_j \subset B_{z_j}$ and $z_j \in \Sigma_j$, in the limit $h \to 0$, $\mathbb{P}^{\nu_h}\left[X_{\tau_\Omega} \in \bigcup_{j=1}^{n_0} \Sigma_j\right] = 1 + O(h)$. Actually, this result can be proven with an exponentially small residual ($O(h)$ is replaced by $O\left(e^{-c/h}\right)$ for some positive c) in a more general setting . Let us refer to [17] where we discuss this result in a more general setting (for example f can have several critical points in Ω and the assumptions (B.20) and (B.21) are not needed).

Corollary B.9. *Let us assume that hypotheses of Theorem B.1 are satisfied. Let for $i \in \{1,\dots,n\}$, Σ_i be an open subset of $\partial\Omega$ which contains z_i and which is such that*

$\overline{\Sigma}_i \subset B_{z_i}$. *Using the notation of Section B.1.4.3, assume that* Σ_i *is the common boundary between* Ω *and another domain* $\Omega_i \subset \mathbb{R}^d$. *Then, the transition rate given by* (B.15), *to go from* Ω *to* Ω_i *satisfies, in the limit* $h \to 0$,

$$k_{0,i} = \frac{1}{\sqrt{\pi h}} \partial_n f(z_i) \frac{\sqrt{\det \text{ Hess} f(x_0)}}{\sqrt{\det \text{ Hess} f_{|\partial\Omega}(z_i)}} e^{-\frac{2}{h}(f(z_i)-f(x_0))}(1+O(h)). \tag{B.25}$$

This corollary thus gives a justification of the Eyring-Kramers formula and the Transition State Theory to build Markov models. As stated in the assumptions, the exit rates are obtained assuming $\partial_n f > 0$ on $\partial\Omega$: the local minima $z_1, \ldots, z_n$ of V on $\partial\Omega$ are therefore not saddle points of f but so-called *generalized saddle points* (see [34,47]). In a future work, we intend to extend these results to the case where the points $(z_i)_{1\leq i\leq n}$ are saddle points of f, in which case we expect to prove the same result (B.25) for the exit rates, with a modified prefactor:

$$k_{0,i} = \frac{1}{\pi} |\lambda^-(z_j)| \frac{\sqrt{\det \text{Hess } f(x_0)}}{\sqrt{|\det \text{Hess } f(z_j)|}} e^{-\frac{2}{h}(f(z_i)-f(x_0))}(1+O(h))$$

(this formula can be obtained using formal expansions on the exit time and Laplace's method). Notice that the latter formula differs from (B.6)–(B.7) by a multiplicative factor 1/2 since λ_h is the exit rate from Ω and not the transition rate to one of the neighboring state (see the remark on page 408 in [5] on this multiplicative factor 1/2 and the results on asymptotic exit times in [50] for example). This factor is due to the fact that once on the saddle point, the process has a probability one half to go back to Ω, and a probability one half to effectively leave Ω. This multiplicative factor does not have any influence on the law of the next visited state which only involves ratio of the rates $k_{0,i}$, see Section B.1.4.3 and Equation (B.24).

B.1.6 Discussion and generalizations

As explained above, the interest of Theorem B.1 is that it justifies the use of the Eyring-Kramers formula to model the exit event using a jump Markov model including the prefactors. It gives in particular the relative probability to leave Ω through each of the local minima z_i of f on the boundary $\partial\Omega$. Moreover, one obtains an estimate of the relative error on the exit probabilities (and not only on the logarithm of the exit probabilities as in (B.8)): it is of order h, see Equation (B.24).

In Section B.1.6.1, we explain how this result can be generalized to a situation where the process $(X_t)_{t\geq 0}$ is assumed to start under another initial condition than the quasi stationary distribution. The importance of the geometric assumption (B.20)-(B.21) (resp. assumption (B.26)) to obtain the asymptotic result of Corollary B.8 (resp. its generalization to deterministic initial conditions, see Corollary B.10) is discussed in Section B.1.6.2. Finally, in Section B.1.6.3, we discuss extensions to less stringent conditions than (B.20)-(B.21). Moreover the exit through subsets of $\partial\Omega$ which do not necessarily contain one of the local minima z_i of $f|_{\partial\Omega}$ is considered: this shows in particular the interest of estimating the prefactors in the asymptotic approximations of the exit rates.

B.1.6.1 Extension of the result to other initial conditions

The question we would like to address in this section is how to generalize Corollary B.8, to a deterministic initial condition: $X_0 = x$ for $x \in \Omega$.

Corollary B.10. *Let us assume that all the hypotheses of Corollary B.8 are satisfied, and that in addition there exists $i_0 \in \{2, \dots, n\}$ such that*

$$2(f(z_{i_0}) - f(z_1)) < f(z_1) - f(x_0). \tag{B.26}$$

Let $i \in \{1, \dots, i_0\}$ and let $\alpha \in \mathbb{R}$ be such that

$$f(x_0) < \alpha < 2f(z_1) - f(z_i).$$

Then, for $i \in \{1, \dots, n\}$ and for all open sets $\Sigma_i \subset \partial\Omega$ containing z_i and such that $\overline{\Sigma}_i \subset B_{z_i}$, we have uniformly in $x \in f^{-1}((-\infty, \alpha]) \cap \Omega$, in the limit $h \to 0$:

$$\mathbb{P}^x[X_{\tau_\Omega} \in \Sigma_i] = \frac{\partial_n f(z_i)}{\sqrt{\det \text{ Hess} f_{|\partial\Omega}(z_i)}} \left(\sum_{k=1}^{n_0} \frac{\partial_n f(z_k)}{\sqrt{\det \text{ Hess} f_{|\partial\Omega}(z_k)}} \right)^{-1} e^{-\frac{2}{h}(f(z_i) - f(z_1))}(1 + O(h)). \tag{B.27}$$

Let us give a simple example to illustrate this result. In a situation where $n = 2$, this corollary shows that the estimates we have obtained on the probability to exit in a neighborhood of z_2 under the assumption $X_0 \sim \nu_h$ are still valid if $X_0 = x$ for $x \in f^{-1}((-\infty, 2f(z_1) - f(z_2))) \cap \Omega$ under the assumption $f(z_1) - f(x_0) > 2(f(z_2) - f(z_1))$, which is a stronger assumption than (B.21).

B.1.6.2 On the geometric assumptions (B.20), (B.21) and (B.26)

On the geometric assumption (B.20).

The question we would like to address is the following: is the assumption (B.20) necessary for the result on the exit point density (B.24) to hold?

In order to test this assumption numerically, we consider the following simple two-dimensional setting. The potential function is

$$f(x, y) = x^2 + y^2 - ax,$$

with $a \in (0, 1/9)$, and the domain Ω is defined by (see Figure B.2):

$$\Omega = [0, 1]^2 \cup \left\{(x, y) \,|x^2 + (y - 1)^2 < 1\right\} \cup \left\{(x, y) \,|x^2 + (y + 1)^2 < 1\right\}.$$

The two local minima of f on $\partial\Omega$ are $z_1 = (1, 0)$ and $z_2 = (-1, 0)$. Notice that $f(z_2) - f(z_1) = 2a > 0$. The potential f has a unique critical point in Ω, namely the global minimum $x_0 = (a/2, 0)$. Let us check that the assumptions of Theorem B.1 are satisfied in this setting (i.e. for $a \in (0, \frac{1}{9})$). Indeed, the inequality $f(z_1) - f(x_0) > f(z_2) - f(z_1)$ is satisfied if and only if $1 - 3a + \frac{a^2}{4} > 0$ i.e. if and only if $a \notin (2(3 - \sqrt{8}), 2(3 + \sqrt{8}))$. Moreover, using Proposition B.34, the inequality $d_a(z_1, B^c_{z_1}) > f(z_2) - f(z_1)$ is satisfied. Finally, to check that the inequality $d_a(z_2, B^c_{z_2}) > f(z_2) - f(z_1)$ is satisfied we use Proposition B.33 with $W = \{(x, y) \in \mathbb{R}^2, |(x, y) - z_2| \leq \frac{1}{3}\} \cap \overline{\Omega}$ and $W' = \{(x, y) \in$

$\mathbb{R}^2$, $|(x,y)-z_2| \leq \frac{2}{3}\} \cap \overline{\Omega}$. In that case, one has $\alpha = \frac{1}{3}$ (where α is defined by (B.88)) and thus the inequality

$$\alpha \inf_{x \in \overline{W' \setminus W}} g(x) = \frac{1}{3} \min\left(\frac{2}{3}, \left|2\left(-1+\frac{2}{3}\right)-a\right|\right) = \frac{1}{3} \min\left(\frac{2}{3}, \frac{2}{3}+a\right) > f(z_2) - f(z_1) = 2a$$

is satisfied if and only if $a < \frac{1}{9}$.

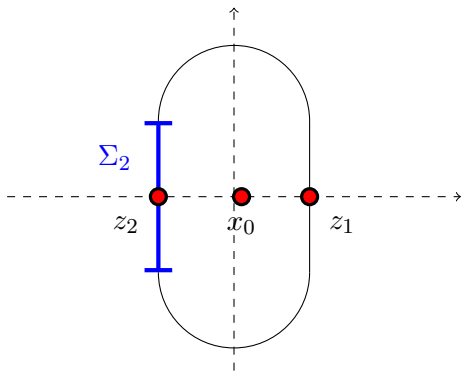

Figure B.2: The domain Ω.

Let us consider the segment Σ_2 joining the two points $(-1,-1)$ and $(-1,1)$. This subset of $\partial\Omega$ contains the highest saddle point z_2 and is included in B_{z_2}. From Theorem B.1, we expect that, in the limit $h \to 0$,

$$\mathbb{P}^{\nu_h}\left[X_{\tau_\Omega} \in \Sigma_2\right] = \exp\left(G\left(\frac{2}{h}\right)\right)(1+O(h))$$

where

$$G(x) = \ln\left[\frac{\partial_n f(z_2)\sqrt{\det \text{Hess} f|_{\partial\Omega}(z_1)}}{\partial_n f(z_1)\sqrt{\det \text{Hess} f|_{\partial\Omega}(z_2)}}\right] - x\left(f(z_2)-f(z_1)\right).$$

The function G is compared to the numerically estimated function F such that $F\left(\frac{2}{h}\right) = \ln\left(\mathbb{P}^{\nu_h}\left[X_{\tau_\Omega} \in \Sigma_2\right]\right)$. In practice, the quasi stationary distribution ν_h is sampled using a Fleming-Viot particle system (the convergence diagnostics being a Gelman-Rubin statistics, see [3]) composed of 10^5 particles. The probability $\mathbb{P}^{\nu_h}(X_{\tau_\Omega} \in \Sigma_2)$ is estimated using a Monte Carlo procedure using 6×10^5 particles distributed according to the quasi stationary distribution ν_h. The dynamics (B.1) is discretized in time using an Euler-Maruyama scheme with a timestep Δt which is made precise in the captions of the figures. On Figures B.3 and B.4, we observe an excellent agreement between the theory and the numerical results.

Now, the potential function f is modified such that the assumption (B.20) is not satisfied anymore. More precisely, the potential function is

$$f(x,y) = \left(y^2 - 2\,a(x)\right)^3,$$

with $a(x) = a_1 x^2 + b_1 x + 0.5$ where a_1 and b_1 are chosen such that $a(-1+\delta) = 0$, $a(1) = 1/4$ for $\delta = 0.05$. We have $f(z_1) = -1/8$ and $f(z_2) = -8(a(-1))^3 > 0 > f(z_1)$.

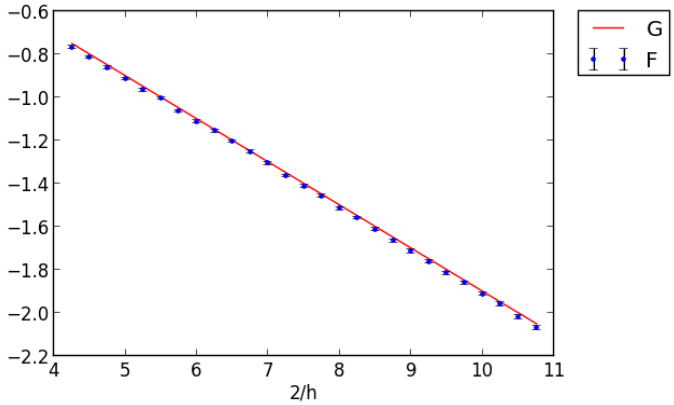

Figure B.3: Logarithm of the probability $\mathbb{P}^{\nu_h}(X_{\tau_\Omega} \in \Sigma_2)$ as a function of $\frac{2}{h}$: comparison of the theoretical result function (G) with the numerical result (function F, $\Delta t = 5.10^{-3}$); $a = 1/10$.

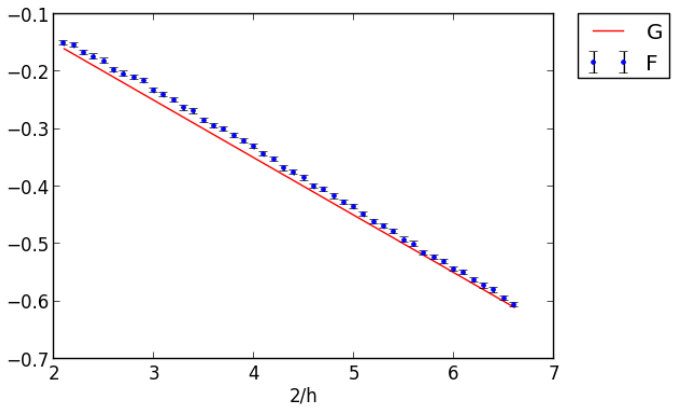

Figure B.4: Logarithm of the probability $\mathbb{P}^{\nu_h}(X_{\tau_\Omega} \in \Sigma_2)$ as function of $\frac{2}{h}$ as a function of $\frac{2}{h}$: comparison of the theoretical result function (G) with the numerical result (function F, $\Delta t = 2.10^{-3}$); $a = 1/20$.

Moreover, two 'corniches' (which are in the level set $f^{-1}(\{0\})$ of f, and on which $|\nabla f| = 0$) on the 'slopes of the hills' of the potential f join the point $(-1+\delta, 0)$ to $B^c_{z_2}$ (at the points $(1, 1/\sqrt{2}) \in B^c_{z_2}$ and $(1, -1/\sqrt{2}) \in B^c_{z_2}$) so that $\inf_{z \in B^c_{z_2}} d_a(z, z_2) < f(z_2) - f(z_1)$. Indeed, in that case assumption (B.20) is not satisfied since

$$\begin{aligned}
\inf_{z \in B^c_{z_2}} d_a(z, z_2) &\leq d_a\left(z_2, (1, 1/\sqrt{2})\right) \\
&\leq d_a\left(z_2, (0, -1+\delta)\right) + d_a\left((0, -1+\delta), (1, 1/\sqrt{2})\right) \\
&= f(z_2) - f(0, -1+\delta) + 0 \\
&= f(z_2) < f(z_2) - f(z_1).
\end{aligned}$$

Notice that the Hessians $(\text{Hess } f|_{\partial\Omega})(z_1)$ and $(\text{Hess } f|_{\partial\Omega})(z_2)$ are nonsingular. The functions $f_{|\Omega}$ and $f|_{\partial\Omega}$ are not Morse functions, but an arbitrarily small perturbation

(which we neglect here) turns them into Morse functions. When comparing the numerically estimated probability $\mathbb{P}^{\nu_h}(X_{\tau_\Omega} \in \Sigma_2)$, with the theoretical asymptotic result in the limit $h \to 0$, we observe a discrepancy on the prefactors, see Figure B.5.

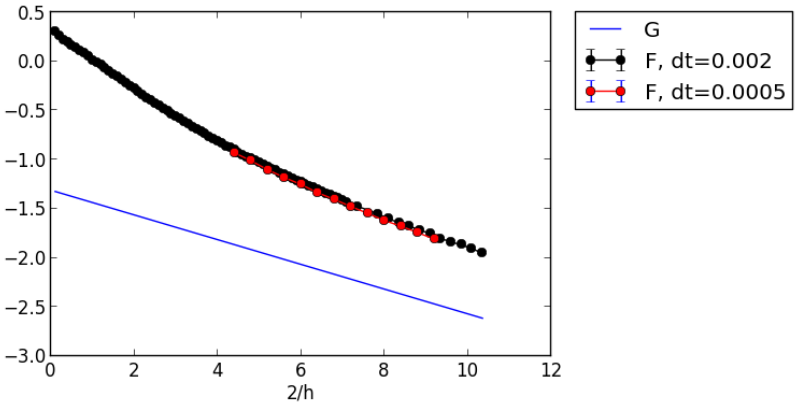

Figure B.5: Logarithm of the probability $\mathbb{P}^{\nu_h}(X_{\tau_\Omega} \in \Sigma_2)$ as a function of $\frac{2}{h}$: comparison of the theoretical result function (G) with the numerical result (function F, $\Delta t = 2.10^{-3}$ and $\Delta t = 5.10^{-4}$).

Therefore, it seems that assumption (B.20) is indeed required to get an accurate description of the dynamics by the jump Markov process using the Eyring-Kramers law to estimate the rates between the neighboring states.

On the geometric assumptions (B.21) and (B.26).

To discuss the necessity of the assumptions (B.26) in Corollary B.10 and (B.21) in Corollary B.8, we consider a one-dimensional case, where the law of X_{τ_Ω} when $X_0 = x$ has an explicit expression. Let $f : \mathbb{R} \to \mathbb{R}$ be C^∞ and let $z_1, z_2 \in \mathbb{R}$ such that $z_1 < z_2$. Let us assume that $f'(z_1) < 0$, $f'(z_2) > 0$, $f(z_1) < f(z_2)$ and f has only one critical point in (z_1, z_2) denoted by x_0. This implies in particular that $f(x_0) = \min_{[z_1,z_2]} f < f(z_1)$. Moreover let us assume that $f''(x_0) > 0$. Therefore, the hypotheses **[H1]**-**[H2]**-**[H3]** hold. For $x \in [z_1, z_2]$, let us denote by $w_h(x) = \mathbb{P}_x[X_{\tau_{(z_1,z_2)}} = z_2]$. It is standard that using a Feynman-Kac formula, w_h solves the elliptic boundary value poblem

$$\frac{2}{h} g'' - g' f' = 0, \;\; g(z_1) = 0, \;\; g(z_2) = 1.$$

Therefore, one has for $x \in [z_1, z_2]$: $w_h(x) = \dfrac{\displaystyle\int_{z_1}^{x} e^{\frac{2}{h} f}}{\displaystyle\int_{z_1}^{z_2} e^{\frac{2}{h} f}}$. Let $x \in [z_1, z_2]$. Using Laplace's method, if $f(x) < f(z_1)$, one obtains in the limit $h \to 0$:

$$\mathbb{P}^x[X_{\tau_{(z_1,z_2)}} = z_2] = -\frac{f'(z_2)}{f'(z_1)} e^{-\frac{2}{h}(f(z_2)-f(z_1))}(1 + O(h)),$$

if $f(x) = f(z_1)$, $x \neq z_1$, it holds in the limit $h \to 0$:

$$\mathbb{P}^x[X_{\tau_{(z_1,z_2)}} = z_2] = f'(z_2) \left(\frac{1}{f'(x)} - \frac{1}{f'(z_1)} \right) e^{-\frac{2}{h}(f(z_2)-f(z_1))}(1 + O(h)),$$

and if $f(x) > f(z_1)$, it holds in the limit $h \to 0$:

$$\mathbb{P}^x[X_{\tau_{(z_1,z_2)}} = z_2] = \frac{f'(z_2)}{f'(x)} e^{-\frac{2}{h}(f(z_2)-f(x))}(1+O(h)).$$

Therefore, in dimension one, the estimate (B.27) holds if and only if $x \in f^{-1}((-\infty, f(z_1)))$. In accordance with Corollary B.10, the asymptotic (B.27) only holds for initial conditions which are sufficiently low in energy. However, we observe that in this simple one-dimensional setting, the assumption (B.26) is not needed. We do not know if the result of Corollary B.10 would hold in general without the assumption (B.26).

Let us now discuss the assumption (B.21) in the framework of Theorem B.1 and Corollary B.8. From (B.13), one has:

$$\mathbb{P}^{\nu_h}[X_{\tau_{(z_1,z_2)}} = z_2] = \frac{\displaystyle\int_{z_1}^{z_2} u_h w_h e^{-\frac{2}{h}f}}{\displaystyle\int_{z_1}^{z_2} u_h e^{-\frac{2}{h}f}}.$$

Using Lemma B.60, Lemma B.18 and (B.61), one has for some $c > 0$, for any $\delta > 0$ and for h small enough:

$$u_h(x) = \frac{\chi(x)}{\sqrt{\int_{z_1}^{z_2} \chi^2 e^{-\frac{2}{h}f}}}(1+\alpha_h) + r(x), \text{ for } x \in \overline{\Omega}$$

with $\alpha_h \in \mathbb{R}$, $\alpha_h = O(e^{-\frac{c}{h}})$, $\int_{z_1}^{z_2} r^2 e^{-\frac{2}{h}f} = O(e^{-\frac{1}{h}(f(z_1)-f(x_0)-\delta)})$ and where $\chi \in C_c^\infty(z_1, z_2)$ is given by Lemma B.60. Therefore, one has:

$$\mathbb{P}^{\nu_h}[X_{\tau_{(z_1,z_2)}} = z_2] = \frac{1}{\int_{z_1}^{z_2} u_h e^{-\frac{2}{h}f}} \left[\frac{\int_{z_1}^{z_2} \chi(x) \int_{z_1}^{x} e^{\frac{2}{h}(f(y)-f(x))} dy dx}{\int_{z_1}^{z_2} e^{\frac{2}{h}f} \sqrt{\int_{z_1}^{z_2} \chi^2 e^{-\frac{2}{h}f}}}(1+\alpha_h) + \int_{z_1}^{z_2} r w_h e^{-\frac{2}{h}f} \right].$$

Using Proposition B.6 and Laplace's method, one gets for any $\delta > 0$, in the limit $h \to 0$:

$$\mathbb{P}^{\nu_h}[X_{\tau_{(z_1,z_2)}} = z_2] = -\frac{f'(z_2)}{f'(z_1)} e^{-\frac{2}{h}(f(z_2)-f(z_1))}(1+O(h)) + O(e^{-\frac{1}{h}(f(z_2)-f(x_0)+f(z_1)-f(x_0)-\delta)}).$$

Therefore, the result of Corollary B.8 holds if

$$2(f(z_1) - f(x_0)) > f(z_2) - f(z_1). \tag{B.28}$$

This explicit computation in dimension one shows that the result of Corollary 1 indeed requires an assumption of the type: the height of the energy barrier to leave the well $f(z_1) - f(x_0)$ is sufficiently large compared to the largest difference in energy of the saddle points $f(z_2) - f(z_1)$. Notice that (B.28) differs from (21) by a multiplicative factor $\frac{1}{2}$. We do not know if the result of Corollary B.8 would hold in general under the weaker assumption (B.28). Finally, let us mention that when $d = 1$, (B.20) is always satisfied.

B.1.6.3 Extension of the result to more general subsets of $\partial\Omega$

It is actually possible to generalize the result of Theorem B.1 and Corollary B.8 to less stringent conditions than (B.20)-(B.21) and to more general subsets $\Sigma \subset \partial\Omega$.

Theorem B.2. *Assume that **[H1]**, **[H2]** and **[H3]** hold. Assume that there exist $k_0 \in \{1, \dots, n\}$ and $f^* \in \mathbb{R}$ such that $f(z_{k_0}) \leq f^* \leq f(z_{k_0+1})$ (with the convention $f(z_{k_0+1}) = +\infty$ if $k_0 = n$),*

$$\begin{cases} \forall i \in \{1, \dots, k_0\}, \ \inf\limits_{z \in B^c_{z_i}} d_a(z, z_i) > \max[f^* - f(z_i), f(z_i) - f(z_1)], \\ \forall i \in \{k_0 + 1, \dots, n\}, \ \inf\limits_{z \in B^c_{z_i}} d_a(z, z_i) > f^* - f(z_1), \end{cases} \tag{B.29}$$

and,

$$f(z_1) - f(x_0) > f^* - f(z_1). \tag{B.30}$$

Let u_h be the eigenfunction associated with the smallest eigenvalue of $-L^{D,(0)}_{f,h}(\Omega)$ (see Proposition B.3) which satisfies (B.11).

1. *For all $i \in \{1, \dots, k_0\}$ and for all smooth open set $\Sigma_i \subset \partial\Omega$ containing z_i and such that $\overline{\Sigma}_i \subset B_{z_i}$, the limit* (B.22) *holds for $\int_{\Sigma_i} (\partial_n u_h)\, e^{-\frac{2}{h}f} d\sigma$ and the limit* (B.24) *holds for $\mathbb{P}^{\nu_h}[X_{\tau_\Omega} \in \Sigma_i]$. Moreover, if $f(z_{k_0+1}) > f(z_{k_0})$, for all $i \in \{k_0+1, \dots, n\}$ and for all smooth open set $\Sigma_i \subset \partial\Omega$ containing z_i and such that $\overline{\Sigma}_i \subset B_{z_i}$, there exist $\varepsilon > 0$ and $h_0 > 0$ such that for all $h \in (0, h_0)$*

$$\int_{\Sigma_i} (\partial_n u_h)\, e^{-\frac{2}{h}f} d\sigma = \left(\int_{\Sigma_{k_0}} (\partial_n u_h)\, e^{-\frac{2}{h}f} d\sigma \right) O\left(e^{-\frac{\varepsilon}{h}}\right), \tag{B.31}$$

and

$$\mathbb{P}^{\nu_h}[X_{\tau_\Omega} \in \Sigma_i] = \mathbb{P}^{\nu_h}[X_{\tau_\Omega} \in \Sigma_{k_0}]\, O\left(e^{-\frac{\varepsilon}{h}}\right) \tag{B.32}$$

2. *Let $j_0 \in \{1, \dots, k_0\}$ and $\Sigma \subset \partial\Omega$ be a smooth open set such that $\overline{\Sigma} \subset B_{z_{j_0}}$ and $\inf_\Sigma f = f^*$. Let $(B^*, p^*) \in \mathbb{R}^*_+ \times \mathbb{R}$ be such that*

$$\int_\Sigma (\partial_n f)\, e^{-\frac{2}{h}f} d\sigma = B^*\ h^{p^*}\ e^{-\frac{2}{h}f^*}\, (1 + O(h)). \tag{B.33}$$

Then, one obtains in the limit $h \to 0$

$$\int_\Sigma (\partial_n u_h)\, e^{-\frac{2}{h}f}\ d\sigma = -\frac{2B^* \left(\det \operatorname{Hess} f(x_0)\right)^{\frac{1}{4}}}{\pi^{\frac{d}{4}}} h^{p^* - \frac{d}{4} - 1} e^{-\frac{1}{h}(2f^* - f(x_0))}\, (1 + O(h)) \tag{B.34}$$

and

$$\mathbb{P}^{\nu_h}[X_{\tau_\Omega} \in \Sigma] = \frac{B^*}{\pi^{\frac{d-1}{2}}} \left(\sum_{k=1}^{n_0} \frac{\partial_n f(z_k)}{\sqrt{\det \operatorname{Hess} f_{|\partial\Omega}(z_k)}} \right)^{-1} h^{p^* - \frac{d-1}{2}} e^{-\frac{2}{h}(f^* - f(z_1))}\, (1 + O(h)). \tag{B.35}$$

In practice, the expansion (B.33) is given by Laplace's method. Theorem B.2 is a generalization of Theorem B.1. Indeed, (B.29)-(B.30) is weaker than (B.20)-(B.21) ((B.20)-(B.21) implies (B.29)-(B.30) for $k_0 = n$ and $f^* = f(z_n)$) and item 2 gives an asymptotic result on the exit probability through $\Sigma \subset B_{z_{j_0}}$ even if $z_{j_0} \notin \overline{\Sigma}$.

As an illustration, let us state a corollary of this theorem, which demonstrates the importance of obtaining a precise asymptotic result including the prefactors. Let us consider a simple situation with only two local minima z_1 and z_2 on the boundary, with $f(z_1) < f(z_2)$. Let us now compare the two exit probabilities (see Figure B.6 for a schematic representation of the geometric setting):

- The probability to leave through Σ_2 such that $\overline{\Sigma_2} \subset B_{z_2}$ and $z_2 \in \Sigma_2$;
- The probability to leave through Σ such that $\overline{\Sigma} \subset B_{z_1}$ and $\inf_\Sigma f = f(z_2)$.

By classic results from the large deviation theory (see for example (B.8)) the probability to exit through Σ and Σ_2 both scale like a prefactor times $\mathrm{e}^{-\frac{2}{h}(f(z_2)-f(z_1))}$: the difference can only be read from the prefactors. Actually, using item 2 in Theorem B.2, one obtains the existence of $C > 0$ such that in the limit $h \to 0$ (see Corollary B.11 below),

$$\frac{\mathbb{P}^{\nu_h}(X_{\tau_\Omega} \in \Sigma)}{\mathbb{P}^{\nu_h}(X_{\tau_\Omega} \in \Sigma_2)} \sim C\sqrt{h}. \tag{B.36}$$

The probability to leave through Σ_2 (namely through the generalized saddle point z_2) is thus larger than through Σ, even though the two regions are at the same height. This result explains why the local minima of f on the boundary (namely the generalized saddle points) play such an important role when studying the exit event. Let us now state the precise result.

Corollary B.11. *Assume **[H1]**, **[H2]**, **[H3]**. Assume that $f|_{\partial\Omega}$ has only two local minima z_1 and z_2 such that $f(z_1) < f(z_2)$ and,*

- *for $j \in \{1, 2\}$,*
$$\inf_{z \in B^c_{z_j}} d_a(z, z_j) > f(z_2) - f(z_1), \tag{B.37}$$
- $$f(z_1) - f(x_0) > f(z_2) - f(z_1). \tag{B.38}$$

Let $\Sigma \subset \partial\Omega$ be a smooth open set such that $\overline{\Sigma} \subset B_{z_1}$. Assume moreover that $\inf_\Sigma f = f(z_2)$ and that the infimum is attained at a single point z^*: $\inf_\Sigma f = f(z^*)$ (necessarily $z^* \in \partial\Sigma$). Finally, let us assume that z^* is a non degenerate minimum of $f_{|\partial\Sigma}$ and $\partial_{n(\partial\Sigma)} f_{|\partial\Sigma}(z^*) < 0$ where $n(\partial\Sigma)$ is the unit outward normal to $\partial\Sigma \subset \partial\Omega$. Then, one has the following asymptotic expansion of $\mathbb{P}^{\nu_h}[X_{\tau_\Omega} \in \Sigma]$ in the limit $h \to 0$:

$$\begin{aligned}\mathbb{P}^{\nu_h}[X_{\tau_\Omega} \in \Sigma] &= -\frac{\sqrt{h}}{2\sqrt{\pi}} \frac{\partial_n f(z^*)}{\partial_{n(\partial\Sigma)} f(z^*) \sqrt{\det \mathrm{Hess} f_{|\partial\Sigma}(z^*)}} \left(\sum_{k=1}^{n_0} \frac{\partial_n f(z_k)}{\sqrt{\det \mathrm{Hess} f_{|\partial\Omega}(z_k)}} \right)^{-1} \\ &\quad \times e^{-\frac{2}{h}(f(z_2)-f(z_1))}(1 + O(h)),\end{aligned}$$

with by convention, $\det \mathrm{Hess} f_{|\partial\Sigma}(z^*) = 1$ *if* $d = 2$.

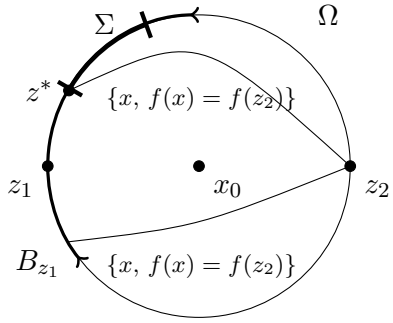

Figure B.6: Schematic representation of the geometric setting of Corollary B.11. The subset Σ is such that $\overline{\Sigma} \subset B_{z_1}$ and $\inf_\Sigma f = f(z_2)$.

Corollaries B.8, B.10 and B.11 imply the result (B.36) announced above.

Remark B.3. *By using Laplace's method, one can check that the asymptotic results obtained in Corollaries B.8, B.10 and B.11 on the law of X_{τ_Ω} can be obtained by writing that the density of X_{τ_Ω} with respect to the Lebesgue measure on $\partial\Omega$ is, in the limit $h \to 0$,*

$$z \in \partial\Omega \mapsto \frac{\partial_n f(z)\, e^{-\frac{2}{h} f(z)}}{\int_{\partial\Omega} \partial_n f\, e^{-\frac{2}{h} f}\, d\sigma}(1 + O(h)). \tag{B.39}$$

This indeed yields exactly the same asymptotic results on the exit distribution. This is reminiscent of previous results obtained in [42, 59], where the authors proved that, starting from a deterministic initial condition in Ω, X_{τ_Ω} has a density with respect to the Lebesgue measure on $\partial\Omega$ which satisfies, in the limit $h \to 0$, $z \in \partial\Omega \mapsto \frac{\partial_n f(z)\, e^{-\frac{2}{h} f(z)}}{\int_{\partial\Omega} \partial_n f\, e^{-\frac{2}{h} f}\, d\sigma} + o(1)$, which is a less precise estimate than (B.39).

B.1.7 Strategy of the proof of Theorem B.1

The aim of this section is to give an overview of the strategy for the proof of Theorem B.1. In view of (B.22), we would like to identify the asymptotic behavior of the normal derivative $\partial_n u_h$ on $\partial\Omega$ in the limit $h \to 0$. We recall that (λ_h, u_h) are defined by the eigenvalue problem (B.12). By differentiating (B.12), we observe that ∇u_h satisfies

$$\begin{cases} L^{(1)}_{f,h} \nabla u_h = -\lambda_h \nabla u_h \text{ on } \Omega, \\ \nabla_T u_h = 0 \text{ on } \partial\Omega, \\ \left(\dfrac{h}{2}\mathrm{div} - \nabla f \cdot\right) \nabla u_h = 0 \text{ on } \partial\Omega, \end{cases} \tag{B.40}$$

where

$$L^{(1)}_{f,h} = \frac{h}{2}\Delta - \nabla f \cdot \nabla - \mathrm{Hess}\, f \tag{B.41}$$

is an operator acting on 1-forms (namely on vector fields). Therefore ∇u_h is an eigen-1-form of the operator $-L^{(1)}_{f,h}$ with tangential Dirichlet boundary conditions (see (C.33)), associated with the small eigenvalue λ_h.

It is known (see for example [34]) that in our geometric setting, $-L_{f,h}^{D,(0)}(\Omega)$ admits exactly one eigenvalue smaller than $\frac{\sqrt{h}}{2}$, namely λ_h with associated eigenfunction u_h (this is because f has only one local minimum in Ω) and that $-L_{f,h}^{D,(1)}(\Omega)$ admits exactly n eigenvalues smaller than $\frac{\sqrt{h}}{2}$ (where, we recall, n is the number of local minima of f on $\partial\Omega$). Actually, all these small eigenvalues are exponentially small in the regime $h \to 0$, the other eigenvalues being bounded from below by a constant in this regime. The idea is then to construct an appropriate basis (with so called quasi-modes, which are localized on the generalized saddle points $(z_i)_{i=1,\dots,n}$) of the eigenspace associated with small eigenvalues for $L_{f,h}^{D,(1)}(\Omega)$, and then to decompose ∇u_h along this basis.

The article is organized as follows. In Section B.2, we introduce the general setting for the proof of our results, and the Gram-Schmidt procedure which allows, starting from a set of quasi-modes, to compute the projection of (an approximation of) ∇u_h along the quasi-modes. In order to quantify the distance between the space spanned by these quasi-modes and the eigenspace of $L_{f,h}^{D,(1)}(\Omega)$ associated with small eigenvalues, we need to use so-called Agmon estimates. Section B.3 is devoted to a presentation of the main properties of the Agmon distance which intervenes in these estimates. The most technical part is the effective construction of the quasi-modes using auxiliary simpler eigenvalue problems associated with each of the local minima $(z_i)_{i=1,\dots,n}$. This is explained in Section B.4 which concludes the proof of Theorem B.1. Finally, Section B.5 concludes the paper by providing the proofs of all the other results stated above, in particular Theorem B.2.

B.2 General setting and strategy for the proof of Theorem B.1

The general setting for proving the results presented in Section B.1 will be the following: $\overline{\Omega}$ is a C^∞ oriented connected compact Riemannian manifold of dimension d with boundary $\partial\Omega$ and the function f is a C^∞ real valued function defined on $\overline{\Omega}$. One defines $\Omega := \overline{\Omega} \setminus \partial\Omega$. In particular, Theorem B.1 will actually be proven in this framework. Notice that the assumptions **[H1]**, **[H2]** and **[H3]** are still meaningful in this more general setting.

In order to use previous results from the literature on semi-classical analysis, we will transform the original problem (B.12) on (λ_h, u_h) associated with weighted Hilbert space $H_w^q(\Omega)$ to an eigenvalue problem on the standard (non-weighted) Hilbert spaces $H^q(\Omega)$, by using a unitary transformation which relates the operator $L_{f,h}^{(p)}$ to the Witten Laplacians $\Delta_{f,h}^{(p)}$. This is explained in Section B.2.1, together with some first well-known results on the spectrum of Witten Laplacians. Then, in Section B.2.2, we explain what are the requirements on the quasi-modes we will build in order to obtain the estimate (B.22), see Proposition B.17. Section B.2.3 is finally devoted to the proof of Proposition B.17.

B.2.1 Witten Laplacians

B.2.1.1 Notations for Sobolev spaces

For $p \in \{0, \dots, d\}$, one denotes by $\Lambda^p C^\infty(\overline{\Omega})$ the space of C^∞ p-forms on $\overline{\Omega}$. Moreover, $\Lambda^p C^\infty_T(\overline{\Omega})$ is the set of C^∞ p-forms v such that $\mathbf{t}v = 0$ on $\partial\Omega$, where $\mathbf{t}$ denotes the tangential trace on forms. Likewise, the set $\Lambda^p C^\infty_N(\overline{\Omega})$ is the set of C^∞ p-forms v such that $\mathbf{n}v = 0$ on $\partial\Omega$, where $\mathbf{n}$ denotes the normal trace on forms defined by: for all $w \in \Lambda^p C^\infty(\overline{\Omega})$, $\mathbf{n}w := w|_{\partial\Omega} - \mathbf{t}w$.

For $p \in \{0, \dots, d\}$ and $q \in \mathbb{N}$, one denotes by $\Lambda^p H^q_w(\Omega)$ the weighted Sobolev spaces of p forms with regularity index q, for the weight $e^{-\frac{2}{h}f(x)}dx$ on Ω: $v \in \Lambda^p H^q_w(\Omega)$ if and only if for all multi-index α with $|\alpha| \leq q$, the α derivative of v is in $\Lambda^p L^2_w(\Omega)$ where $\Lambda^p L^2_w(\Omega)$ is the completion of the space $\Lambda^p C^\infty(\overline{\Omega})$ for the norm

$$w \in \Lambda^p C^\infty(\overline{\Omega}) \mapsto \int_\Omega |w|^2 e^{-\frac{2}{h}f}.$$

See for example [65] for an introduction to Sobolev spaces on manifolds with boundaries. For $p \in \{0, \dots, d\}$ and $q > \frac{1}{2}$, the set $\Lambda^p H^q_{w,T}(\Omega)$ is defined by

$$\Lambda^p H^q_{w,T}(\Omega) := \{v \in \Lambda^p H^q_w(\Omega) \,|\, \mathbf{t}v = 0 \text{ on } \partial\Omega\}.$$

Notice that $\Lambda^p L^2_w(\Omega)$ is the space $\Lambda^p H^0_w(\Omega)$ and that $\Lambda^0 H^1_{w,T}(\Omega)$ is the space $H^1_{w,0}(\Omega)$ than we introduced in Proposition C.2 to define the domain of $L^{D,(0)}_{f,h}(\Omega)$. Likewise for $p \in \{0, \dots, d\}$ and $q > \frac{1}{2}$, the set $\Lambda^p H^q_{w,T}(\Omega)$ is defined by

$$\Lambda^p H^q_{w,N}(\Omega) := \{v \in \Lambda^p H^q_w(\Omega) \,|\, \mathbf{n}v = 0 \text{ on } \partial\Omega\}.$$

We will denote by $\|.\|_{H^q_w}$ the norm on the weighted space $\Lambda^p H^q_w(\Omega)$. Moreover $\langle \cdot, \cdot \rangle_{L^2_w}$ denotes the scalar product in $\Lambda^p L^2_w(\Omega)$.

Finally, we will also use the same notation without the index w to denote the standard Sobolev spaces defined with respect to the Lebesgue measure on Ω.

B.2.1.2 Definition of Witten Laplacians

Let us first recall some basic properties of Witten Laplacians, as well as the link between those and the operators $L^{(p)}_{f,h}$ introduced above (see (B.10) and (B.41)). As already explained above, we will actually need in this article to work only with 0 and 1-forms ($p \in \{0, 1\}$). For an introduction to the Hodge theory and the Hodge Laplacians on manifolds with boundary, one can refer to [65].

Denote by d the exterior derivative on Ω,

$$d^{(p)} : \Lambda^p C^\infty(\Omega) \to \Lambda^{p+1} C^\infty(\Omega),$$

and $(d^{(p)})^*$ its adjoint. The exterior derivative is 2 nilpotent,

$$d^{(p+1)} \circ d^{(p)} = 0,$$

and therefore $(d^{(p)})^* \circ (d^{(p+1)})^* = 0$. In all what follows, the superscript (p) may be omitted when there is no ambiguity.

Let us now introduce the so called distorted exterior derivative

$$d_{f,h}^{(p)} := e^{-\frac{f}{h}}\, h\, d^{(p)}\, e^{\frac{f}{h}} = h d^{(p)} + df\wedge \tag{B.42}$$

and its formal adjoint

$$(d_{f,h}^{(p)})^* := e^{\frac{f}{h}}\, h\, (d^{(p)})^*\, e^{\frac{-f}{h}} = h(d^{(p)})^* + \mathbf{i}_{\nabla f}. \tag{B.43}$$

The distorted exterior derivative was firstly introduced by Witten in [74].

Definition B.5. *The Witten Laplacian is the non negative differential operator*

$$\Delta_{f,h}^{(p)} := \left(d_{f,h}^{(p)} + \left(d_{f,h}^{(p)}\right)^*\right)^2.$$

An equivalent expression of the Witten Laplacians is

$$\Delta_{f,h}^{(p)} = h^2\Delta_H^{(p)} + |\nabla f|^2 + h\left(\mathcal{L}_{\nabla f} + \mathcal{L}_{\nabla f}^*\right),$$

where $\mathcal{L}$ stands for the Lie derivative, ∇ is the covariant derivative associated to the metric g on Ω and $\Delta_H^{(p)}$ is the Hodge Laplacian acting on p-forms, defined by:

$$\Delta_H^{(p)} := \left(d^{(p)} + \left(d^{(p)}\right)^*\right)^2.$$

We recall that $\Delta_H^{(p)}$ is a positive operator (in $\mathbb{R}^d$, $\Delta_H^{(0)} = -\sum_{i=1}^d \partial_{x_i,x_i}^2$). The operator $\mathcal{L}_{\nabla f} + \mathcal{L}_{\nabla f}^*$ is an operator of order 0 (namely a multiplicative operator). On 0-forms, namely on functions, the Witten Laplacian has the following expression

$$\Delta_{f,h}^{(0)} = h^2\Delta_H^{(0)} + |\nabla f|^2 + h\,\Delta_H^{(0)} f. \tag{B.44}$$

Let us recall the complex structure associated with the Witten Laplacians defined on a manifold with boundary. This requires to use appropriate boundary conditions (see [34]).

Proposition B.12. *The Dirichlet realization of $\Delta_{f,h}^{(p)}$ on Ω is the operator $\Delta_{f,h}^{D,(p)}(\Omega)$ with domain*

$$D\left(\Delta_{f,h}^{D,(p)}(\Omega)\right) = \left\{v \in \Lambda^p H^2(\Omega) |\ \mathbf{t}v = 0,\ \mathbf{t}d_{f,h}^* v = 0\right\}.$$

The Neumann realization of $\Delta_{f,h}^{(p)}$ on Ω is the operator $\Delta_{f,h}^{N,(p)}(\Omega)$ with domain

$$D\left(\Delta_{f,h}^{N,(p)}(\Omega)\right) = \left\{v \in \Lambda^p H^2(\Omega) |\ \mathbf{n}v = 0,\ \mathbf{n}d_{f,h} v = 0\right\}.$$

The operators $\Delta_{f,h}^{D,(p)}(\Omega)$ and $\Delta_{f,h}^{N,(p)}(\Omega)$ are both self adjoint operators with compact resolvent.

We recall that $\mathbf{t}$ denotes the tangential trace on forms and that $\mathbf{n}\omega = \omega - \mathbf{t}\omega$ is the normal trace. The proof of Proposition B.12 can be found in [34, Section 2.4] and

in [47, Section 4.2.3]. It is a generalization of what is stated in [65] for the Hodge Laplacians. One can check that the operator $\Delta_{f,h}^{D,(p)}(\Omega)$ is actually the Friedrichs extension associated to the quadratic form

$$v \in \Lambda^p H_T^1(\Omega) \mapsto \left\| d_{f,h}^{(p)} v \right\|_{L^2}^2 + \left\| \left(d_{f,h}^{(p)} \right)^* v \right\|_{L^2}^2 . \tag{B.45}$$

The following properties are easily checked

$$d_{f,h}\Delta_{f,h}^{D,(p)}(\Omega) = \Delta_{f,h}^{D,(p+1)}(\Omega) d_{f,h} \text{ and } d_{f,h}^* \Delta_{f,h}^{D,(p+1)}(\Omega) = \Delta_{f,h}^{D,(p)}(\Omega) d_{f,h}^*. \tag{B.46}$$

Similar relations hold for $\Delta_{f,h}^{N}(\Omega)$. The relations (B.46) allows us to define the Dirichlet complex structure (see [10], [34] and [45]):

$$\{0\} \longrightarrow D\left(\Delta_{f,h}^{D,(0)}(\Omega)\right) \xrightarrow{d_{f,h}} D\left(\Delta_{f,h}^{D,(1)}(\Omega)\right) \xrightarrow{d_{f,h}} \cdots D\left(\Delta_{f,h}^{D,(d)}(\Omega)\right) \xrightarrow{d_{f,h}} \{0\}$$

$$\{0\} \xleftarrow{d_{f,h}^*} D\left(\Delta_{f,h}^{D,(0)}(\Omega)\right) \xleftarrow{d_{f,h}^*} D\left(\Delta_{f,h}^{D,(1)}(\Omega)\right) \cdots \xleftarrow{d_{f,h}^*} D\left(\Delta_{f,h}^{D,(d)}(\Omega)\right) \longleftarrow \{0\}.$$

One can define similarly the Neumann complex structure (see [47]).

One can relate the infinitesimal generator $L_{f,h}^{(0)}$ of the diffusion (B.1) to the Witten Laplacian $\Delta_{f,h}^{(0)}$ through the unitary transformation:

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

Indeed, one can check that

$$\Delta_{f,h}^{D,(0)}(\Omega) = -2\, h\, e^{-\frac{f}{h}}\, L_{f,h}^{D,(0)}(\Omega)\, e^{\frac{f}{h}}. \tag{B.47}$$

Let us now generalize this to p-forms, using extensions of $L_{f,h}^{(0)}$ to p-forms.

Proposition B.13. *The Friedrichs extension associated with the quadratic form*

$$v \in \Lambda^p C_T^\infty(\Omega) \mapsto \frac{h}{2}\left[\left\| d^{(p)} v \right\|_{L_w^2(\Omega)}^2 + \left\| e^{\frac{2f}{h}} \left(d^{(p)} \right)^* e^{-\frac{2f}{h}} v \right\|_{L_w^2(\Omega)}^2 \right]$$

on $\Lambda^p L_w^2(\Omega)$, is denoted $\left(-L_{f,h}^{D,(p)}(\Omega),\ D\left(-L_{f,h}^{D,(p)}(\Omega)\right)\right)$. The operator $-L_{f,h}^{D,(p)}(\Omega)$ is a positive unbounded self adjoint operator on $\Lambda^p L_w^2(\Omega)$. Besides, one has

$$D\left(-L_{f,h}^{D,(p)}(\Omega)\right) = \left\{ v \in \Lambda^p H_w^2(\Omega) \,|\, \mathbf{t} v = 0,\ \mathbf{t} d^* \left(e^{-\frac{2f}{h}} v \right) = 0 \right\}.$$

For $p = 0$, the differential operator

$$L_{f,h}^{(0)} = -\frac{h}{2}\Delta_H^{(0)} - \nabla f \cdot \nabla$$

is the infinitesimal generator (B.10) of the overdamped Langevin dynamics (B.1). For $p = 1$ one gets

$$L_{f,h}^{(1)} = -\frac{h}{2}\Delta_H^{(1)} - \nabla f \cdot \nabla - \operatorname{Hess} f, \tag{B.48}$$

where we recall Hess f is the Hessian of f, see Remark B.1.

The generalisation of (B.47) for p-forms is:

$$\Delta_{f,h}^{D,(p)}(\Omega) = -2\,h\,e^{-\frac{f}{h}}\left(L_{f,h}^{D,(p)}(\Omega)\right)\,e^{\frac{f}{h}}. \tag{B.49}$$

The commutation relation (B.46) writes on $L_{f,h}^{D,(p)}(\Omega)$:

$$L_{f,h}^{D,(p+1)}(\Omega)d = dL_{f,h}^{D,(p)}(\Omega) \text{ and } L_{f,h}^{D,(p-1)}(\Omega)d_{2f,h}^{*} = d_{2f,h}^{*}L_{f,h}^{D,(p)}(\Omega). \tag{B.50}$$

Thanks to the relation (B.49), the operators $L_{f,h}^{D,(p)}(\Omega)$ and $\Delta_{f,h}^{D,(p)}(\Omega)$ have the same spectral properties. In particular the operators $L_{f,h}^{D,(p)}(\Omega)$ and $\Delta_{f,h}^{D,(p)}(\Omega)$ both have compact resolvents, and thus a discrete spectrum. The generalization of Proposition B.3 is the following:

Proposition B.14. *The smallest eigenvalue of $-L_{f,h}^{D,(0)}(\Omega)$, denoted by λ_h, is positive and non degenerate. The associated eigenfunction u_h has sign on Ω. Moreover $u_h \in C^{\infty}\left(\overline{\Omega},\mathbb{R}\right)$.*

Without loss of generality, one can assume that u_h satisfies normalization (B.11). The couple (λ_h, u_h) satisfies the following relation

$$\begin{cases} -L_{f,h}^{(0)}u_h = \lambda_h\,u_h \text{ on } \Omega, \\ \qquad u_h = 0 \text{ on } \partial\Omega. \end{cases} \tag{B.51}$$

Thanks to the relation (B.49), the couple $(\mu_h, v_h) := \left(2h\lambda_h, u_h\,e^{-\frac{f}{h}}\right)$ is the first eigenvalue and eigenfunction of $\Delta_{f,h}^{D,(0)}(\Omega)$. The couple (μ_h, v_h) satisfies

$$\begin{cases} \Delta_{f,h}^{(0)}\,v_h = \mu_h\,v_h \text{ on } \Omega, \\ \qquad v_h = 0 \text{ on } \partial\Omega. \end{cases} \tag{B.52}$$

Moreover, $v_h > 0$ on Ω and

$$\int_{\Omega} v_h^2(x)\,dx = 1.$$

The following lemma will be instrumental throughout this work.

Lemma B.15. *Let $(A, D(A))$ be a non negative self adjoint operator on a Hilbert Space $(\mathcal{H}, \|.\|)$ with associated quadratic form $q_A(u) = (u, Au)$ with domain $D(q_A)$. Then for any $u \in D(q_A)$ and $b > 0$*

$$\left\|\pi_{[b,+\infty)}(A)\,u\right\|^2 \leq \frac{q_A(u)}{b}$$

where, for $E \subset \mathbb{R}$ a Borel set, $\pi_E(A)$ is the spectral projection of the operator A on E.

Proof. The inequality is easily obtained for $u \in D(A)$ by writing A as an integral using its spectral measure [32, Theorem 8.15]:

$$\begin{aligned}(u, Au) &= \int_{[0,\infty)} \lambda\,d(\pi_\lambda(A)u, u) \\ &\geq \int_{(b,\infty)} \lambda\,d(\pi_\lambda(A)u, u) \geq b(\pi_{[b,+\infty)}(A)\,u, u) = b\left\|\pi_{[b,+\infty)}(A)\,u\right\|^2.\end{aligned}$$

The inequality also holds for $u \in D(q_A)$ thanks to the density of $D(A)$ in $D(q_A)$. ∎

This lemma will be in particular applied to the non negative self adjoint operators $\Delta_{f,h}^{D,(p)}(\Omega)$ and $-L_{f,h}^{D,(p)}(\Omega)$ and their associated quadratic forms.

B.2.1.3 Small eigenvalues of $\Delta_{f,h}^{D,(0)}(\Omega)$ and $L_{f,h}^{D,(0)}(\Omega)$

The dimension of the range of the orthogonal projectors $\pi_{[0,h^{3/2})}\left(\Delta_{f,h}^{D,(0)}(\Omega)\right)$ and $\pi_{[0,h^{3/2})}\left(\Delta_{f,h}^{D,(1)}(\Omega)\right)$ in the regime $h \to 0$ have already been studied in [34, Section 3]: when $\nabla f \neq 0$ on $\partial\Omega$ and when f and $f_{|\partial\Omega}$ are Morse functions, the dimension of $\mathrm{Ran}\left(\pi_{[0,h^{\frac{3}{2}})}\left(\Delta_{f,h}^{D,(0)}(\Omega)\right)\right)$ (respectively $\mathrm{Ran}\left(\pi_{[0,h^{\frac{3}{2}})}\left(\Delta_{f,h}^{D,(1)}(\Omega)\right)\right)$) is equal to the number of local minima of f (respectively to the number of generalized critical points of index 1). A generalized critical point of index 1 for $\Delta_{f,h}^{D,(1)}(\Omega)$ is either a local minimum of $f|_{\partial\Omega}$ such that $\partial_n f(z_i) > 0$ or a saddle point of index 1 of f inside Ω. In our setting, thanks to assumptions **[H1]**, **[H2]** and **[H3]**, there are n generalized critical points of index 1, which are the local minima $(z_i)_{i=1,\dots,n}$ of $f|_{\partial\Omega}$.

Proposition B.16. *Under **[H1]**, **[H2]**, and **[H3]**, there exists $h_0 > 0$ such that for all $h \in (0, h_0)$*

$$\dim\ \mathrm{Ran}\,\pi_{[0,h^{3/2})}\left(\Delta_{f,h}^{D,(0)}(\Omega)\right) = 1,$$

and

$$\dim\ \mathrm{Ran}\,\pi_{[0,h^{3/2})}\left(\Delta_{f,h}^{D,(1)}(\Omega)\right) = n.$$

Proof. We refer to [34, Theorem 3.2.3] for the proof of this proposition. ∎

Let us denote by $\mu_h^{(1),1} \leq \ldots \leq \mu_h^{(1),n}$ the eigenvalues of $\Delta_{f,h}^{D,(1)}(\Omega)$ smaller than $h^{3/2}$. It can actually be shown that, when $h \to 0$, they are exponentially small: for $j \in \{1, \ldots, n\}$,

$$\lim_{h\to 0} h \ln(\mu_h^{(1),j}) < 0.$$

Thanks to (B.49), similar results hold for $L_{f,h}^{D,(p)}(\Omega)$: there exists $h_0 > 0$ such that for all $h \in (0, h_0)$

$$\dim\ \mathrm{Ran}\,\pi_{[0,\frac{\sqrt{h}}{2})}\left(-L_{f,h}^{D,(0)}(\Omega)\right) = 1 \text{ and } \dim\ \mathrm{Ran}\,\pi_{[0,\frac{\sqrt{h}}{2})}\left(-L_{f,h}^{D,(1)}(\Omega)\right) = n.$$

The spectral projection $\pi_{[0,\frac{\sqrt{h}}{2})}\left(-L_{f,h}^{D,(0)}(\Omega)\right)$ is the orthogonal projection in $L_w^2(\Omega)$ on $\mathrm{span}(u_h)$ and thanks to the commutation property (B.50), we have the following crucial property:

$$\nabla u_h \in \mathrm{Ran}\,\pi_{[0,\frac{\sqrt{h}}{2})}\left(-L_{f,h}^{D,(1)}(\Omega)\right). \tag{B.53}$$

For the ease of notation, for $p \in \{1, 2\}$, we use in the following the notation:

$$\pi_h^{(p)} := \pi_{[0,\frac{\sqrt{h}}{2})}\left(-L_{f,h}^{D,(p)}(\Omega)\right). \tag{B.54}$$

B.2.2 Statement of the assumptions required for the quasi-modes

B.2.2.1 Statement of Proposition B.17

The next proposition gives the assumption we need on the quasi-modes $(\tilde{\psi}_i)_{i=1,\dots,n}$ whose span approximates $\operatorname{Ran}\pi_h^{(1)}$, and $\tilde{u}$ whose span approximates $\operatorname{Ran}\pi_h^{(0)}$, in order to prove Theorem B.1.

Proposition B.17. *Assume **[H1]**, **[H2]** and **[H3]**. As in the statement of Theorem B.1, for all $i \in \{1,\dots,n\}$, Σ_i denotes an open set included in $\partial\Omega$ containing z_i and such that $\overline{\Sigma}_i \subset B_{z_i}$.*

Let us assume in addition that there exist n quasi-modes $(\tilde{\psi}_i)_{i=1,\dots,n}$ and a family of quasi-modes $(\tilde{u} = \tilde{u}_\delta)_{\delta>0}$ satisfying the following conditions:

1. *For all $i \in \{1,\dots,n\}$, $\tilde{\psi}_i \in \Lambda^1 H^1_{w,T}(\Omega)$ and $\tilde{u} \in \Lambda^0 H^1_{w,T}(\Omega)$. The function $\tilde{u}$ is non negative in Ω. Moreover, one assumes the following normalization: for all $i \in \{1,\dots,n\}$,*
$$\left\|\tilde{\psi}_i\right\|_{L^2_w} = \|\tilde{u}\|_{L^2_w} = 1.$$

2. (a) *There exists $\varepsilon_1 > 0$ such that for all $i \in \{1,\dots,n\}$, in the limit $h \to 0$:*
$$\left\|\left(1-\pi_h^{(1)}\right)\tilde{\psi}_i\right\|^2_{H^1_w} = O\left(e^{-\frac{2}{h}(\max[f(z_n)-f(z_i),f(z_i)-f(z_1)]+\varepsilon_1)}\right). \tag{B.55}$$

   (b) *For any $\delta > 0$, in the limit $h \to 0$: $\|\nabla\tilde{u}\|^2_{L^2_w} = O\left(e^{-\frac{2}{h}(f(z_1)-f(x_0)-\delta)}\right)$.*

3. *There exists $\varepsilon_0 > 0$ such that $\forall (i,j) \in \{1,\dots,n\}^2$ with $i<j$, in the limit $h \to 0$:*
$$\left\langle \tilde{\psi}_i, \tilde{\psi}_j \right\rangle_{L^2_w} = O\left(e^{-\frac{1}{h}(f(z_j)-f(z_i)+\varepsilon_0)}\right).$$

4. (a) *There exist constants $(C_i)_{i=1,\dots,n}$ and p which do not depend on h such that for all $i \in \{1,\dots,n\}$, in the limit $h \to 0$:*
$$\left\langle \nabla\tilde{u}, \tilde{\psi}_i \right\rangle_{L^2_w} = C_i\ h^p e^{-\frac{1}{h}(f(z_i)-f(x_0))}\ (1+O(h)).$$

   (b) *There exist constants $(B_i)_{i=1,\dots,n}$ and m which do not depend on h such that for all $(i,j) \in \{1,\dots,n\}^2$, in the limit $h \to 0$:*
$$\int_{\Sigma_i} \tilde{\psi}_j \cdot n\ e^{-\frac{2}{h}f} d\sigma = \begin{cases} B_i\ h^m\ e^{-\frac{1}{h}f(z_i)}\ (1+O(h)) & \text{if } i=j \\ 0 & \text{if } i \neq j. \end{cases}$$

Then, for all $i \in \{1,\dots,n\}$, in the limit $h \to 0$:
$$\int_{\Sigma_i} (\partial_n u_h)\, e^{-\frac{2}{h}f} d\sigma = C_i B_i\ h^{p+m}\, e^{-\frac{1}{h}(2f(z_i)-f(x_0))}\ (1+O(h)),$$

where u_h is the eigenfunction associated with the smallest eigenvalue of $-L^{D,(0)}_{f,h}(\Omega)$ (see Proposition B.14) which satisfies (B.11).

Let us comment on the assumptions made on the quasi-modes. Assumption 1 gives the proper functional setting and the normalization. Assumption 2 will be used to show that $\mathrm{span}(\tilde{\psi}_i,\, i=1,\dots,n)$ (respectively $\mathrm{span}(\tilde{u})$) is included in $\mathrm{Ran}(\pi_h^{(1)})$ (respectively in $\mathrm{Ran}(\pi_h^{(0)}) = \mathrm{span}(u_h)$) up to exponentially small terms. Assumption 3 states the quasi-orthonormality of the quasi-modes $(\tilde{\psi}_i)_{i=1,\dots,n}$. Finally, Assumption 4(a) gives the components of the decomposition of $\nabla\tilde{u}$ over $\mathrm{span}(\tilde{\psi}_i,\, i=1,\dots,n)$, and Assumption 4(b) is then used to find the asymptotic behavior of $\int_{\Sigma_i}(\partial_n u_h)\, e^{-\frac{2}{h}f} d\sigma$, knowing those of $\int_{\Sigma_i}\tilde{\psi}_j\cdot n\, e^{-\frac{2}{h}f} d\sigma$.

Theorem B.1 is a consequence of this proposition. The construction of appropriate quasi-modes $\tilde{u}$ and $(\tilde{\psi}_i)_{i=1,\dots,n}$ satisfying the requirements of Proposition B.17 will be the focus of Section B.4, where explicit values for the constants B_i, C_i, p and m will be given (see (B.231) and (B.235)).

B.2.2.2 Rewriting the hypotheses on $(\tilde{\psi}_i)_{i\in\{1,\dots,n\}}$ in Proposition B.17

The quasi-modes $(\tilde{\psi}_i)_{i\in\{1,\dots,n\}}$ will be built using eigenforms of some Witten Laplacians. It will thus be more convenient to work in non weighted Sobolev spaces, and to actually consider the 1-forms (see (B.47)): for $i\in\{1,\dots,n\}$,

$$\tilde{\phi}_i := e^{-\frac{1}{h}f}\tilde{\psi}_i \in \Lambda^1 H^1_T(\Omega). \tag{B.56}$$

For further references, let us rewrite the hypotheses on the 1-forms $(\tilde{\psi}_j)_{j=1,\dots,n}$ stated in Proposition B.17 in terms of the 1-forms $(\tilde{\phi}_j)_{j=1,\dots,n}$ defined by (B.56):

1. For all $i\in\{1,\dots,n\}$, $\tilde{\phi}_i\in\Lambda^1 H^1_T(\Omega)$ and
$$\left\|\tilde{\phi}_i\right\|_{L^2} = 1.$$

2. There exist $\varepsilon_1>0$ such that for all $i\in\{1,\dots,n\}$, in the limit $h\to 0$:
$$\left\|\left(1-\pi_{[0,h^{\frac{3}{2}})}\left(\Delta^{D,(1)}_{f,h}(\Omega)\right)\right)\tilde{\phi}_i\right\|^2_{H^1} = O\left(e^{-\frac{2}{h}(\max[f(z_n)-f(z_i),f(z_i)-f(z_1)]+\varepsilon_1)}\right). \tag{B.57}$$

3. There exists $\varepsilon_0>0$ such that $\forall (i,j)\in\{1,\dots,n\}^2$, $i<j$, in the limit $h\to 0$:
$$\int_\Omega \tilde{\phi}_i(x)\cdot\tilde{\phi}_j(x)\,dx = O\left(e^{-\frac{1}{h}[f(z_j)-f(z_i)+\varepsilon_0]}\right). \tag{B.58}$$

4. (a) There exist constants $(C_i)_{i=1,\dots,n}$ and p which do not depend on h such that for all $i\in\{1,\dots,n\}$, in the limit $h\to 0$:
$$\int_\Omega \nabla\tilde{u}\cdot\tilde{\phi}_i\; e^{-\frac{1}{h}f} = C_i\; h^p e^{-\frac{1}{h}(f(z_i)-f(x_0))}\;(1+O(h)). \tag{B.59}$$

   (b) There exist constants $(B_i)_{i=1,\dots,n}$ and m which do not depend on h such that for all $(i,j)\in\{1,\dots,n\}^2$, in the limit $h\to 0$:
$$\int_{\Sigma_i}\tilde{\phi}_j\cdot n\; e^{-\frac{1}{h}f} d\sigma = \begin{cases} B_i\; h^m\; e^{-\frac{1}{h}f(z_i)}\;(1+O(h)) & \text{if } i=j,\\ 0 & \text{if } i\neq j.\end{cases} \tag{B.60}$$

As mentioned above, the construction of quasi-modes $\tilde{u}$ and $(\tilde{\phi}_i)_{i=1,\dots,n}$ satisfying those estimates will be the purpose of Section B.4.

Let us comment on the equivalence between the first assumption here (namely (B.57)) and assumption 2(a) in Proposition B.17 (namely (B.55)). This equivalence is a consequence of the following relation between the projectors which comes from (B.49):

$$\pi_{[0,h^{\frac{3}{2}})}\left(\Delta_{f,h}^{D,(1)}(\Omega)\right) = e^{-\frac{1}{h}f}\pi_h^{(1)}e^{\frac{1}{h}f}.$$

Indeed, using this relation, one has:

$$\|e^{-\frac{1}{h}f}(1-\pi_h^{(1)})\tilde{\psi}_i\|_{H^1} = \left\|\left(1-\pi_{[0,h^{\frac{3}{2}})}\left(\Delta_{f,h}^{D,(1)}(\Omega)\right)\right)\tilde{\phi}_i\right\|_{H^1}.$$

Moreover, one easily checks that there exists $C>0$ such that, for all $h\in(0,1)$ and for all $u\in\Lambda^p H^1(\Omega)$,

$$\|u\|_{H^1_w} \leq \frac{C}{h}\left\|u\,e^{-\frac{1}{h}f}\right\|_{H^1}.$$

Therefore

$$\|(1-\pi_h^{(1)})\tilde{\psi}_i\|_{H^1_w} \leq \frac{C}{h}\left\|\left(1-\pi_{[0,h^{\frac{3}{2}})}\left(\Delta_{f,h}^{D,(1)}(\Omega)\right)\right)\tilde{\phi}_i\right\|_{H^1}$$

which shows that (B.57) (with ε_1) implies (B.55) (with $\varepsilon_1/2$). A similar reasoning shows that (B.55) also implies (B.57), but this will not be used in the following.

B.2.3 Proof of Proposition B.17

In all this section, we assume that the hypotheses **[H1]**, **[H2]** and **[H3]** hold and we assume the existence of $n+1$ quasi-modes $(\tilde{u},(\tilde{\psi}_i)_{i=1,\dots,n})$ satisfying the conditions of Proposition B.17. In the following, ε denotes a positive constant independent of h, smaller than $\min(\varepsilon_1,\varepsilon_0)$, and whose precise value may vary (a finite number of times) from one occurrence to the other.

Let us start the proof with two preliminary lemmas relating $\tilde{u}$ with u_h on the one hand, and span $\left(\tilde{\psi}_j, j=1,\dots,n\right)$ with $\operatorname{Ran}\pi_h^{(1)}$ on the other hand.

Lemma B.18. *Let us assume that the assumptions of Proposition B.17 hold. Then there exist $c>0$ and $h_0>0$ such that for $h\in(0,h_0)$,*

$$\left\|\pi_h^{(0)}\tilde{u}\right\|_{L^2_w} = 1+O\left(e^{-\frac{c}{h}}\right).$$

Proof. Since $\tilde{u}\in\Lambda^0 H^1_{w,T}$, $\left\|(1-\pi_h^{(0)})\tilde{u}\right\|_{L^2_w}$ is bounded from above by $\sqrt{2}h^{1/4}\|\nabla\tilde{u}\|_{L^2_w}$ thanks to Lemma C.8. In addition since $\|\nabla\tilde{u}\|^2_{L^2_w} = O\left(e^{-\frac{2}{h}[f(z_1)-f(x_0)-\delta]}\right)$ (see assumption 2(b) in Proposition B.17), by taking $\delta\in(0,f(z_1)-f(x_0))$, one gets that $\left\|\pi_h^{(0)}\tilde{u}\right\|_{L^2_w} = 1+O\left(e^{-\frac{c}{h}}\right)$. ∎

As a direct consequence of Lemma B.18, one has that for h small enough $\pi_h^{(0)}\tilde{u}\neq 0$ and therefore (since moreover $\tilde{u}$ is non negative in Ω: $\langle u_h,\pi_h\tilde{u}\rangle_{L^2_w} = \langle u_h,\tilde{u}\rangle_{L^2_w}\geq 0$),

$$u_h = \frac{\pi_h^{(0)}\tilde{u}}{\left\|\pi_h^{(0)}\tilde{u}\right\|_{L^2_w}}. \tag{B.61}$$

Additionally, one has the following lemma concerning the 1-forms.

Lemma B.19. *Let us assume that the assumptions of Proposition B.17 hold. Then there exists h_0 such that for all $h \in (0, h_0)$,*

$$\operatorname{span}\left(\pi_h^{(1)}\tilde{\psi}_i,\, i = 1, \dots, n\right) = \operatorname{Ran} \pi_h^{(1)}.$$

Proof. The determinant of the Gram matrix of the 1-forms $\left(\pi_h^{(1)}\tilde{\psi}_i\right)_{i=1,\dots,n}$ is $1 + O(e^{-c/h})$ thanks to the following identity

$$\left\langle \pi_h^{(1)}\tilde{\psi}_i, \pi_h^{(1)}\tilde{\psi}_j \right\rangle_{L^2_w} = -\left\langle \left(\pi_h^{(1)} - 1\right)\tilde{\psi}_i, \left(\pi_h^{(1)} - 1\right)\tilde{\psi}_j \right\rangle_{L^2_w} + \left\langle \tilde{\psi}_i, \tilde{\psi}_j \right\rangle_{L^2_w} \tag{B.62}$$

and the fact that, from assumptions 1, 2(a) and 3 in Proposition B.17, there exist $h_0 > 0$, $c > 0$ such that for $h \in (0, h_0)$,

$$\left\langle \tilde{\psi}_i, \tilde{\psi}_j \right\rangle_{L^2_w} = (1 - \delta_{i,j})O(e^{-\frac{c}{h}}) + \delta_{i,j} \text{ and } \left\| \left(1 - \pi_h^{(1)}\right)\tilde{\psi}_i \right\|^2_{H^1_w} = O\left(e^{-\frac{c}{h}}\right).$$

Moreover, from Proposition B.16, $\dim \operatorname{Ran} \pi_h^{(1)} = n$. This proves Lemma B.19. ∎

Thanks to Lemma B.19, one can build on orthonormal basis $(\psi_i)_{i=1,\dots,n}$ of $\operatorname{Ran}\left(\pi_h^{(1)}\right)$ using a Gram-Schmidt orthonormalization procedure on $(\pi_h^{(1)}(\tilde{\psi}_i))_{i=1,\dots,n}$. This will be done in Section B.2.3.1 below. Then, since

$$\nabla u_h \in \operatorname{Ran}\left(\pi_h^{(1)}\right) = \operatorname{span}\left(\psi_j, j = 1, \dots, n\right)$$

(see (B.53)) and $\|\psi_j\|_{L^2_w} = 1$, one has

$$\int_{\Sigma_k} (\partial_n u_h)\, e^{-\frac{2}{h}f} d\sigma = \sum_{j=1}^{n} \langle \nabla u_h, \psi_j \rangle_{L^2_w} \int_{\Sigma_k} \psi_j \cdot n\, e^{-\frac{2}{h}f} d\sigma. \tag{B.63}$$

The proof of Proposition B.17 then consists in replacing (in the right-hand side of (B.63)) u_h by its expression (B.61) in terms of $\tilde{u}$, and the $(\psi_i)_{i=1,\dots,n}$ by the $(\tilde{\psi}_i)_{i=1,\dots,n}$, and to use the assumptions of Proposition B.17 to get an estimate of $\int_{\Sigma_k} (\partial_n u_h)\, e^{-\frac{2}{h}f} d\sigma$. Section B.2.3.2 provides estimates on $\langle \nabla u_h, \psi_j \rangle_{L^2_w}$. Section C.3.2.3 provides estimates of $\int_{\Sigma_k} \psi_j \cdot n\, e^{-\frac{2}{h}f}$. All these results are then gathered to conclude the proof of Proposition B.17 in Section B.2.3.4.

B.2.3.1 Gram-Schmidt orthonormalization

Using a Gram-Schmidt procedure, one obtains the following result.

Lemma B.20. *Let us assume that the assumptions of Proposition B.17 hold. Then for all $j \in \{1, \dots, n\}$, there exist $(\kappa_{ji})_{i=1,\dots,j-1} \subset \mathbb{R}^{j-1}$ such that the 1-forms*

$$v_j := \pi_h^{(1)}\left[\tilde{\psi}_j + \sum_{i=1}^{j-1} \kappa_{ji}\, \tilde{\psi}_i\right], \tag{B.64}$$

(with the convention $\sum_{i=1}^{0} = 0$) satisfy

- *for all* $k \in \{1, \dots, n\}$, $\operatorname{span}(v_i, i = 1, \dots, k) = \operatorname{span}\left(\pi_h^{(1)} \tilde{\psi}_i, i = 1, \dots, k\right)$,
- *for all* $i \neq j$, $\langle v_i, v_j \rangle_{L^2_w} = 0$.

In the following, we denote by

$$Z_j := \|v_j\|_{L^2_w} \text{ and } \psi_j := \frac{v_j}{Z_j} \tag{B.65}$$

the normalized 1-forms.

We are first interested in estimating κ_{ji} and Z_j.

Lemma B.21. *Let us assume that the assumptions of Proposition B.17 hold. There exist* $\varepsilon > 0$ *and* $h_0 > 0$ *such that for all* $(i, j) \in \{1, \dots, n\}^2$ *with* $i < j$ *and all* $h \in (0, h_0)$

$$\left\langle \pi_h^{(1)} \tilde{\psi}_i, \pi_h^{(1)} \tilde{\psi}_j \right\rangle_{L^2_w} = O\left(e^{-\frac{1}{h}(f(z_j) - f(z_i) + \varepsilon)}\right).$$

Proof. Using assumption 2(a) in Proposition B.17, one gets: for $i < j$,

$$\begin{aligned}
\left\langle \left(1 - \pi_h^{(1)}\right) \tilde{\psi}_j, \left(1 - \pi_h^{(1)}\right) \tilde{\psi}_i \right\rangle_{L^2_w} &\leq \left\| \left(1 - \pi_h^{(1)}\right) \tilde{\psi}_k \right\|_{H^1_w} \left\| \left(1 - \pi_h^{(1)}\right) \tilde{\psi}_k \right\|_{H^1_w} \\
&= O\left(e^{-\frac{1}{h}(f(z_n) - f(z_i) + f(z_j) - f(z_1) + \varepsilon)}\right) \\
&= O\left(e^{-\frac{1}{h}(f(z_j) - f(z_i) + \varepsilon)}\right).
\end{aligned}$$

The result is then a consequence of assumption 3 in Proposition B.17 and the identity (C.130). ∎

Notice that since $\pi_h^{(1)}$ is an L^2_w-projection, $\left\langle \pi_h^{(1)} \tilde{\psi}_i, \pi_h^{(1)} \tilde{\psi}_j \right\rangle_{L^2_w} = \left\langle \pi_h^{(1)} \tilde{\psi}_i, \tilde{\psi}_j \right\rangle_{L^2_w}$. This will be used extensively in the following.

Lemma B.22. *Let us assume that the assumptions of Proposition B.17 hold. Then there exist* $h_0 > 0$, $\varepsilon > 0$ *and* $c > 0$ *such that for all* $j \in \{1, \dots, n\}$, $i \in \{1, \dots, j-1\}$ *and* $h \in (0, h_0)$

$$\kappa_{ji} = O\left(e^{-\frac{1}{h}(f(z_j) - f(z_i) + \varepsilon)}\right) \text{ and } Z_j = 1 + O\left(e^{-\frac{c}{h}}\right).$$

Proof. Let us introduce the notation: for all $i \in \{1, \dots, n\}$,

$$r_i := \left\| \left(1 - \pi_h^{(1)}\right) \tilde{\psi}_i \right\|^2_{H^1_w}.$$

Let us prove this lemma by induction. Concerning ψ_1, one has from Lemma B.20

$$\psi_1 = \frac{v_1}{Z_1} \text{ with } v_1 = \pi_h^{(1)} \tilde{\psi}_1.$$

Since $\|\tilde{\psi}_1\|_{L^2_w} = 1$, one has $Z_1 = \|\pi_h^{(1)} \tilde{\psi}_1\|_{L^2_w} \leq 1$. In addition, by Pythagorean Theorem and by assumption 2(a) in Proposition B.17 on r_1, there exists $c > 0$ such that for h small enough

$$Z_1^2 \geq 1 - \left\| \left(1 - \pi_h^{(1)}\right) \tilde{\psi}_1 \right\|^2_{L^2_w} \geq 1 - r_1 \geq 1 - e^{-\frac{c}{h}}.$$

Thus $Z_1 = 1 + O\left(e^{-\frac{c}{h}}\right)$. Now, concerning ψ_2, one has

$$\psi_2 = \frac{v_2}{Z_2} \text{ with } v_2 = \pi_h^{(1)}\tilde{\psi}_2 - \left\langle \pi_h^{(1)}\tilde{\psi}_2, \psi_1 \right\rangle_{L^2_w} \psi_1,$$

and thus $\kappa_{21} = -\frac{1}{Z_1^2}\left\langle \pi_h^{(1)}\tilde{\psi}_1, \tilde{\psi}_2 \right\rangle_{L^2_w} = O\left(e^{-\frac{1}{h}(f(z_2)-f(z_1)+\varepsilon)}\right)$ (by Lemma B.21). Then one obtains that $Z_2 = 1 + O\left(e^{-\frac{c}{h}}\right)$ by a similar reasoning as the one we used above for Z_1.

In order to prove Lemma B.22 by induction, let us now assume that for $k \in \{1, \dots, n\}$ and for all $j \in \{1, \dots, k\}$, $i \in \{1, \dots, j-1\}$,

$$\kappa_{ji} = O\left(e^{-\frac{1}{h}[f(z_j)-f(z_i)+\varepsilon]}\right) \text{ and } Z_j = 1 + O\left(e^{-\frac{c}{h}}\right).$$

One gets by the Gram-Schmidt procedure which defines the $(\psi_i)_{i=1,\dots,n}$,

$$\psi_{k+1} = \frac{v_{k+1}}{Z_{k+1}}$$

where, using the notation $\kappa_{ii} = 1$,

$$\begin{aligned} v_{k+1} &= \pi_h^{(1)}\tilde{\psi}_{k+1} - \sum_{j=1}^{k} \langle \pi_h^{(1)}\tilde{\psi}_{k+1}, \psi_j \rangle_{L^2_w} \psi_j \\ &= \pi_h^{(1)}\tilde{\psi}_{k+1} - \sum_{j=1}^{k} \sum_{l,q=1}^{j} \frac{1}{Z_j^2} \langle \pi_h^{(1)}\tilde{\psi}_{k+1}, \pi_h^{(1)}\tilde{\psi}_l \rangle_{L^2_w} \ \kappa_{jl}\kappa_{jq} \ \pi_h^{(1)}\tilde{\psi}_q \\ &= \pi_h^{(1)}\tilde{\psi}_{k+1} - \sum_{q=1}^{k} \pi_h^{(1)}\tilde{\psi}_q \sum_{j=q}^{k} \sum_{l=1}^{j} \frac{1}{Z_j^2} \langle \pi_h^{(1)}\tilde{\psi}_{k+1}, \pi_h^{(1)}\tilde{\psi}_l \rangle_{L^2_w} \ \kappa_{jl}\kappa_{jq}. \end{aligned}$$

Then for $q \in \{1, \dots, k\}$,

$$\kappa_{(k+1)q} = -\sum_{j=q}^{k} \sum_{l=1}^{j} \frac{1}{Z_j^2} \langle \pi_h^{(1)}\tilde{\psi}_{k+1}, \pi_h^{(1)}\tilde{\psi}_l \rangle_{L^2_w} \ \kappa_{jl}\kappa_{jq}. \tag{B.66}$$

Since $Z_j = 1 + O\left(e^{-\frac{c}{h}}\right)$, one gets $Z_j^{-1} = 1 + O\left(e^{-\frac{c}{h}}\right)$. Using Lemma B.21, one obtains $\left\langle \pi_h^{(1)}\tilde{\psi}_{k+1}, \pi_h^{(1)}\tilde{\psi}_l \right\rangle_{L^2_w} = O\left(e^{-\frac{1}{h}[f(z_{k+1})-f(z_l)+\varepsilon]}\right)$, since $l < k+1$. Moreover one notices that $l \leq j$ and $q \leq j$. If $q < j$, $\kappa_{jl}\kappa_{jq} = O\left(e^{-\frac{1}{h}[f(z_j)-f(z_q)+\varepsilon]}\right)$, and thus

$$\begin{aligned} \left\langle \pi_h^{(1)}\tilde{\psi}_{k+1}, \pi_h^{(1)}\tilde{\psi}_l \right\rangle_{L^2_w} \kappa_{jl}\kappa_{jq} &= O\left(e^{-\frac{1}{h}[f(z_{k+1})-f(z_l)+f(z_j)-f(z_q)+\varepsilon]}\right) \\ &= O\left(e^{-\frac{1}{h}[f(z_{k+1})-f(z_q)+\varepsilon]}\right). \end{aligned}$$

If $l < j$ and if $q = j$,

$$\kappa_{jl}\kappa_{jq} = O\left(e^{-\frac{1}{h}[f(z_j)-f(z_l)+\varepsilon]}\right).$$

Since, if $l < j$ and $q = j$, $f(z_q) = f(z_j) \geq f(z_l)$ one obtains that

$$\left\langle \pi_h^{(1)} \tilde{\psi}_{k+1}, \pi_h^{(1)} \tilde{\psi}_l \right\rangle_{L^2_w} \kappa_{jl}\kappa_{jq} = O\left(e^{-\frac{1}{h}[f(z_{k+1})-f(z_l)+f(z_j)-f(z_l)+\varepsilon]}\right)$$
$$= O\left(e^{-\frac{1}{h}[f(z_{k+1})-f(z_l)+\varepsilon]}\right) = O\left(e^{-\frac{1}{h}[f(z_{k+1})-f(z_q)+\varepsilon]}\right).$$

If $l = q = j$, $\kappa_{jl}\kappa_{jq} = 1$. Thus one has: for $q \in \{1, \ldots, k\}$,

$$\kappa_{(k+1)q} = O\left(e^{-\frac{1}{h}[f(z_{k+1})-f(z_q)+\varepsilon]}\right).$$

The estimate $Z_{k+1} = 1 + O\left(e^{-\frac{c}{h}}\right)$ is a consequence of the fact that $(\kappa_{(k+1)q})_{q\in\{1,\ldots,k\}}$ are exponentially small and the estimate

$$\left\| \pi_h^{(1)} \tilde{\psi}_{k+1} \right\|_{L^2_w} = 1 + O\left(e^{-\frac{c}{h}}\right).$$

This concludes the proof by induction. ∎

B.2.3.2 Estimates on the interaction terms $\left(\langle \nabla u_h, \psi_j \rangle_{L^2_w}\right)_{j\in\{1,\ldots,n\}}$

Lemma B.23. *Let us assume that the assumptions of Proposition B.17 hold. Then for $j \in \{1, \ldots, n\}$, one has*

$$\langle \nabla u_h, \psi_j \rangle_{L^2_w} = C_j \; h^p e^{-\frac{1}{h}(f(z_j)-f(x_0))} \; (1 + O(h)).$$

Proof. From (B.50), for any $\phi \in H^1_{w,T}(\Omega)$ and $v \in L^2_w(\Omega)$, it holds,

$$\langle \nabla \pi_h^{(0)} \phi, \pi_h^{(1)} v \rangle_{L^2_w} = \langle \nabla \phi, \pi_h^{(1)} v \rangle_{L^2_w}. \tag{B.67}$$

Using (B.61)–(B.64)–(B.65)–(B.67), for all $j \in \{1, \ldots, n\}$, one has

$$\begin{aligned}
\langle \nabla u_h, \psi_j \rangle_{L^2_w} &= \frac{Z_j^{-1}}{\left\| \pi_h^{(0)} \tilde{u} \right\|_{L^2_w}} \left[\left\langle \nabla \tilde{u}, \pi_h^{(1)} \tilde{\psi}_j \right\rangle_{L^2_w} + \sum_{i=1}^{j-1} \kappa_{ji} \; \left\langle \nabla \tilde{u}, \pi_h^{(1)} \tilde{\psi}_i \right\rangle_{L^2_w} \right] \\
&= \frac{Z_j^{-1}}{\left\| \pi_h^{(0)} \tilde{u} \right\|_{L^2_w}} \left[\left\langle \nabla \tilde{u}, \tilde{\psi}_j \right\rangle_{L^2_w} + \left\langle \nabla \tilde{u}, \left(\pi_h^{(1)} - 1\right) \tilde{\psi}_j \right\rangle_{L^2_w} \right] \\
&\quad + \frac{Z_j^{-1}}{\left\| \pi_h^{(0)} \tilde{u} \right\|_{L^2_w}} \left[\sum_{i=1}^{j-1} \kappa_{ji} \; \left(\left\langle \nabla \tilde{u}, \tilde{\psi}_i \right\rangle_{L^2_w} + \left\langle \nabla \tilde{u}, \left(\pi_h^{(1)} - 1\right) \tilde{\psi}_i \right\rangle_{L^2_w} \right) \right].
\end{aligned} \tag{B.68}$$

From Lemmata B.18 and B.22, one has $\frac{Z_j^{-1}}{\left\| \pi_h^{(0)} \tilde{u} \right\|_{L^2_w}} = 1 + O\left(e^{-\frac{c}{h}}\right)$. Using assumptions 2 and 4(a) in Proposition B.17 and Lemma B.22, there exists $\delta_0 > 0$ such that for all

$\delta \in (0, \delta_0)$,

$$\begin{aligned}\langle \nabla u_h, \psi_j \rangle_{L^2_w} &= C_j h^p e^{-\frac{1}{h}[f(z_j)-f(x_0)]}(1+O(h)) \\ &+ O\left(e^{-\frac{1}{h}[f(z_1)-f(x_0)-\delta+f(z_j)-f(z_1)+\varepsilon]}\right) \\ &+ \sum_{i=1}^{j-1} O\left(e^{-\frac{1}{h}[f(z_j)-f(z_i)+\varepsilon+f(z_i)-f(x_0)-\delta]}\right) \\ &+ \sum_{i=1}^{j-1} O\left(e^{-\frac{1}{h}[f(z_j)-f(z_i)+\varepsilon+f(z_1)-f(x_0)-\delta+f(z_i)-f(z_1)+\varepsilon]}\right).\end{aligned}$$

Therefore choosing $\delta < \varepsilon$, there exists $\varepsilon' > 0$ such that

$$\langle \nabla u_h, \psi_j \rangle_{L^2_w} = C_j h^p e^{-\frac{1}{h}[f(z_j)-f(x_0)]}(1+O(h)) + O\left(e^{-\frac{1}{h}[f(z_j)-f(x_0)+\varepsilon']}\right).$$

This concludes the proof of Lemma B.23. ∎

B.2.3.3 Estimates on the boundary terms $\left(\int_{\Sigma_k} \psi_j \cdot n\, e^{-\frac{2}{h}f} d\sigma\right)_{(j,k)\in\{1,\dots,n\}^2}$

One denotes for $k \in \{1, \dots, n\}$, $K_k := \max(f(z_n) - f(z_k), f(z_k) - f(z_1)) \geq 0$.

Lemma B.24. *Let us assume that the assumptions of Proposition B.17 hold. Then for all $(j,k) \in \{1,\dots,n\}^2$, there exists $\varepsilon > 0$ such that it holds*

$$\int_{\Sigma_k} \psi_j \cdot n\, e^{-\frac{2}{h}f} d\sigma = \begin{cases} O\left(e^{-\frac{1}{h}[f(z_j)+\varepsilon]}\right) & \text{if } k < j, \\ B_j h^m\, e^{-\frac{1}{h}f(z_j)}\,(1+O(h)) & \text{if } k = j, \\ O\left(e^{-\frac{1}{h}[K_j+f(z_k)+\varepsilon]}\right) + \sum_{i=1}^{j-1} O\left(e^{-\frac{1}{h}[f(z_j)-f(z_i)+K_i+f(z_k)+\varepsilon]}\right) & \text{if } k > j. \end{cases}$$

Proof. Using (B.64)–(B.65) and writing $\pi_h^{(1)}\tilde{\psi}_i = \tilde{\psi}_i + \left(\pi_h^{(1)} - 1\right)\tilde{\psi}_i$, one obtains that

$$\int_{\Sigma_k} \psi_j \cdot n\, e^{-\frac{2}{h}f} d\sigma = a_{jk} + b_{jk} + \sum_{i=1}^{j-1}(c_{jki} + d_{jki})$$

with for $(j,k) \in \{1,\dots,n\}^2$ and $i \in \{1,\dots,j-1\}$,

$$a_{jk} = Z_j^{-1} \int_{\Sigma_k} \tilde{\psi}_j \cdot n\, e^{-\frac{2}{h}f} d\sigma \ , \ b_{jk} = Z_j^{-1} \int_{\Sigma_k} \left(\pi_h^{(1)} - 1\right) \tilde{\psi}_j \cdot n\, e^{-\frac{2}{h}f} d\sigma$$

$$c_{jki} = Z_j^{-1}\kappa_{ji} \int_{\Sigma_k} \tilde{\psi}_i \cdot n\, e^{-\frac{2}{h}f} d\sigma \text{ and } d_{jki} = Z_j^{-1}\kappa_{ji} \int_{\Sigma_k} \left(\pi_h^{(1)} - 1\right) \tilde{\psi}_i \cdot n\, e^{-\frac{2}{h}f} d\sigma.$$

Using the trace theorem and assumption 2(a) in Proposition B.17, one has, for some universal constant C,

$$\begin{aligned}\int_{\Sigma_k} \left(\pi_h^{(1)} - 1\right) \tilde{\psi}_j \cdot n\, e^{-\frac{2}{h}f} d\sigma &\leq \frac{C}{h} \left\| \left(\pi_h^{(1)} - 1\right) \tilde{\psi}_j \right\|_{H^1_w} \sqrt{\int_{\Sigma_k} e^{-\frac{2}{h}f}} \\ &= O\left(e^{-\frac{1}{h}[K_j+f(z_k)+\varepsilon]}\right). \end{aligned} \tag{B.69}$$

If $k = j$ and $i \in \{1, \dots, j-1\}$, one gets, using (B.69), Lemma B.22 and assumption 4(b) in Proposition B.17:

$$a_{jk} = B_j h^m \; e^{-\frac{1}{h} f(z_j)} (1 + O(h)) \; , \; b_{jk} = O\left(e^{-\frac{1}{h}[K_j + f(z_j) + \varepsilon]}\right),$$

$$c_{jki} = 0 \text{ and } d_{jki} = O\left(e^{-\frac{1}{h}[f(z_j) - f(z_i) + K_i + f(z_j) + \varepsilon]}\right).$$

If $k \neq j$ and $i \in \{1, \dots, j-1\}$, one gets using again (B.69), Lemma B.22 and assumption 4(b) in Proposition B.17:

$$a_{jk} = 0 \; , \; b_{jk} = O\left(e^{-\frac{1}{h}[K_j + f(z_k) + \varepsilon]}\right),$$

$$c_{jki} = \begin{cases} O\left(e^{-\frac{1}{h}[f(z_j) + \varepsilon]}\right) & \text{if } k = i, \\ 0 & \text{if } k \neq i, \end{cases} \text{ and } d_{jki} = O\left(e^{-\frac{1}{h}[f(z_j) - f(z_i) + K_i + f(z_k) + \varepsilon]}\right).$$

Notice that $c_{jki} = 0$ if $j < k$ and that if $j > k$ there exists only one i such that $c_{jki} \neq 0$, namely $i = k$. This concludes the proof of the Lemma C.36. ∎

B.2.3.4 Estimates on $\left(\int_{\Sigma_k} (\partial_n u_h)\, e^{-\frac{2}{h} f} d\sigma\right)_{k \in \{1, \dots, n\}}$

We are now in position to conclude the proof of Proposition B.17, by proving that for $k \in \{1, \dots, n\}$, one has

$$\int_{\Sigma_k} (\partial_n u_h)\, e^{-\frac{2}{h} f} d\sigma = C_k B_k \; h^{p+m} e^{-\frac{1}{h}(2f(z_k) - f(x_0))} \, (1 + O(h)).$$

Proof. Let us assume that the assumptions of Proposition B.17 hold. Let us recall the decomposition (B.63):

$$\int_{\Sigma_k} (\partial_n u_h)\, e^{-\frac{2}{h} f} d\sigma = \sum_{j=1}^{n} \langle \nabla u_h, \psi_j \rangle_{L^2_w} \int_{\Sigma_k} \psi_j \cdot n \, e^{-\frac{2}{h} f} d\sigma.$$

Using Lemmas B.23 and C.36 , we can now estimate the terms in the sum in the right-hand side. If $j > k$, there exist $\varepsilon > 0$ and $h_0 > 0$ such that for all $h \in (0, h_0)$

$$\begin{aligned} \langle \nabla u_h, \psi_j \rangle_{L^2_w} \int_{\Sigma_k} \psi_j \cdot n \; e^{-\frac{2}{h} f} d\sigma &= C_j h^p O\left(e^{-\frac{1}{h}[f(z_j) - f(x_0)]} e^{-\frac{1}{h}[f(z_j) + \varepsilon]}\right) \\ &= C_j h^p O\left(e^{-\frac{1}{h}[2f(z_j) - f(x_0) + \varepsilon]}\right) \\ &= C_j h^p O\left(e^{-\frac{1}{h}[2f(z_k) - f(x_0) + \varepsilon]}\right). \end{aligned}$$

If $j < k$, there exist $\varepsilon > 0$ and $h_0 > 0$ such that for all $h \in (0, h_0)$

$$\begin{aligned}
\langle \nabla u_h, \psi_j \rangle_{L^2_w} \int_{\Sigma_k} \psi_j \cdot n \; e^{-\frac{2}{h} f} d\sigma &= O\left(e^{-\frac{1}{h}[f(z_j)-f(x_0)+K_j+f(z_k)+\varepsilon]}\right) \\
&\quad + \sum_{i=1}^{j-1} O\left(e^{-\frac{1}{h}[f(z_j)-f(x_0)+f(z_j)-f(z_i)+K_i+f(z_k)+\varepsilon]}\right) \\
&= O\left(e^{-\frac{1}{h}[f(z_j)-f(x_0)+f(z_n)-f(z_j)+f(z_k)+\varepsilon]}\right) \\
&\quad + \sum_{i=1}^{j-1} O\left(e^{-\frac{1}{h}[f(z_j)-f(x_0)+f(z_j)-f(z_i)+f(z_n)-f(z_i)+f(z_k)+\varepsilon]}\right) \\
&= O\left(e^{-\frac{1}{h}[f(z_n)+f(z_k)-f(x_0)+\varepsilon]}\right) \\
&\quad + \sum_{i=1}^{j-1} O\left(e^{-\frac{1}{h}[f(z_n)+f(z_k)-f(x_0)+2(f(z_j)-f(z_i))+\varepsilon]}\right) \\
&= O\left(e^{-\frac{1}{h}[2f(z_k)-f(x_0)+\varepsilon]}\right).
\end{aligned}$$

Finally if $j = k$, $\exists \varepsilon > 0$ and $\exists h_0 > 0$ such that for all $h \in (0, h_0)$

$$\langle \nabla u_h, \psi_k \rangle_{L^2_w} \int_{\Sigma_k} \psi_k \cdot n \; e^{-\frac{2}{h} f} d\sigma = C_k B_k \; h^{p+m} e^{-\frac{1}{h}(2f(z_k)-f(x_0))}(1 + O(h)). \tag{B.70}$$

From these estimates, for a fixed $k \in \{1, \ldots, n\}$, the dominant term in the sum in the right-hand side of (B.63) is the one with index $j = k$, namely (B.70). This concludes the proof of Proposition B.17. ∎

B.3 On the Agmon distance

In this section, we present the main properties of the Agmon distance introduced in Definition B.3. The Agmon distance is useful to quantify the decay of eigenforms of some Witten Laplacians away from critical points of f and $f|_{\partial\Omega}$. The Agmon distance on a domain without boundary has been extensively analyzed in many previous works (see in particular [35–37, 39]). The aim of this section is to generalize well-known results in the case without boundary to our context, namely for bounded domains. Indeed, to the best of our knowledge, this has not been done in the literature before in a comprehensive way.

For simplicity, all the proofs in this section are made for a bounded connected open connected C^∞ domain $\Omega \subset \mathbb{R}^d$ (equipped with the geodesic Euclidean distance (B.85)) and for a C^∞ function $f : \overline{\Omega} \to \mathbb{R}$. The generalization to a C^∞ compact connected Riemannian manifold of dimension d with boundary is straightforward. The notation $|x - y|$ denotes the Euclidean distance between x and y in $\mathbb{R}^d$. If one deals with a compact connected Riemannian manifold of dimension d with boundary, this distance has to be replaced by the geodesic distance on $\overline{\Omega}$ for the initial metric and the scalar product between two vectors of $\mathbb{R}^d$ has to be replaced by the one induced by the initial metric on the tangent space of $\overline{\Omega}$.

This section is organized as follows. Section B.3.1 is devoted to an equivalent definition of the Agmon distance, which will be crucial in the following. In Section B.3.2, we then give a few useful properties of the Agmon distance. As already mentioned in Section B.1.5.1, there is a link between the Agmon distance and the eikonal equation. This is explained in Section B.3.3 and B.3.5. This link is useful in order to build explicit curves realizing the Agmon distance, as explained in Section B.3.4.

B.3.1 The set $A(x,y)$ and an equivalent definition of the Agmon distance

In order to study the Agmon distance, it will be more convenient for technical reasons to restrict the class of curves appearing in the definition of the Agmon distance (see Definition B.3).

Definition B.6. *For $x, y \in \overline{\Omega}$, we denote by $A(x,y)$ the set of curves $\gamma : [0,1] \to \overline{\Omega}$ which are Lipschitz with $\gamma(0) = x$, $\gamma(1) = y$ and such that the set $\partial\{t \in [0,1] \big| \gamma(t) \in \partial\Omega\}$ is finite.*

Here $\partial\{t \in [0,1],\, \gamma(t) \in \partial\Omega\}$ denotes the boundary of the set $\{t \in [0,1],\, \gamma(t) \in \partial\Omega\}$. The main result of this section is that, under assumption **[H3]**, the Agmon distance d_a satisfies (compare with (B.18)):

$$\forall\, (x,y) \in \overline{\Omega}^2,\, d_a(x,y) = \inf_{\gamma \in A(x,y)} L(\gamma, (0,1)). \tag{B.71}$$

See Corollary B.28 below.

The following lemma will be needed several times throughout this section. It motivates the use of the set $A(x,y)$ appearing in Definition B.6.

Lemma B.25. *Let $x, y \in \overline{\Omega}$ and $\gamma \in A(x,y)$. Then for any $h : \overline{\Omega} \to \mathbb{R}$ which is C^1, one gets*

$$h(y) - h(x) = \int_{\{t \in [0,1],\, \gamma(t) \in \Omega\}} (\nabla h)(\gamma) \cdot \gamma' + \int_{\mathrm{int}\{t \in [0,1],\, \gamma(t) \in \partial\Omega\}} (\nabla_T h)(\gamma) \cdot \gamma'. \tag{B.72}$$

Here the notation int *stands for the interior of a domain.*

Proof. Since γ is Lipschitz, $h \circ \gamma$ is Lipchitz and thus absolutely continuous. Therefore, one has:

$$\begin{aligned} h(y) - h(x) &= \int_0^1 \frac{d}{dt}(h \circ \gamma) \\ &= \int_{\{t \in [0,1],\, \gamma(t) \in \Omega\}} \frac{d}{dt}(h \circ \gamma) + \int_{\mathrm{int}\{t \in [0,1],\ \gamma(t) \in \partial\Omega\}} \frac{d}{dt}(h \circ \gamma) \\ &\quad + \int_{\partial\{t \in [0,1],\, \gamma(t) \in \partial\Omega\}} \frac{d}{dt}(h \circ \gamma). \end{aligned}$$

By definition of the set $A(x,y)$ (see Definition B.6) the set $\partial\{t \in [0,1],\ \gamma(t) \in \partial\Omega\}$ has Lebesgue measure zero,

$$\int_{\partial\{t \in [0,1],\, \gamma(t) \in \partial\Omega\}} \frac{d}{dt}(h \circ \gamma) = 0.$$

The curve γ is continuous and thus the set $\{t \in [0,1],\ \gamma(t) \in \Omega\}$ is open in $[0,1]$. Thus, using in addition that since γ is Lipschitz, it is almost everywhere differentiable (by the Rademacher Theorem), one has for almost every $t \in [0,1]$:

$$\frac{d}{dt}h(\gamma)(t) = \begin{cases} (\nabla h)(\gamma(t)) \cdot \dfrac{d}{dt}\gamma(t) \ \text{ a.e. on } \{t \in [0,1],\ \gamma(t) \in \Omega\} \\ (\nabla_T h)(\gamma(t)) \cdot \dfrac{d}{dt}\gamma(t) \ \text{ a.e. on int} \{t \in [0,1],\ \gamma(t) \in \partial\Omega\}. \end{cases}$$

This proves (B.72). ∎

Remark B.4. *Notice that there exist Lipschitz curves γ such that $\partial\{t \in [0,1],\ \gamma(t) \in \partial\Omega\}$ has a positive Lebesgue measure. Let us give an example. Consider $\Omega = (0,1) \times (0,2)$ and the curve*

$$\gamma : t \in [0,1] \mapsto \left(t, \inf_{y \in K} |t-y|\right) \in [0,1]^2,$$

where K is the Smith-Volterra-Cantor set in $[0,1]$, such that K is closed, has a positive Lebesgue measure and has an empty interior (see [60, Section 2.5]). Notice that the distance $\inf_{y\in K}|t-y|$ to K is a Lipschitz function of $t \in (0,1)$, so that γ is a Lipschitz function. The set K is closed and thus

$$\{t \in [0,1], \gamma(t) \in \partial\Omega\} = \{t \in [0,1], \gamma(t) = 0\} = K.$$

Therefore $\partial\{t \in [0,1],\ \gamma(t) \in \partial\Omega\} = \overline{K} \setminus (\text{int}K) = K$.

The following results will be useful to prove the equality (B.71) and to prove the existence of curves realizing the Agmon distance (see Section B.3.4).

Proposition B.26. *Assume that **[H3]** holds. Let $\gamma : [0,1] \to \overline{\Omega}$ be a Lipschitz curve and assume that there exists a time $t^* \in [0,1]$ such that $\gamma(t^*) \in \partial\Omega$. Then there exists $(a,b) \in [0,1]^2$, with $a \le t^* \le b$ and $a < b$ such that for all $(t_1,t_2) \in [0,1]^2$, with $a \le t_1 < t_2 \le b$, there exists a Lipschitz curve $\gamma_{12} : [t_1,t_2] \to \overline{\Omega}$ satisfying*

$$\gamma_{12}(t_1) = \gamma(t_1) \text{ and } \gamma_{12}(t_2) = \gamma(t_2),$$

$$L(\gamma,(t_1,t_2)) \ge L(\gamma_{12},(t_1,t_2)) \tag{B.73}$$

and, either $\{t \in [t_1,t_2],\ \gamma_{12}(t) \in \partial\Omega\}$ is empty, or its boundary $\partial\{t \in [t_1,t_2],\ \gamma_{12}(t) \in \partial\Omega\}$ consists of isolated points in $\{t \in [t_1,t_2],\ \gamma_{12}(t) \in \partial\Omega\}$. Moreover, if the following is satisfied:

$$\exists (s_1,s_2,s_3) \in [t_1,t_2]^3, s_1 < s_2 < s_3,\ \gamma(s_1) \in \partial\Omega, \gamma(s_2) \in \Omega \text{ and } \gamma(s_3) \in \partial\Omega, \tag{B.74}$$

then the inequality (B.73) *is strict.*

Remark B.5. *Notice that if $t^* \in \partial\{t \in [0,1],\ \gamma(t) \in \partial\Omega\}$ is not isolated in $\partial\{t \in [0,1],\ \gamma(t) \in \partial\Omega\}$, then there exits a neighborhood $[t_1,t_2]$ of t^* in $[0,1]$ such that* (B.74) *is satisfied and thus the inequality* (B.73) *is strict. Therefore if a Lipschitz curve γ realizes the infimum of L on $\text{Lip}(x,y)$, then $\partial\{t \in [0,1],\ \gamma(t) \in \partial\Omega\}$ is finite. This motivates the introduction of the set $A(x,y)$.*

Proof. Let $t^* \in [0,1]$ be such that $\gamma(t^*) \in \partial\Omega$. The proof is divided into three steps.

Step 1: Introduction of a normal system of coordinates and definition of a and b. Let us consider a neighborhood $V_{\partial\Omega}$ of $\gamma(t^*)$ in $\partial\Omega$, and a smooth local system of coordinates in $V_{\partial\Omega} \subset \partial\Omega$, denoted by $x_T : V_{\partial\Omega} \to \mathbb{R}^{d-1}$. Let us now extend it to a tangential and normal system of coordinates around $\gamma(t^*)$ in $\overline{\Omega}$, denoted by $\phi(x) = (x_T, x_N)$. The function ϕ is defined from a neighborhood of $\gamma(t^*)$ in $\overline{\Omega}$ to $\mathbb{R}^d$. Moreover, one has $x_N(x) \geq 0$ and for all x, $x_N(x) = 0$ if and only if $x \in \partial\Omega$. One can assume without loss of generality that ϕ is defined on a neighborhood V_α of $\gamma(t^*)$ in $\overline{\Omega}$ such that $\phi(V_\alpha) = U \times [0,\alpha]$ for $\alpha > 0$, and $U \subset \mathbb{R}^{d-1}$. For this normal system of coordinates, the metric tensor G is such that: $\forall (x_T, x_N) \in U \times [0,\alpha]$,

$$G(x_T, x_N) = \begin{pmatrix} \tilde{G}(x_T, x_N) & 0 \\ 0 & G_{NN}(x_T, x_N) \end{pmatrix},$$

where $\tilde{G}(x_T, x_N) \in \mathbb{R}^{(d-1)\times(d-1)}$ and $G_{NN}(x_T, x_N) \in \mathbb{R}$ are smooth functions of (x_T, x_N). The existence of such a system of coordinates is a consequence of the collar theorem, see [65].

Under assumption **[H3]** (namely $\partial_n f > 0$ on $\partial\Omega$), there exist constants $A > 1$ and $\varepsilon_1 > 0$ such that for all $x_N \in (0, \varepsilon_1]$ and for all $x_T \in U$, (see (B.17) for the definition of g)

$$g(\phi^{-1}(x_T, x_N)) \geq A\, g(\phi^{-1}(x_T, 0)). \tag{B.75}$$

Since the local change of coordinates is smooth, for all $\varepsilon \in (0,1)$, there exists $\eta > 0$ such that for all $x_N \in [0,\eta]$ and for all $x_T \in U$, one has

$$\tilde{G}\,(x_T, x_N) \geq (1-\varepsilon)^2 \tilde{G}(x_T, 0).$$

Let us choose $\varepsilon > 0$ such that $(1-\varepsilon)\,A > 1$. One can reduce V_α such that $0 \leq x_N(x) \leq \min(\eta, \varepsilon_1)$ for all $x \in V_\alpha$. By continuity of γ, there exist $(a,b) \in [0,1]^2$, with $a \leq t^* \leq b$ and $a < b$ such that for all $t \in [a,b]$, $\gamma(t) \in V_\alpha$. Let us introduce the components of γ in the normal system of coordinates: $(\gamma_T(t), \gamma_N(t)) = \phi(\gamma(t))$. Let us now define: for $t \in [a,b]$,

$$\tilde{\gamma}(t) := \phi^{-1}\left(\gamma_T(t), 0\right) \in \partial\Omega.$$

For almost every $t \in (a,b)$, if $\gamma(t) \in \partial\Omega$, $\gamma(t) = \phi^{-1}(\gamma_T(t), 0) = \tilde{\gamma}(t)$, $g(\gamma(t)) = g(\tilde{\gamma}(t))$ and

$$\begin{aligned} |\gamma'(t)|^2 &= \left[(\gamma_T, \gamma_N)'\right]^{Tr} G\left(\gamma_T(t), 0\right) (\gamma_T, \gamma_N)' \\ &= \left[\gamma_T'(t)\right]^{Tr} \tilde{G}(\gamma_T(t), 0)\, \gamma_T'(t) + G_{NN}\left(\gamma_T(t), 0\right) \gamma_N'(t)^2 \\ &\geq \left[\gamma_T'(t)\right]^{Tr} \tilde{G}\left(\gamma_T(t), 0\right) \gamma_T'(t) = \left|\tilde{\gamma}'(t)\right|^2, \end{aligned}$$

where the supersript ^{Tr} stands for the transposition operator. For almost every $t \in (a,b)$, if $\gamma(t) \in \Omega$,

$$\begin{aligned} |\gamma'(t)|^2 &= \left[(\gamma_T, \gamma_N)'\right]^{Tr} G\left((\gamma_T, \gamma_N)\right) (\gamma_T, \gamma_N)' \\ &= \left[\gamma_T'(t)\right]^{Tr} \tilde{G}\left((\gamma_T, \gamma_N)\right) \gamma_T'(t) + G_{NN}\left((\gamma_T, \gamma_N)\right) \gamma_N'(t)^2 \\ &\geq (1-\varepsilon)^2 \left[\gamma_T'(t)\right]^{Tr} \tilde{G}\left(\gamma_T(t), 0\right) \gamma_T'(t) = (1-\varepsilon)^2 \left|\tilde{\gamma}'(t)\right|^2. \end{aligned}$$

Step 2: Definition of γ_{12}. Let $(t_1, t_2) \in [0,1]^2$, with $a \leq t_1 < t_2 \leq b$. Let us distinguish between two cases.

- If the set $\{t \in [t_1, t_2],\, \gamma(t) \in \partial\Omega\}$ is non empty, let us consider $t_1^+ := \inf\{t \in [t_1, t_2],\, \gamma(t) \in \partial\Omega\}$ and $t_2^- := \sup\{t \in [t_1, t_2],\, \gamma(t) \in \partial\Omega\}$. The curve $\gamma_{12} : [t_1, t_2] \to \overline{\Omega}$ is then defined by

$$\gamma_{12}(t) = \begin{cases} \gamma(t) & \text{if } t \in (t_1, t_1^+), \\ \tilde{\gamma}(t) & \text{if } t \in (t_1^+, t_2^-), \\ \gamma(t) & \text{if } t \in (t_2^-, t_2). \end{cases}$$

  Observe that for all $t \in (t_1, t_1^+) \cup (t_2^-, t_2)$, $\gamma(t) = \gamma_{12}(t)$, which implies $g(\gamma(t))|\gamma'(t)| = g(\gamma_{12}(t))|\tilde{\gamma}'_{12}(t)|$ almost everywhere in $(t_1, t_1^+) \cup (t_2^-, t_2)$. Moreover, using the fact that $A(1-\varepsilon) > 1$, for almost every $t \in (t_1^+, t_2^-)$,

$$g(\gamma(t))|\gamma'(t)| \geq A(1-\varepsilon) g(\phi^{-1}(\gamma_T(t), 0))|\tilde{\gamma}'(t)| > g(\tilde{\gamma})|\tilde{\gamma}'(t)| = g(\gamma_{12})|\gamma'_{12}(t)|. \tag{B.76}$$

  Therefore (B.73) is satisfied.

- If the set $\{t \in [t_1, t_2],\, \gamma(t) \in \partial\Omega\}$ is empty, which means that $\forall t \in [t_1, t_2]$, $\gamma(t) \in \Omega$, then one simply defines the curve $\gamma_{12} : [t_1, t_2] \to \overline{\Omega}$ by $\gamma_{12} = \gamma$.

In both cases, the curve γ_{12} is Lipschitz, $\gamma_{12}(t_j) = \gamma(t_j)$ for $j \in \{1, 2\}$ and (B.73) is satisfied. Moreover by construction of γ_{12}, the set $\partial\{t \in [t_1, t_2],\, \gamma_{12}(t) \in \partial\Omega\}$ consists of isolated points in $\{t \in [t_1, t_2],\, \gamma_{12}(t) \in \partial\Omega\}$, or is empty.

Step 3: On the strict inequality in (B.73). Assume that (B.74) holds and let us show that the inequality (B.73) is strict. Indeed, in that case $t_1^+ \leq s_1 < s_3 \leq t_2^-$ and by continuity of γ, there exists $(u_1, u_2) \in (s_1, s_3)^2$ such that $u_1 < s_2 < u_2$ and $\gamma([u_1, u_2]) \subset \Omega$. Thus, the inequality (B.76) holds almost everywhere on the open nonempty interval (u_1, u_2) which implies that $L(\gamma, (u_1, u_2)) > L(\gamma_{12}, (u_1, u_2))$. This concludes the proof of Proposition B.26.

∎

A consequence of the previous proposition is the following result.

Proposition B.27. *Let $x, y \in \overline{\Omega}$ and assume that **[H3]** holds. For any Lipschitz curve $\gamma : [0,1] \to \overline{\Omega}$ with $\gamma(0) = x$ and $\gamma(0) = y$, there exists $\gamma_1 \in A(x, y)$ such that $L(\gamma, (0,1)) \geq L(\gamma_1, (0,1))$.*

Proof. The set $\partial\{t \in [0,1],\, \gamma(t) \in \partial\Omega\}$ is closed, so its limit points are its non isolated points. Let us define $\mathrm{Ad}(\gamma)$ as the set of limit points of $\partial\{t \in [0,1],\, \gamma(t) \in \partial\Omega\}$. If $\mathrm{Ad}(\gamma)$ is empty, then $\partial\{t \in [0,1],\, \gamma(t) \in \partial\Omega\}$ is empty or consists of isolated points in $\partial\{t \in [0,1],\, \gamma(t) \in \partial\Omega\}$ and since $\partial\{t \in [0,1],\, \gamma(t) \in \partial\Omega\}$ is compact, this implies that $\gamma \in A(x, y)$ and Proposition B.27 is thus proved by simply taking $\gamma_1 = \gamma$.

If $\mathrm{Ad}(\gamma)$ is non empty, we will construct a curve $\gamma_1 \in A(x, y)$ such that

$$L(\gamma, (0,1)) \geq L(\gamma_1, (0,1)).$$

Without loss of generality, one can assume that 0 and 1 are not in $\mathrm{Ad}(\gamma)$. Otherwise one could modify γ in neighborhoods of 0 and 1 without increasing $L(\gamma, (0,1))$ and without

changing the end points using Proposition B.26. To prove the result, we will show by induction on $N \geq 1$ the following property $\mathcal{P}_N$: for all $\{t_1, \ldots, t_N\} \subset \mathrm{Ad}(\gamma)$, denote by $(a_j, b_j)_{j=1,\ldots,N}$ the open intervals given by Proposition B.26 for each t_i; then, it is possible to change γ to construct a Lipschitz curve $\gamma_1 : [0,1] \to \overline{\Omega}$ with $\gamma_1(0) = x$ and $\gamma_1(0) = y$, such that $\gamma_1 = \gamma$ on $[0,1] \setminus \left(\bigcup_{j=1}^N (a_j, b_j)\right)^c$, $\mathrm{Ad}(\gamma_1) \cap \bigcup_{j=1}^N (a_j, b_j) = \emptyset$ and $L(\gamma, (0,1)) \geq L(\gamma_1, (0,1))$.

The first step to prove $\mathcal{P}_1$ is just a straightforward application of Proposition B.26 (choosing $t_1 = a_1$ and $t_2 = b_2$). Now, let us prove $\mathcal{P}_{N+1}$ assuming $\mathcal{P}_N$. Let us consider $\{t_1, \ldots, t_N, t_{N+1}\} \subset \mathrm{Ad}(\gamma)$ and denote by $(a_j, b_j)_{j=1,\ldots,N,N+1}$ the open intervals given by Proposition B.26 for each t_i. Applying $\mathcal{P}_N$, it is possible to change γ to construct a Lipschitz curve $\gamma_1 : [0,1] \to \overline{\Omega}$ with $\gamma_1(0) = x$ and $\gamma_1(0) = y$, such that $\mathrm{Ad}(\gamma_1) \cap \bigcup_{j=1}^N (a_j, b_j) = \emptyset$ and $L(\gamma, (0,1)) \geq L(\gamma_1, (0,1))$. If $(a_{N+1}, b_{N+1}) \subset \bigcup_{j=1}^N (a_j, b_j)$, then $\mathcal{P}_{N+1}$ holds taking γ_1. Otherwise, there exist $K \in \mathbb{N}^*$ and $(q_1, \ldots, q_K, d_1, \ldots, d_K) \in [0,1]^{2K}$ such that

$$(a_{N+1}, b_{N+1}) \cap \left[\bigcup_{j=1}^N (a_j, b_j)\right]^c = \bigcup_{i=1}^K [(q_i, d_i)],$$

with $0 < q_1 < d_1 < q_2 < d_2 < \ldots < q_K < d_K < 1$; the notation $[($ and $)]$ mean that the extremities can or not belong to the interval. In addition, for $i \in \{1, \ldots, K\}$, $q_i \in \{a_{N+1}\} \cup \{b_1, \ldots, b_N\}$ and $d_i \in \{b_{N+1}\} \cup \{a_1, \ldots, a_N\}$. Then applying Proposition B.26 to γ_1 on each interval $(q_i, d_i) \subset (a_{N+1}, b_{N+1})$, one gets that it is possible to construct a Lipschitz curve γ_2 with $\gamma_2(0) = x$ and $\gamma_2(0) = y$, such that

$$L(\gamma_1, (0,1)) \geq L(\gamma_2, (0,1)), \ \mathrm{Ad}(\gamma_2) \cap \bigcup_{i=1}^K (q_i, d_i) = \emptyset.$$

If for some $k \in \{1, \ldots, K\}$ and $j \in \{1, \ldots, N\}$ $q_k = b_j$, then q_k is isolated from the left in $\{t \in [0,1], \gamma_1(t) \in \partial\Omega\}$ from the construction of γ_1 (see Proposition B.26) and, by construction of γ_2, q_k is also isolated from the right in $\{t \in [0,1], \gamma_2(t) \in \partial\Omega\}$. Thus, since there exits $s \in [0, q_k)$ such that $\gamma_2 = \gamma_1$ on $[s, q_k]$, one has $q_k \notin \mathrm{Ad}(\gamma_2)$. A similar reasoning holds for the points d_k. Thus

$$\mathrm{Ad}(\gamma_2) \cap (a_{N+1}, b_{N+1}) \cap \left[\bigcup_{j=1}^N (a_j, b_j)\right]^c = \emptyset.$$

This proves that $\mathrm{Ad}(\gamma_2) \cap \bigcup_{j=1}^{N+1} (a_j, b_j) = \emptyset$ and thus $\mathcal{P}_{N+1}$.

By induction, we thus have proven $\mathcal{P}_N$ for all $N \geq 1$. Now, notice that by a compactness argument, there exist $N \geq 0$ and $\{t_1, \ldots, t_N\} \subset \mathrm{Ad}(\gamma)$ such that if one denotes by $(a_j, b_j)_{j=1,\ldots,N}$ the open intervals given by Proposition B.26 for each t_i, then

$$\mathrm{Ad}(\gamma) \subset \bigcup_{i=1}^N (a_i, b_i).$$

Applying $\mathcal{P}_N$ yields the desired result. ∎

A direct consequence of Proposition B.27 is the following.

Corollary B.28. *Assume that **[H3]** holds. Then the Agmon distance d_a introduced in Definition B.3 satisfies* (B.71)*: for all $(x,y) \in \overline{\Omega}^2$*

$$d_a(x,y) = \inf_{\gamma \in A(x,y)} L(\gamma, (0,1)).$$

In all what follows, we will often use the formula (B.71) to study the property of the Agmon distance.

B.3.2 First properties of the Agmon distance

In this section, we aim at giving the basic properties of the Agmon distance.

B.3.2.1 Upper bounds and topology of $(\overline{\Omega}, d_a)$

Proposition B.29. *There exists a constant C such that for all $x, y \in \overline{\Omega}$,*

$$d_a(x,y) \leq C|x-y|. \tag{B.77}$$

For any fixed $y \in \overline{\Omega}$, $x \in \overline{\Omega} \mapsto d_a(x,y)$ is Lipschitz. Its gradient is well defined almost everywhere and satisfies for $y \in \overline{\Omega}$ and for almost every $x \in \Omega$,

$$|\nabla_x d_a(x,y)| \leq |\nabla f(x)|. \tag{B.78}$$

*Moreover, if **[H3]** holds, for all $x, y \in \overline{\Omega}$, we have*

$$|f(x) - f(y)| \leq d_a(x,y). \tag{B.79}$$

Proof. Let us first prove the inequality (B.79). For any $\gamma \in A(x,y)$, using Lemma B.25, one has:

$$\begin{aligned}
|f(x) - f(y)| &= \left| \int_0^1 \frac{d}{dt}(f \circ \gamma)\, dt \right| \\
&= \left| \int_{\{t \in [0,1],\ \gamma(t) \in \Omega\}} (\nabla f)(\gamma) \cdot \gamma'\, dt + \int_{\mathrm{int}\{t \in [0,1],\ \gamma(t) \in \partial\Omega\}} (\nabla_T f)(\gamma) \cdot \gamma'\, dt \right| \\
&\leq \int_0^1 g(\gamma(t))\, |\gamma'(t)|\, dt.
\end{aligned}$$

Therefeore (B.79) is proved by taking the infimum over $\gamma \in A(x,y)$ in the right-hand side (see Corollary B.28). The second inequality (B.77) is proven below in Lemma B.30. Let us conclude the proof. Now let $y \in \overline{\Omega}$ and $x \in \Omega$. Since Ω is open, there exists an open ball $B \subset \Omega$ with center x. Let $z \in B$. For $t \in [0,1]$, the path $\gamma(t) = tz + (1-t)x$ is included in B. Then, one obtains

$$\begin{aligned}
|d_a(x,y) - d_a(z,y)| &\leq d_a(x,z) \\
&\leq |x-z| \int_0^1 g(tz + (1-t)x)\, dt \\
&= |x-z| \int_0^1 |\nabla f|(x + t(z-x))\, dt.
\end{aligned}$$

Since f is smooth, up to considering a smaller ball B centered at x, there exists a constant $c > 0$ such that for all $z \in B$, for all $t \in [0,1]$,

$$|\nabla f|(x + t(z - x)) \leq |\nabla f|(x) + c\,|x - z|\,.$$

Thus, for all $z \in B$,

$$|d_a\,(x,y) - d_a(z,y)| \leq |x - z|\,(|\nabla f|(x) + c\,|x - z|)\,.$$

As a consequence, for any fixed $y \in \overline{\Omega}$ and for almost $x \in \Omega$ one gets (B.78), by considering the limit $z \to x$ in the previous inequality. ∎

Let us now give the proof of (B.77).

Lemma B.30. *The function $(x,y) \in \overline{\Omega} \times \overline{\Omega} \mapsto d_a\,(x,y)$ is bounded and satisfies*

$$\sup_{(x,y)\in\overline{\Omega}\times\overline{\Omega}} \frac{d_a\,(x,y)}{|x-y|} < \infty. \tag{B.80}$$

Proof. Let us first prove by contradiction that $(x,y) \in \overline{\Omega} \times \overline{\Omega} \mapsto d_a\,(x,y)$ is bounded. Let us assume that there exists a sequence $(x_k, y_k)_{k\geq 1} \in \overline{\Omega} \times \overline{\Omega}$ such that for all $k \geq 1$,

$$d_a(x_k, y_k) \geq k. \tag{B.81}$$

Up to the extraction of a subsequence, it can be assumed that $\lim_{k\to\infty}(x_k, y_k) = (x,y) \in \overline{\Omega} \times \overline{\Omega}$ (the convergence being for the Euclidean metric). Notice that

$$d_a(x_k, y_k) \leq d_a(x_k, x) + d_a\,(x,y) + d_a(y_k, y). \tag{B.82}$$

Let us consider $d_a(x_k, x)$. If $x \in \Omega$ then there exist an open ball $B \subset \Omega$ centered on x and an integer N such that for all $k \geq N$, $x_k \in B$ and therefore $\gamma(t) = tx_k + (1-t)x \in B$ for all $t \in (0,1)$. Then, by definition of the Agmon distance, for all $k \geq 1$,

$$d_a(x_k, x) \leq \|g\|_{L^\infty(B)}\,|x - x_k|.$$

If $x \in \partial\Omega$ then there exist $r > 0$ and a C^∞ bijective map $\phi\ :\ B(x,r) \to B(0,1)$ such that $\phi(x) = 0$, $\phi(B(x,r) \cap \partial\Omega) = Q_0$ and $\phi(B(x,r) \cap \overline{\Omega}) = Q_-$, where $Q_0 := \{y = (y_1, \ldots, y_d),\ |y| \leq 1,\ y_d = 0\}$ and $Q_- := \{y = (y_1, \ldots, y_d),\ |y| \leq 1,\ y_d \leq 0\}$. Moreover, there exists N such that for all $k \geq N$, $x_k \in B(x,r) \cap \overline{\Omega}$. Now, for any $k \geq N$, let us consider

$$\gamma(t) = \phi^{-1}((1-t)\phi(x_k) + t\phi(x)).$$

Notice that $\gamma \in A(x_k, x)$ and satisfies $\gamma([0,1]) \subset B(x,r)$. Moreover $c(t) = \phi\,(\gamma(t)) = (1-t)\phi(x_k) + t\phi(x) \in Q_-$ for $t \in [0,1]$. Then, one has:

$$\begin{aligned}
d_a(x_k, x) &\leq \int_0^1 g(\gamma)|\gamma'|, \\
&\leq \|g\|_{L^\infty(B(x,r))} \int_0^1 |\gamma'|, \\
&= \|g\|_{L^\infty(B(x,r))} \int_0^1 |\mathrm{Jac}(\phi^{-1})(c)c'|, \\
&\leq \|g\|_{L^\infty(B(x,r))} \|\mathrm{Jac}(\phi^{-1})\|_{L^\infty(B(0,1))} |\phi(x_k) - \phi(x)|
\end{aligned}$$

and therefore, since ϕ is Lipschitz,

$$d_a(x_k, x) \leq C|x_k - x|, \tag{B.83}$$

where C is a constant independent of $k \geq N$. This shows that $d_a(x_k, x)$ is bounded. The same reasoning shows that $d_a(y, y_k)$ is bounded. This yields a contradiction, considering the inequality (B.82) and (B.81).

To show (B.80), one proceeds in the same way. Assume that there exists a sequence $(x_k, y_k) \in \overline{\Omega} \times \overline{\Omega}$ such that

$$d_a(x_k, y_k) \geq k\,|x_k - y_k|\,. \tag{B.84}$$

Up to the extraction of a subsequence, it can be assumed that $\lim_{k\to\infty}(x_k, y_k) = (x, y) \in \overline{\Omega} \times \overline{\Omega}$. If $x \neq y$, then, for k sufficiently large

$$\frac{d_a(x_k, y_k)}{|x_k - y_k|} \leq 2\,\frac{\sup_{(x,y)\in\overline{\Omega}} d_a(x, y)}{|x - y|} < \infty$$

which contradicts (B.84). If $x = y \in \Omega$, then, for all k sufficiently large, the curve $\gamma(t) = tx_k + (1 - t)y_k$ is with values in Ω and therefore for all k sufficiently large

$$d_a(x_k, y_k) \leq \|g\|_{L^\infty(\overline{\Omega})}|y_k - x_k|.$$

This again leads to a contradiction when $k \to \infty$. Finally, if $x = y \in \partial\Omega$, using the same reasoning as above to prove (B.83), one has the existence of a constant C such that for all k sufficiently large,

$$d_a(x_k, y_k) \leq C|x_k - y_k|,$$

which again contradicts (B.84). This concludes the proof of Lemma B.30. ∎

A consequence of the previous lemma is the following proposition.

Proposition B.31. *Assume that **[H1]** holds. The space $\left(\overline{\Omega}, d_a\right)$ is a compact separated metric space. Moreover the topology of the metric space $\left(\overline{\Omega}, d_a\right)$ is equivalent to the topology induced by the Euclidean metric on $\overline{\Omega}$.*

Proof. It is clear that $d_a \geq 0$, and for all $(x, y, z) \in \overline{\Omega}^3$, $d_a\,(x, y) \leq d_a\,(x, z) + d_a\,(z, y)$. Let us show that for any $(x, y) \in \overline{\Omega}^2$, if $x \neq y$ then $d_a\,(x, y) > 0$. Let us denote by d_e the geodesic distance on $\overline{\Omega}$ for the Euclidean metric: for all $x, y \in \overline{\Omega}$,

$$d_e\,(x, y) := \inf_\gamma \int_0^1 \left|\gamma'(t)\right|\,dt, \tag{B.85}$$

where the infimum is taken over all the paths $\gamma : [0, 1] \to \overline{\Omega}$ which are Lipchitz with $\gamma(0) = x$ and $\gamma(1) = y$. Since **[H1]** holds, the functions f and $f|_{\partial\Omega}$ have a finite number of critical points, and, there exist $0 < r_1 < r_2 < d_e(x, y)$ such that the infimum of g on the set $C(r_1, r_2) := \left\{z \in \overline{\Omega},\, r_1 < d_e(x, z) < r_2\right\}$ is positive i.e. $c(r_1, r_2) := \inf_{C(r_1,r_2)} g > 0$. For any path $\gamma \in A\,(x, y)$, one has

$$\int_0^1 |\gamma'(t)|\,g(\gamma(t))\,dt \geq c(r_1, r_2)r(C(r_1, r_2)),$$

where $r(C(r_1,r_2)) := \inf_{x\in C(r_1,r_2)} \sup_{y\in C(r_1,r_2)} d_e(x,y) > 0$. Then $d_a(x,y) > 0$. If $x = y$, it is clear that $d_a(x,y) = 0$ since $L(\gamma,(0,1)) = 0$ where $\gamma(t) = x$ for all $t \in [0,1]$. This shows that $\left(\overline{\Omega}, d_a\right)$ is separated.

The fact that $\left(\overline{\Omega}, d_a\right)$ is compact comes from the inequality (B.77) proved in Lemma B.30. Indeed, since $\left(\overline{\Omega}, d_a\right)$ is a metric space, it is sufficient to prove the sequential compactness. Let $(x_n)_{n\geq 0}$ be a sequence in $\overline{\Omega}$. Since $\overline{\Omega}$ is compact for the Euclidean metric, one can extract a converging subsequence $(x'_n)_{n\geq 0}$ for the Euclidean metric. From (B.77), this subsequence is also converging for d_a, which ends the proof.

Let us finally prove the equivalence of the topologies on $\overline{\Omega}$. From Lemma B.30, it is obvious that if a sequence $(x_n)_{n\geq 0}$ converges to x in $\overline{\Omega}$ for the Euclidean metric, then $d_a(x_n,x)$ converges to 0. Conversely, let us assume that $(x_n)_{n\geq 0}$ is a sequence of $\overline{\Omega}$ such that $d_a(x_n,x)$ converges to 0, for a point $x \in \overline{\Omega}$. Since $\overline{\Omega}$ is compact for the Euclidean metric, it is enough to show that x is the only limit point of the sequence to show that $(x_n)_{n\geq 0}$ converges to x for the Euclidean metric. From Lemma B.30, any limit point y for the Euclidean metric is also an limit point for the Agmon distance, and thus, since $\left(\overline{\Omega}, d_a\right)$ is a separated space, $y = x$. This concludes the proof. ∎

Notice that from the proof, it is obvious that the topology is separated as soon as f and $f|_{\partial\Omega}$ have a finite number of critical points, which is a weaker assumption than **[H1]**.

Finally, the following lemma will be useful in the following.

Lemma B.32. *Assume that **[H3]** holds. Let $I \subset \mathbb{R}$ be an interval and $\gamma : I \to \overline{\Omega}$ a Lipschitz curve such that $\partial\{t \in I,\ \gamma(t) \in \partial\Omega\}$ is finite and such that $x := \lim_{t\to(\inf I)^+} \gamma(t)$ and $y := \lim_{t\to(\sup I)^-} \gamma(t)$ exist. Then one has*

$$d_a(x,y) \leq L(\gamma, I).$$

Proof. Let $(a,b) \in I^2$ with $a < b$ and define for $u \in [0,1]$, $\gamma_{ab}(u) = \gamma(a + u(b-a))$. Then $\gamma_{ab} \in A(\gamma(a),\gamma(b))$. By definition of the Agmon distance (see Definition B.3), $d_a(a,b) \leq L(\gamma_{ab},(0,1)) = L(\gamma,(a,b))$. Taking the limits $a \to (\inf I)^+$, $b \to (\sup I)^-$ and using the continuity of the Agmon distance, one obtains that $d_a(x,y) \leq L(\gamma, I)$. Lemma B.32 is proved. ∎

As a simple consequence of this lemma, we have the following simple remark.

Remark B.6. *Let x^* be a local minimum of f (from **[H3]**, $x^* \in \Omega$). Then, for all x in the basin of attraction of x^* for the dynamics*

$$\gamma' = \begin{cases} -\nabla f(\gamma) \text{ in } \Omega \\ -\nabla_T f(\gamma) \text{ on } \partial\Omega \end{cases} \tag{B.86}$$

it holds $x \in \Omega$ and

$$d_a(x^*,x) = f(x) - f(x^*). \tag{B.87}$$

Indeed, from (B.79)*, we already have $d_a(x^*,x) \geq f(x) - f(x^*)$. To prove the reverse inequality, from Lemma B.32, it is enough to exhibit a Lipschitz curve $\gamma : I \to \overline{\Omega}$ such*

that $\partial\{t \in I,\ \gamma(t) \in \partial\Omega\}$ *is finite,* $L(\gamma, I) = f(x) - f(x^*)$ *and* $\lim_{t\to(\inf I)^+} \gamma(t) = x^*$ *and* $\lim_{t\to(\sup I)^-} \gamma(t) = x$*. Such a curve is given on the interval* $I = [0, \infty)$ *by considering the solution to* (B.86) *with initial condition* $\gamma(0) = x$*. Notice that if* $\exists t_0$ *such that* $\gamma(t_0) \in \partial\Omega$*, then* $\forall t \geq t_0$*,* $\gamma(t) \in \partial\Omega$*. Thus, since* $\lim_{t\to+\infty} \gamma(t) = x^* \in \Omega$*, one has: for all* $t \geq 0, \gamma(t) \in \Omega$*. Therefore,*

$$\begin{aligned} f(x^*) - f(x) &= \int_0^{+\infty} \frac{d}{dt} f \circ \gamma(t)\, dt = \int_0^{+\infty} \nabla f(\gamma(t)) \cdot \gamma'(t)\, dt = -\int_0^{+\infty} |\nabla f(\gamma(t))|^2 dt \\ &= -\int_0^{+\infty} |\nabla f(\gamma(t))| \left|\gamma'(t)\right| dt = -\int_0^{+\infty} g\left(\gamma(t)\right) \left|\gamma'(t)\right| dt \\ &= -\lim_{t\to+\infty} L(\gamma, (0, t)). \end{aligned}$$

This concludes the proof of (B.87)*.*

Notice that for $\varepsilon > 0$ *small enough, the set* $f^{-1}\left([f(x^*), f(x^*) + \varepsilon)\right) \cap B(x^*, \varepsilon) \subset \Omega$ *is a neighborhood of* x^* *which is included in the basin of attraction of* x^* *for the dynamics* (B.86)*. Therefore* (B.87) *holds in a neighborhood of* x^**.*

B.3.2.2 A lower bound on the Agmon distance

In this section, easily computable lower bounds on the Agmon distance are provided. This is in particular useful to check if the hypothesis (B.20) appearing in Theorem B.1 is satisfied, see for example Section B.1.6.2.

Proposition B.33. *Let* $z \in \overline{\Omega}$ *and denote by* W *and* W' *two closed neighborhoods of* z *in* $\overline{\Omega}$ *with* $W \subset W'$*. Define*

$$\alpha := \inf\{d_e\left(x, y\right),\, x \in \overline{\Omega} \setminus W',\, y \in W\}, \tag{B.88}$$

where d_e *denotes the geodesic distance for the Euclidean metric, see* (B.85)*. Assume that* $\alpha > 0$ *and that there exists* $K > 0$ *such that*

$$\inf_{x \in \overline{W' \setminus W}} g(x) > \frac{K}{\alpha},$$

where g *has been introduced in Definition B.2. Then, for all set* $B \subset \overline{\Omega}$ *such that* $B \cap \overline{W'} = \emptyset$*,*

$$\inf_{y \in B} d_a(z, y) > K,$$

where d_a *is the Agmon distance (see Definition B.3).*

Proof. By assumption, there exists $\varepsilon > 0$ such that

$$\inf_{x \in \overline{W' \setminus W}} g(x) \geq \frac{K}{\alpha} + \varepsilon.$$

Let $y \in B$ and $\gamma \in \mathrm{Lip}(z, y)$. Let us define

$$t_2 = \inf\{t \in [0, 1],\, \gamma(t) \notin W'\},\ t_1 = \sup\{t \in [0, 1],\, t < t_2,\, \gamma(t) \in W\}.$$

Since γ is continuous and $\alpha > 0$, it holds $0 < t_1 < t_2 < 1$ and one has $\gamma(t) \in \overline{W' \setminus W}$ for all $t \in [t_1, t_2]$, $\gamma(t_1) \in \overline{W} = W$ and $\gamma(t_2) \in \overline{\overline{\Omega} \setminus W'}$. Then, one has:

$$\begin{aligned}\int_0^1 g(\gamma(t)) \left|\gamma'(t)\right| dt &\geq \int_{t_1}^{t_2} g(\gamma(t)) \left|\gamma'(t)\right| dt \\ &\geq \left(\frac{K}{\alpha} + \varepsilon\right) \int_{t_1}^{t_2} \left|\gamma'(t)\right| dt \\ &\geq \left(\frac{K}{\alpha} + \varepsilon\right) \alpha = K + \varepsilon\alpha.\end{aligned}$$

Since $\varepsilon\alpha$ is independent of $y \in B$ and since $\varepsilon\alpha$ is also independent of the curve γ, one can take the infimum over γ and $y \in B$. Thus $\inf_{y \in B} d_a(z, y) > K$. ∎

We now give a simple sufficient condition for the hypotheses (B.20) to hold, in the case where $f|_{\partial\Omega}$ has only two local minima. This result is based on Proposition B.49 that will be proven in Section B.3.4.3 below and which shows that

$$d_a(z_1, z_2) > f(z_2) - f(z_1).$$

In particular, the condition stated in the following proposition has been used in Section B.1.6.2 in order to check hypothesis (B.20).

Proposition B.34. *Assume that **[H1]** and **[H3]** hold and assume in addition that $f|_{\partial\Omega}$ has only two local minima z_1 and z_2 (with $f(z_1) \leq f(z_2)$) on $\partial\Omega$. Then, if z_2 is the only global minimum of $f|_{\partial\Omega}$ on $B_{z_1}^c$, one has*

$$\inf_{z \in B_{z_1}^c} d_a(z_1, z) > f(z_2) - f(z_1).$$

Proof. Proposition B.49 and the continuity of the Agmon distance ensure that there exist an open ball $B_2 \subset B_{z_1}^c$ centered at z_2, and $\varepsilon > 0$ such that for all $z \in B_2$

$$d_a(z_1, z) \geq f(z_2) - f(z_1) + \varepsilon.$$

Since z_2 is the only global minimum of $f|_{\partial\Omega}$ on $B_{z_1}^c$, there exists $\varepsilon' > 0$, such that for all $z \in B_{z_1}^c \setminus B_2$, $f(z) \geq f(z_2) + \varepsilon'$. In addition, from the inequality (B.79), for all $z \in B_{z_1}^c \setminus B_2$, it holds

$$d_a(z_1, z) \geq f(z) - f(z_1) \geq f(z_2) - f(z_1) + \varepsilon'.$$

Consequently $\inf_{z \in B_{z_1}^c} d_a(z_1, z) > f(z_2) - f(z_1)$. ∎

B.3.3 Agmon distance near critical points of f or $f|_{\partial\Omega}$ and eikonal equation

We will show that the Agmon distance d_a locally solves the eikonal equation in a neighborhood of any critical point of $f|_{\partial\Omega}$ or f (or equivalently, any point x such that $g(x) = 0$, see (B.17)).

B.3.3.1 The Agmon distance near critical points of f

Proposition B.35. *Let us assume that **[H1]** holds. Let $x^* \in \Omega$ be such that $\nabla f(x^*) = 0$. Let us denote by $(\mu_1, \dots, \mu_d) \in (\mathbb{R}^*)^d$ the eigenvalues of the Hessian of f at x^*. Then there exist a neighborhood V^* of x^* in Ω and a C^∞ function $\Phi : V^* \to \mathbb{R}$ such that*

$$\begin{cases} |\nabla \Phi|^2 = |\nabla f|^2, \\ \Phi(x_1, \dots, x_d) = \displaystyle\sum_{i=1}^{d} |\mu_i| \, (x_i - x_i^*)^2 + O\left(|x - x^*|^3\right). \end{cases} \tag{B.89}$$

Moreover, one has the following uniqueness result: if $\widetilde{\Phi}$ is a C^∞ real valued function defined on a neighborhood $\widetilde{V^*}$ of x^* satisfying (B.89)*, then $\widetilde{\Phi} = \Phi$ on $V^* \cap \widetilde{V^*}$.*

Let us notice that $\Phi(x^*) = 0$. In addition, up to choosing a smaller neighborhood V^* of x^*, one can assume that Φ is positive on $V^* \setminus \{x^*\}$. The point x^* is then a non degenerate minimum of Φ.

Proof. The proof is made in [31, Proposition 2.3.6] in the more general setting where $|\nabla f|^2$ is replaced in (B.89) by a smooth positive function W around a non degenerate minimum y^* of W such that $W(y^*) = 0$. Here $W = |\nabla f|^2$ and $y^* = x^*$. This leads to $\nabla W = 2\mathrm{Hess} f \, (\nabla f)$ and thus $\mathrm{Hess} W(x^*) = 2 \, (\mathrm{Hess} f)^2 \, (x^*)$ is a non degenerate matrix. Therefore x^* is indeed a non degenerate minimum of $W = |\nabla f|^2$. ∎

Proposition B.36. *Let us assume that **[H1]** and **[H3]** hold. Let $x^* \in \Omega$ be such that $\nabla f(x^*) = 0$. Then there exists a neighborhood U^* of x^* in Ω such that for all $x \in U^*$*

$$d_a(x^*, x) = \Phi(x), \tag{B.90}$$

where Φ is the smooth solution of (B.89) and d_a is the Agmon distance.

Proof. Notice that hypothesis **[H3]** allows us to use Corollary B.28. Let Φ be a smooth solution of (B.89) on a neighborhood V^* of x^*, as defined in Proposition B.35 and such that Φ is positive on $V^* \setminus \{x^*\}$. There exists $\varepsilon > 0$ such that $U^* := \Phi^{-1}([0, \varepsilon)) \subset V^*$ is a neighborhood of x^* (consider for example $\varepsilon = \inf \{\Phi(x), x \in V^* \setminus B(x^*, r)\} > 0$ where $r > 0$ is such that $B(x^*, 2r) \subset V^*$).

Let us first prove that for $x \in U^*$, $\Phi(x) \leq d_a(x, x^*)$. For $x \in U^*$, one has $\Phi(x) < \varepsilon$ and thus $\Phi^{-1}([0, \Phi(x))) \subset U^*$. Let γ belong to $A\,(x^*, x)$. Let us define the time $t_0 := \inf \left\{t \in [0, 1],\ \gamma(t) \notin \Phi^{-1}([0, \Phi(x)))\right\}$. By continuity of the curve γ, one has $t_0 > 0$, $\Phi(\gamma(t_0)) = \Phi(x)$ and for all $t \in [0, t_0)$, $\gamma(t) \in \Phi^{-1}([0, \Phi(x))) \subset U^*$. Thus, since the curve γ is Lipschitz and since for all $t \in [0, t_0)$, $\gamma(t) \in \Omega$, one has

$$\begin{aligned} \Phi(x) &= \int_0^{t_0} \frac{d}{dt} \Phi(\gamma)(t) \, dt = \int_0^{t_0} \nabla \Phi(\gamma(t)) \cdot \gamma'(t) \, dt \\ &\leq \int_0^{t_0} |\nabla \Phi(\gamma(t))| \left|\gamma'(t)\right| \, dt \\ &\leq \int_0^{t_0} |\nabla f(\gamma(t))| \left|\gamma'(t)\right| \, dt \leq \int_0^1 g\,(\gamma(t)) \left|\gamma'(t)\right| \, dt = L\,(\gamma, (0, 1)). \end{aligned}$$

Taking the infimum on the right-hand side over $\gamma \in A(x^*, x)$, one gets $\Phi(x) \leq d_a(x^*, x)$, for all $x \in U^*$. Let us now prove the reverse inequality: for $x \in U^*$, $\Phi(x) \geq d_a(x, x^*)$. For $x \in U^*$, let us define a curve $\gamma : \mathbb{R}_+ \to U^*$ by

$$\forall t \geq 0,\ \gamma'(t) = -\nabla\Phi(\gamma(t)) \text{ and } \gamma(0) = x.$$

Since the function $t \mapsto \Phi(\gamma(t))$ is decreasing, the curve γ always belongs to U^* and is defined on $\mathbb{R}_+$. Moreover γ is C^∞ and satisfies

$$\lim_{t\to+\infty} \gamma(t) = x^*.$$

Since γ is with values in $U^* \subset \Omega$, one has

$$\begin{aligned}
-\Phi(x) &= \int_0^{+\infty} \frac{d}{dt}\Phi \circ \gamma(t)\, dt = \int_0^{+\infty} \nabla\Phi(\gamma(t)) \cdot \gamma'(t)\, dt = -\int_0^{+\infty} |\nabla\Phi(\gamma(t))|^2 dt \\
&= -\int_0^{+\infty} |\nabla\Phi(\gamma(t))| \left|\gamma'(t)\right| dt = -\int_0^{+\infty} g(\gamma(t)) \left|\gamma'(t)\right| dt = -\lim_{t\to+\infty} L(\gamma, (0,t)).
\end{aligned}$$

Thanks to Lemma B.32,

$$d_a(x, x^*) \leq L(\gamma, (0, +\infty)) = \Phi(x).$$

Therefore $\Phi(x) = d_a(x^*, x)$ for all $x \in U^*$. ∎

Remark B.7. *Let us mention a simple consequence of the previous proof that will be useful in the following. If $x^* \in \Omega$ is such that $\nabla f(x^*) = 0$, there exists a neighborhood U^* of x^* in Ω such that for all $x \in U^*$, there exists a C^∞ curve $\gamma : \mathbb{R}_+ \to \Omega$ such that*

$$d_a(x^*, x) = \int_0^{+\infty} |\nabla f(\gamma(t))| \left|\gamma'(t)\right| dt,$$

with $\gamma(0) = x$ and $\lim_{t\to+\infty} \gamma(t) = x^*$. The curve γ is defined by

$$\gamma'(t) = -\nabla\Phi(\gamma(t)), \quad \gamma(0) = x,$$

where Φ solves (B.89). In addition $\{t \in [0, \infty),\ \gamma(t) \in \partial\Omega\}$ is empty.

B.3.3.2 The Agmon distance near critical points of $f|_{\partial\Omega}$

Let us first define the Agmon distance in the boundary $\partial\Omega$.

Definition B.7. *The Agmon distance between $x \in \partial\Omega$ and $y \in \partial\Omega$ in the boundary $\partial\Omega$ is defined by*

$$d_a^{\partial\Omega}(x, y) = \inf_\gamma \int_0^1 |\nabla_T f(\gamma(t))| \left|\gamma'(t)\right| dt, \tag{B.91}$$

where the infimum is taken over all the paths $\gamma : [0, 1] \to \partial\Omega$ which are Lipschitz with $\gamma(0) = x$ and $\gamma(1) = y$.

Similarly to Remark B.6, one has:

Remark B.8. *If x^* is a local minimum of $f|_{\partial\Omega}$, one has $d_a^{\partial\Omega}(x^*, x) = f(x) - f(x^*)$ for all $x \in \partial\Omega$ which is in the basin of attraction of x^* in $\partial\Omega$ for the gradient dynamics $\gamma' = -\nabla_T f(\gamma)$.*

The next proposition is the equivalent of Proposition B.36 for that Agmon distance in $\partial\Omega$. Since $\partial\Omega$ is a smooth manifold without boundary, the next result is a direct consequence of well known results from [30], [19] and [22].

Proposition B.37. *Let us assume that **[H1]** holds. Let $x^* \in \partial\Omega$ be such that $\nabla_T f(x^*) = 0$. Then there exists a neighborhood U^* of x^* in $\partial\Omega$ such that $y \mapsto d_a^{\partial\Omega}(x^*, y)$ is smooth on U^* and $\forall x \in U^*$,*

$$\left|\nabla_T d_a^{\partial\Omega}(x^*, x)\right|^2 = |\nabla_T f(x)|^2. \tag{B.92}$$

Proof. The boundary $\partial\Omega$ is a C^∞ compact manifold and x^* is a non degenerate minimum of $|\nabla_T f|^2$. The proof is made in [31, Proposition 2.3.6] in the more general setting where $|\nabla_T f|^2$ is replaced in (B.92) and in (B.91) by a smooth non negative function W around a non degenerate minimum y^* of W such that $W(y^*) = 0$. Here $W = |\nabla_T f|^2$ and $y^* = x^*$. This leads to $\nabla W = 2\,\mathrm{Hess}\,(f|_{\partial\Omega})\,(\nabla_T f)$ and therefore x^* is a critical point of $W = |\nabla_T f|^2$ (which turns out to be a minimum). In addition, since $\nabla_T f(x^*) = 0$, one gets that $\mathrm{Hess} W(x^*) = 2\,(\mathrm{Hess}\,(f|_{\partial\Omega}))^2\,(x^*)$ which is a non degenerate matrix. ∎

Proposition B.38. *Let us assume that **[H1]** and **[H3]** hold. Let $x^* \in \partial\Omega$ be such that $\nabla_T f(x^*) = 0$. Then there exist a neighborhood V^* of x^* in $\overline{\Omega}$ and a C^∞ function $\Phi : V^* \to \mathbb{R}$ such that*

$$\begin{cases} |\nabla\Phi|^2 = |\nabla f|^2 \text{ in } \Omega \cap V^*, \\ \quad \Phi = d_a^{\partial\Omega}(x^*, .) \text{ on } \partial\Omega \cap V^*, \\ \partial_n \Phi < 0 \text{ on } \partial\Omega \cap V^*. \end{cases} \tag{B.93}$$

Moreover, one has the following uniqueness results: if $\widetilde{\Phi}$ is a C^∞ real valued function defined on a neighborhood $\widetilde{V^*}$ of x^* satisfying (B.93)*, then $\widetilde{\Phi} = \Phi$ on $\widetilde{V^*} \cap V^*$.*

Finally, up to choosing a smaller neighborhood V^* of x^*, one can assume that Φ is positive on $V^* \setminus \{x^*\}$, so that x^* is a non degenerate minimum of Φ on V^*.

Proof. From Proposition B.37, the function $x \in \partial\Omega \mapsto d_a^{\partial\Omega}(x^*, x)$ is smooth near x^*. Then, the result stated can be proven using the method of characteristics, see [19, Theorem 1.5] or [22, Section 3.2]. Let us mention that the proof crucially relies on the assumption $\partial_n f(x^*) > 0$. The fact that one can reduce V^* such that Φ is positive on $V^* \setminus \{x^*\}$ is a consequence of $\partial_n \Phi < 0$ on $\partial\Omega \cap V^*$ together with the fact that x^* is the only minimum of $d_a^{\partial\Omega}(x^*, .)$ (which is positive on $\partial\Omega \setminus \{x^*\}$). ∎

Let us state a simple corollary of Proposition B.38 and Remark B.8.

Corollary B.39. *Let us assume that **[H1]** and **[H3]** hold. Let $x^* \in \partial\Omega$ be a local minimum of $f|_{\partial\Omega}$. Then there exist a neighborhood V^* of x^* in $\overline{\Omega}$ and a C^∞ function $\Phi : V^* \to \mathbb{R}$ such that*

$$\begin{cases} |\nabla\Phi|^2 = |\nabla f|^2 \text{ in } \Omega \cap V^*, \\ \quad \Phi = f - f(x^*) \text{ on } \partial\Omega \cap V^*, \\ \partial_n \Phi < 0 \text{ on } \partial\Omega \cap V^*. \end{cases} \tag{B.94}$$

Moreover, one has the following uniqueness results: if $\widetilde{\Phi}$ is a C^∞ real valued function defined on a neighborhood $\widetilde{V^*}$ of x^* satisfying (B.93)*, then $\widetilde{\Phi} = \Phi$ on $\widetilde{V^*} \cap V^*$.*

Finally, up to choosing a smaller neighborhood V^* of x^*, one can assume that Φ is positive on $V^* \setminus \{x^*\}$, and that $\Phi - f > -f(x^*)$ in $V^* \cap (\partial\Omega)^c$. As a consequence,

$$\{x \in V^*,\, \Phi(x) = f(x) - f(x^*)\} \subset \partial\Omega. \tag{B.95}$$

Proof. All the statements but (B.95) are direct consequences of Proposition B.38 and the fact that $d_a^{\partial\Omega}(x^*, x) = f(x) - f(x^*)$, thanks to Remark B.8. Now, notice that on $\partial\Omega \cap V^*$, $\Phi - f = -f(x^*)$ and $\partial_n(\Phi - f) < 0$ so that, up to choosing a smaller neighborhood V^* of x^*, one can assume that $\Phi - f > -f(x^*)$ in $V^* \cap (\partial\Omega)^c$. This concludes the proof of (B.95). ∎

We are now in position to state the main result of this section.

Proposition B.40. *Let us assume that **[H1]** and **[H3]** hold. Let $x^* \in \partial\Omega$ be such that $\nabla_T f(x^*) = 0$. Then there exists a neighborhood U^* of x^* in $\overline{\Omega}$ such that for all $x \in U^*$*

$$d_a\,(x, x^*) = \Phi(x),$$

where Φ solves (B.93) and d_a is the Agmon distance.

Proof. Notice that hypothesis **[H3]** allows us to use Corollary B.28. The proof is similar to the one of Proposition B.36. Let $x^* \in \partial\Omega$ be such that $\nabla_T f(x^*) = 0$. Let Φ be the smooth solution of (B.93) on a neighborhood V^* of x^* and such that Φ is positive on $V^* \setminus \{x^*\}$, as defined in Proposition B.38. One chooses $\varepsilon > 0$ sufficiently small such that $U^* := \Phi^{-1}([0, \varepsilon)) \subset V^*$ is a neighborhood of x^* in $\overline{\Omega}$.

Step 1. Let us first prove that for all $x \in U^*$, $\Phi(x) \le d_a(x^*, x)$. For $x \in U^*$, one has $\Phi(x) < \varepsilon$ and thus $\Phi^{-1}([0, \Phi(x))) \subset U^*$. Let γ belong to $A\,(x^*, x)$. Let us define the time $t_0 := \inf\left\{t \in [0,1],\ \gamma(t) \notin \Phi^{-1}([0, \Phi(x)))\right\}$. By continuity of the curve γ, one has $t_0 > 0$, $\Phi(\gamma(t_0)) = \Phi(x)$ and for all $t \in [0, t_0)$, $\gamma(t) \in \Phi^{-1}([0, \Phi(x))) \subset U^*$. Thus, using Lemma B.25, one obtains

$$\begin{aligned}\Phi(x) &= \int_0^{t_0} \frac{d}{dt}\Phi \circ \gamma(t)\, dt = \int_0^{t_0} \nabla\Phi(\gamma(t)) \cdot \gamma'(t)\, dt \\ &= \int_{\mathrm{int}\{t\in(0,t_0),\ \gamma(t)\in\partial\Omega\}} \nabla_T\Phi(\gamma(t)) \cdot \gamma'(t)\, dt + \int_{\{t\in(0,t_0),\ \gamma(t)\in\Omega\}} \nabla\Phi(\gamma(t)) \cdot \gamma'(t)\, dt.\end{aligned}$$

On the one hand,

$$\begin{aligned}\int_{\mathrm{int}\{t\in(0,t_0),\ \gamma(t)\in\partial\Omega\}} \nabla_T\Phi(\gamma(t)) \cdot \gamma'(t)\, dt &= \int_{\mathrm{int}\{t\in(0,t_0),\ \gamma(t)\in\partial\Omega\}} \nabla_T d_a^{\partial\Omega}(x^*, \gamma(t)) \cdot \gamma'(t)\, dt \\ &\le \int_{\mathrm{int}\{t\in(0,t_0),\ \gamma(t)\in\partial\Omega\}} \left|\nabla_T d_a^{\partial\Omega}\,(x^*, \gamma(t))\right| \left|\gamma'(t)\right|\, dt \\ &\le \int_{\mathrm{int}\{t\in(0,t_0),\ \gamma(t)\in\partial\Omega\}} |\nabla_T f(\gamma(t))| \left|\gamma'(t)\right|\, dt,\end{aligned}$$

where one used the relations (B.93) and (B.92). On the other hand, using (B.93), one obtains

$$\int_{\{t\in(0,t_0),\ \gamma(t)\in\Omega\}} \nabla\Phi(\gamma(t))\cdot\gamma'(t)\,dt \le \int_{\mathrm{int}\{t\in(0,t_0),\ \gamma(t)\in\Omega\}} |\nabla\Phi(\gamma(t))|\left|\gamma'(t)\right|\,dt$$
$$\le \int_{\mathrm{int}\{t\in(0,t_0),\ \gamma(t)\in\Omega\}} |\nabla f(\gamma(t))|\left|\gamma'(t)\right|\,dt.$$

Thus one gets

$$\Phi(x) \le \int_{\mathrm{int}\{t\in(0,t_0),\ \gamma(t)\in\partial\Omega\}} |\nabla_T f(\gamma(t))|\left|\gamma'(t)\right|\,dt + \int_{\{t\in(0,t_0),\ \gamma(t)\in\Omega\}} |\nabla f(\gamma(t))|\left|\gamma'(t)\right|\,dt$$
$$= \int_0^{t_0} g\left(\gamma(t)\right)\left|\gamma'(t)\right|\,dt \le \int_0^1 g\left(\gamma(t)\right)\left|\gamma'(t)\right|\,dt = L\left(\gamma,(0,1)\right).$$

Taking the infimum on the right-hand side over $\gamma\in A\left(x^*,x\right)$, one gets $\Phi(x)\le d_a\left(x^*,x\right)$, for all $x\in U^*$.

Step 2. Let us now prove the reverse inequality: $\forall x\in U^*$, $d_a(x,x^*)\le\Phi(x)$ Let us define the following vector field on U^*

$$X := \begin{cases} -\nabla\Phi \text{ in } \Omega\cap U^*, \\ -\nabla_T\Phi \text{ on } \partial\Omega\cap U^*. \end{cases} \tag{B.96}$$

For $x\in U^*$, let us define the curve γ by

$$\forall t\ge 0,\ \gamma'(t) = X\left(\gamma(t)\right) \text{ and } \gamma(0)=x. \tag{B.97}$$

Since the function $t\mapsto\Phi\left(\gamma(t)\right)$ is decreasing, the curve γ always belongs to U^* and is defined on $\mathbb{R}_+$. If there exists a time t_0 such that $\gamma(t_0)\in\partial\Omega$, then, for all $t\ge t_0$, $\gamma(t)\in\partial\Omega$. The function γ is piecewise C^∞, continuous and satisfies

$$\lim_{t\to+\infty}\gamma(t) = x^*.$$

Let us define $t_{\partial\Omega}=\inf\left\{t\in[0,+\infty),\ \gamma(t)\in\partial\Omega\right\}\in[0,\infty]$. One has

$$\begin{aligned}
-\Phi(x) &= \int_0^{+\infty}\frac{d}{dt}\Phi\circ\gamma(t)\,dt \\
&= \int_0^{t_{\partial\Omega}}\nabla\Phi(\gamma(t))\cdot\gamma'(t)\,dt + \int_{t_{\partial\Omega}}^{+\infty}\nabla_T\Phi(\gamma(t))\cdot\gamma'(t)\,dt \\
&= -\left(\int_0^{t_{\partial\Omega}}|\nabla\Phi(\gamma(t))|^2dt + \int_{t_{\partial\Omega}}^{+\infty}|\nabla_T\Phi(\gamma(t))|^2dt\right) \\
&= -\left(\int_0^{t_{\partial\Omega}}|\nabla\Phi(\gamma(t))|\left|\gamma'(t)\right|\,dt + \int_{t_{\partial\Omega}}^{+\infty}|\nabla_T\Phi(\gamma(t))|\left|\gamma'(t)\right|\,dt\right) \\
&= -\int_0^{+\infty} g\left(\gamma(t)\right)\left|\gamma'(t)\right|\,dt = -\lim_{t\to+\infty}L(\gamma,(0,t)).
\end{aligned}$$

Thanks to Lemma B.32,

$$d_a\left(x,x^*\right)\le L(\gamma,(0,+\infty)) = \Phi(x).$$

In conclusion, $\Phi(x)=d_a\left(x^*,x\right)$ for all $x\in U^*$. ∎

Remark B.9. *Let us mention a simple consequence of the previous proof that will be useful in the following. If $x^* \in \partial\Omega$ is such that $\nabla_T f(x^*) = 0$, there exists a neighborhood U^* of x^* such that for all $x \in U^*$, there exists a piecewise C^∞ and continuous curve $\gamma : \mathbb{R}_+ \to \overline{\Omega}$ such that*

$$d_a(x^*, x) = \int_0^{+\infty} g\left(\gamma(t)\right) \left|\gamma'(t)\right| \, dt,$$

with $\gamma(0) = x$ and $\lim_{t\to+\infty} \gamma(t) = x^*$. In addition $\partial\{t \in [0,\infty),\ \gamma(t) \in \partial\Omega\}$ either consists of one point or is empty.

B.3.4 Curves realizing the Agmon distance

In this section, it is proven that for any two points $x \in \overline{\Omega}$ and $y \in \overline{\Omega}$, their exists a finite number of curves $(\gamma_i)_{i=1,\dots,N}$ such that the sum of their lengths equals the Agmon distance $d_a(x, y)$. The precise statement is given in the following theorem.

Theorem B.3. *Assume that **[H1]** and **[H3]** hold. Let $x, y \in \overline{\Omega}$. Then there exists a finite number of Lipschitz curves $(\gamma_j)_{j=1,\dots,N}$ which are defined on possibly unbounded intervals $I_j \subset \mathbb{R}$, with values in $\overline{\Omega}$, such that for all $j \in \{1, \dots, N\}$, the sets $\partial\{t \in I_j,\ \gamma_j(t) \in \partial\Omega\}$ are finite and*

$$d_a(x, y) = \sum_{j=1}^{N} L\left(\gamma_j, I_j\right).$$

Additionally, by construction, the intervals $(I_j)_{j\in\{1,\dots,N\}}$ are either $[0 + \infty)$, $(-\infty, 0]$ or $[0, 1]$. Moreover, if $I_j = [0, +\infty)$ or $I_j = (-\infty, 0]$, then γ_j is continuous and piecewise C^∞. If $I_j = [0, 1]$, then $\gamma_j \in A(\gamma_j(0), \gamma_j(1))$. Finally the curves $((\gamma_1, I_1), \dots, (\gamma_N, I_N))$ are ordered such that

$$\lim_{t\to(\inf I_1)^+} \gamma_1(t) = x, \qquad \lim_{t\to(\sup I_N)^-} \gamma_N(t) = y,$$

and for all $k \in \{1, \dots, N-1\}$,

$$\lim_{t\to(\sup I_k)^-} \gamma_k(t) = \lim_{t\to(\inf I_{k+1})^+} \gamma_{k+1}(t).$$

This section is entirely dedicated to the proof of Theorem B.3. In the following, one denotes by

$$\{x_1, \dots, x_m\} = \{x \in \overline{\Omega},\ g(x) = 0\},$$

where g is defined by (B.17) (there is a finite number of zeros of g thanks to **[H1]**).

B.3.4.1 Preliminary results

Let us first consider the simple case when the curve realizing the Agmon distance does not meet zeros of g.

Lemma B.41. *Assume that **[H1]** and **[H3]** hold. Let $(x,y) \in \overline{\Omega} \times \overline{\Omega}$. Let $(\gamma_n)_{n\geq 0} \in A(x,y)^{\mathbb{N}}$ be a minimizing sequence of curves for $d_a(x,y)$: $\lim_{n\to\infty} L(\gamma_n,(0,1)) = d_a(x,y)$. In addition, assume that for each $k \in \{1,\dots,m\}$, there exists a neighborhood V_k of x_k in $\overline{\Omega}$, such that:*

$$\forall n \in \mathbb{N},\ \forall k \in \{1,\dots,m\},\ \mathbb{R}an(\gamma_n) \cap V_k = \emptyset.$$

Then, there exists $\gamma \in A(x,y)$ such that

$$L(\gamma,(0,1)) = d_a(x,y).$$

Proof. Let M be such that for all n, $L(\gamma_n,(0,1)) \leq M$ and let us define

$$c := \inf_{\overline{\Omega}\setminus(V_1\cup\dots\cup V_m)} g > 0.$$

One defines for $t \in [0,1]$, $\phi_n(t) = \frac{L(\gamma_n,(0,t))+t}{L(\gamma_n,(0,1))+1}$. The map ϕ_n is strictly increasing and continuous from $[0,1]$ to $[0,1]$. Therefore it admits an inverse. Setting $\tilde{\gamma}_n(u) := \gamma_n \circ \phi_n^{-1}(u)$, one gets $L(\gamma_n,(0,1)) = L(\tilde{\gamma}_n,(0,1))$ and

$$\begin{aligned}
\left|\tilde{\gamma}_n'\right|(\phi_n(t)) &= \frac{|\gamma_n'(t)|}{g(\gamma_n(t))\ |\gamma_n'(t)|+1}\ (L(\gamma_n,(0,1))+1) \\
&\leq \frac{|\gamma_n'(t)|}{c\ |\gamma_n'(t)|+1}\ (L(\gamma_n,(0,1))+1) \\
&\leq \frac{1}{c}\,(L(\gamma_n,(0,1))+1) \\
&\leq \frac{1}{c}\,(M+1).
\end{aligned}$$

Thus, up to replacing γ_n by $\tilde{\gamma}_n$, one may assume that the Lipchitz constants of γ_n are bounded uniformly in n. In addition since for all $t \in [0,1]$, $\gamma_n(t) \in \overline{\Omega}$, the sequence $(\gamma_n)_{n\geq 0}$ is relatively compact in $C^0([0,1],\overline{\Omega})$. Thus, up to the extraction of a subsequence, there exists a Lipschitz curve γ such that $\lim_{n\to\infty}\gamma_n = \gamma$ uniformly on $[0,1]$. Moreover since $(\gamma_n)_{n\geq 0}$ is bounded in $H^1([0,1],\overline{\Omega})$, up to the extraction of a subsequence, $(\gamma_n)_{n\geq 0}$ converges weakly to γ in $H^1([0,1],\overline{\Omega})$. It is not difficult to see that for all $t \in [0,1]$,

$$\liminf_{n\to\infty} g(\gamma_n(t)) \geq g(\gamma(t)).$$

Indeed, for $t \in [0,1]$, there are two cases:

- if $\gamma(t) \in \Omega$, then for n large enough, all the points $\gamma_n(t)$ are in Ω and thus $\liminf_{n\to\infty} g(\gamma_n(t)) = \lim_{n\to\infty} g(\gamma_n(t)) = |\nabla f(\gamma(t))| = g(\gamma(t))$,

- if $\gamma(t) \in \partial\Omega$. Since $\mathbb{N} = \{n,\ \gamma_n(t) \in \partial\Omega\} \cup \{n,\ \gamma_n(t) \in \Omega\}$, one obtains that the set of limit points of $(\gamma_n(t))_{n\geq 0}$ is included in $\{|\nabla f(\gamma(t))|, |\nabla_T f(\gamma(t))|\}$. Therefore, from **[H3]**, one has: $\liminf_{n\to\infty} g(\gamma_n(t)) \geq |\nabla_T f(\gamma(t))| = g(\gamma(t))$.

Then, one obtains

$$\begin{aligned} d_a(x,y) = \lim_{l\to\infty} \int_0^1 g(\gamma_l(t))|\gamma_l'(t)|dt &\geq \liminf_{n\to\infty} \liminf_{p\to\infty} \int_0^1 g(\gamma_p(t))|\gamma_n'(t)|dt \\ &\geq \liminf_{n\to\infty} \int_0^1 \liminf_{p\to\infty} g(\gamma_p(t))|\gamma_n'(t)|dt \\ &\geq \liminf_{n\to\infty} \int_0^1 g(\gamma(t))\,|\gamma_n'(t)|dt \\ &\geq \int_0^1 g(\gamma(t))\,|\gamma'(t)|dt. \end{aligned}$$

In the previous computation, one used Fatou Lemma and the lower semi continuity (for the weak convergence) of the convex functional

$$h \in H^1([0,1],\overline{\Omega}) \mapsto \int_0^1 g(\gamma(t))\left|h'(t)\right| dt.$$

Since **[H3]** holds, using Proposition B.27, there exits a curve $\gamma_1 \in A(x,y)$ such that $L(\gamma,(0,1)) \geq L(\gamma_1,(0,1))$ and thus $d_a(x,y) = L(\gamma_1,(0,1))$. ∎

Let us now introduce a sufficient condition so that a minimizing sequence of curves realizing the Agmon distance avoids a neighborhood of a zero of g. For $x \in \overline{\Omega}$, one introduces the following sets:

$$\forall k \in \{1,\dots,m\},\ A_k(x) := \left\{z \in \overline{\Omega},\ d_a(x,z) = d_a(x,x_k) + d_a(x_k,z)\right\}. \tag{B.98}$$

One notices that $z \in A_k(x)$ if and only if $x \in A_k(z)$.

Proposition B.42. *Assume that **[H1]** and **[H3]** hold. Let $(x,y) \in \overline{\Omega}^2$ and assume that there exists $k \in \{1,\dots,m\}$ such that $y \notin A_k(x)$. If $(\gamma_n)_{n\geq 0} \in A(x,y)^{\mathbb{N}}$ is a minimizing sequence of curves for $d_a(x,y)$, then there exists a neighborhood V_k of x_k in $\overline{\Omega}$ and $n_0 \in \mathbb{N}$, such that for all $n \geq n_0$,*

$$\mathbb{R}an(\gamma_n) \cap V_k = \emptyset.$$

Proof. If $y \notin A_k(x)$, for a $k \in \{1,\dots,m\}$, then $d_a(x,y) < d_a(x,x_k) + d_a(x_k,y)$ and thus $y \neq x_k$ and $x \neq x_k$. Let us define

$$\varepsilon := d_a(x,x_k) + d_a(x_k,y) - d_a(x,y) > 0,$$

and $V_k := B_a\left(x_k, \min\left(\frac{\varepsilon}{3}, \frac{d_a(x_k,y)}{2}\right)\right)$ where

$$\forall z \in \overline{\Omega},\ \forall r > 0,\ B_a(z,r) := \left\{u \in \overline{\Omega},\ d_a(z,u) < r\right\}. \tag{B.99}$$

Notice that $y \notin V_k$. We now prove Proposition B.42 by contradiction. We assume that, up to the extraction of a subsequence, for all $n \in \mathbb{N}$,

$$\mathbb{R}an(\gamma_n) \cap V_k \neq \emptyset,$$

and we define

$$t_0^n := \inf\{t \in [0,1],\ \gamma_n(t) \in V_k\}, \quad t_1^n := \sup\{t \in [0,1],\ \gamma_n(t) \in V_k\}.$$

We have for all $n \in \mathbb{N}$, owing to the triangular inequality,

$$L(\gamma_n, (0, t_0^n)) \geq d_a(x, x_k) - \frac{\varepsilon}{3}, \quad L(\gamma_n, (t_1^n, 1)) \geq d_a(x_k, y) - \frac{\varepsilon}{3}.$$

Thus for all $n \in \mathbb{N}$,

$$\begin{aligned} L(\gamma_n(0,1)) &\geq L(\gamma_n, (0, t_0^n)) + L(\gamma_n, (t_1^n, 1)) \\ &\geq d_a(x, x_k) + d_a(x_k, y) - \frac{2\varepsilon}{3} = d_a(x, y) + \frac{\varepsilon}{3}. \end{aligned}$$

This contradicts the fact that $\lim_{n\to\infty} L(\gamma_n, (0,1)) = d_a(x,y)$. ∎

A direct corollary of Proposition B.42 and Lemma B.41 is the following result:

Corollary B.43. *Assume that **[H1]** and **[H3]** hold. Let $y \in \overline{\Omega}$ and assume that $y \notin A_j(x)$ for all $j \in \{1, \ldots, m\}$. Then there exists a curve $\gamma \in A(x,y)$ such that*

$$d_a(x,y) = L(\gamma, (0,1)).$$

Notice that $y \notin A_j(x)$ for all $j \in \{1, \ldots, m\}$ implies in particular that x and y are not zeros of g. This corollary will be used below to build the curves γ_j associated with intervals $I_j = [0,1]$ in Theorem B.3. The curves γ_j associated with intervals $I_j = [0, +\infty)$ or $I_j = (-\infty, 0]$ with be built using the following lemma, which is a direct consequence of Remarks B.7 and B.9.

Lemma B.44. *Assume that **[H1]** and **[H3]** hold. Let $k \in \{1, \ldots, m\}$. There exists a neighborhood V_k of x_k in $\overline{\Omega}$, such that for all $y \in V_k$, there exists a continuous and piecewise C^∞ curve γ defined on $(-\infty, 0]$ satisfying*

$$d_a(y, x_k) = L(\gamma, (-\infty, 0]), \ \lim_{t\to-\infty} \gamma(t) = x_k,\ \gamma(0) = y.$$

In addition $\partial\{t \in (-\infty, 0],\ \gamma(t) \in \partial\Omega\}$ is either empty or a single point.

Before proving Theorem B.3, we finally need two additional preliminary lemmas.

Lemma B.45. *Assume that **[H1]** and **[H3]** hold. Let $u \in \overline{\Omega}$ and $w \in \overline{\Omega}$. For any $\delta > 0$ small enough, there exists z_δ such that $d_a(u, z_\delta) = \delta$ and $d_a(w,u) = d_a(w, z_\delta) + d_a(z_\delta, u)$.*

Proof. Notice that $d_a(u, z_\delta) = \delta$ is equivalent to $z_\delta \in \partial B_a(u, \delta)$, where B_a is defined by (B.99). We prove Lemma B.45 by contradiction. Assume that there exists $\delta \in \left(0, \frac{d_a(u,w)}{2}\right)$ such that for all $z \in \partial B_a(u, \delta)$,

$$d_a(w,u) < d_a(w,z) + d_a(z,u).$$

By compactness of $\partial B_a(u,\delta)$, there exists $a_\delta > 0$ such that for all $z \in \partial B_a(u,\delta)$,

$$d_a(w,u) + a_\delta \leq d_a(w,z) + d_a(z,u).$$

Thus if $\gamma \in A(u,w)$, since there exists a time t_δ such that $\gamma(t_\delta) \in \partial B_a(u,\delta)$, one has

$$\begin{aligned} L(\gamma,(0,1)) &= L(\gamma,(0,\gamma(t_\delta))) + L(\gamma,(\gamma(t_\delta),1)) \\ &\geq d_a(u,\gamma(t_\delta)) + d_a(\gamma(t_\delta),w) \\ &\geq d_a(u,w) + a_\delta. \end{aligned}$$

This is impossible since by definition $d_a(u,w) = \inf_{\gamma\in A(u,w)} L(\gamma,(0,1))$. ∎

Lemma B.46. *Assume that **[H1]** holds. Let $(x,y) \in \overline{\Omega}^2$ with $x \neq y$. Let us assume that there exists $j \in \{1,\dots,m\}$ such that $y \in A_j(x)$. Then, there exist $N \in \mathbb{N}$ and a sequence $(b_j)_{j\in\{0,\dots,N+1\}} \in \overline{\Omega}^{N+2}$, $b_0 = x$, $b_{N+1} = y$, $(b_j)_{j\in\{1,\dots,N\}} \in \{x_1,\dots,x_m\}^N$ (with the convention $\{x_1,\dots,x_m\}^0 = \emptyset$) such that the following holds:*

1. *For all $i \in \{0,\dots,N\}$, $b_i \neq b_{i+1}$ and*

$$d_a(x,y) = \sum_{i=0}^{N} d_a(b_i,b_{i+1}). \tag{B.100}$$

2. *For all $i \in \{0,\dots,N\}$ and for all $z \in \{x,y,x_1,\dots,x_m\} \setminus \{b_i,b_{i+1}\}$,*

$$d_a(b_i,b_{i+1}) < d_a(b_i,z) + d_a(z,b_{i+1}).$$

Proof. Since $x \neq y$, the following set

$$\begin{aligned} E := \{&(N,b),\ N \in \mathbb{N},\ b = (b_j)_{j\in\{0,\dots,N+1\}} \in \overline{\Omega}^{N+2},\ b_0 = x,\ b_{N+1} = y, \\ &\forall i \in \{0,\dots,N\},\ b_i \neq b_{i+1},\ (b_j)_{j\in\{1,\dots,N\}} \in \{x_1,\dots,x_m\}^N, \text{(B.100) holds}\}, \end{aligned}$$

is not empty since by assumption it contains $(0,\{x,y\})$. For $(N,b) \in E$, one defines the cardinal of (N,b) by the number of different critical points b contains. The cardinal of an element of E belongs to $\{0,\dots,m\}$.

Let us now consider an element $(N,b) \in E$ which is maximal for the cardinal. By construction, this element satisfies point 1 in Lemma B.46. Let us now show that it also satisfies point 2 in Lemma B.46. Notice that $\{b_0,\dots,b_{N+1}\} \subset \{x,y,x_1,\dots,x_m\}$. Let $i \in \{0,\dots,N\}$ and $z \in \{x,y,x_1,\dots,x_m\} \setminus \{b_i,b_{i+1}\}$. If $z \in \{x,y,x_1,\dots,x_m\} \setminus \{b_0,\dots,b_{N+1}\}$, the equality $d_a(b_i,b_{i+1}) = d_a(b_i,z) + d_a(z,b_{i+1})$ cannot hold since b has been chosen maximal in E for the cardinal. Thus, by the triangular inequality $d_a(b_i,b_{i+1}) < d_a(b_i,z) + d_a(z,b_{i+1})$. If $z \in \{b_0,\dots,b_{N+1}\} \setminus \{b_i,b_{i+1}\}$, let us prove that $d_a(b_i,b_{i+1}) < d_a(b_i,z) + d_a(z,b_{i+1})$ by contradiction. By the triangular inequality, if the previous inequality does not hold, one has $d_a(b_i,b_{i+1}) = d_a(b_i,z) + d_a(z,b_{i+1})$ for some $z \in \{b_0,\dots,b_{N+1}\} \setminus \{b_i,b_{i+1}\}$. Let us denote by $j_0 \in \{0,\dots,i-1,i+2,\dots,N+1\}$ the index such that $z = b_{j_0}$. One has $d_a(b_i,b_{i+1}) = d_a(b_i,b_{j_0}) + d_a(b_{j_0},b_{i+1})$. Let us assume without loss of generality that $j_0 < i$ (the case $j_0 > i+1$ is treated similarly). In this

case, one has, using the triangular inequality:

$$\begin{aligned}
d_a(x,y) &= \sum_{j=0}^{N} d_a(b_j,b_{j+1}) \\
&= \sum_{j=0}^{i-1} d_a(b_j,b_{j+1}) + d_a(b_i,b_{j_0}) + d_a(b_{j_0},b_{i+1}) + \sum_{j=i+1}^{N} d_a(b_j,b_{j+1}) \\
&= \sum_{j=0}^{j_0-1} d_a(b_j,b_{j+1}) + d_a(b_{j_0},b_{i+1}) + \sum_{j=i+1}^{N} d_a(b_j,b_{j+1}) + \sum_{j=j_0}^{i-1} d_a(b_j,b_{j+1}) + d_a(b_i,b_{j_0}) \\
&\geq d_a(x,y) + \sum_{j=j_0}^{i-1} d_a(b_j,b_{j+1}) + d_a(b_i,b_{j_0}).
\end{aligned}$$

Thus, $\sum_{j=j_0}^{i-1} d_a(b_j,b_{j+1}) + d_a(b_i,b_{j_0}) = 0$ and $b_{j_0} = b_i$ which is in contradiction with $z \notin \{b_i, b_{i+1}\}$. Therefore $d_a(b_i,b_{i+1}) < d_a(b_i,b_{j_0}) + d_a(b_{j_0},b_{i+1})$. This concludes the proof of Lemma B.46. ∎

B.3.4.2 Proof of Theorem B.3

Let us now prove Theorem B.3. Recall that by assumption, the hypotheses **[H1]** and **[H3]** hold.

Proof. Let $x, y \in \overline{\Omega}$. If $x = y$, then Theorem B.3 is proved by taking the constant curve $\gamma(t) = x$ for all $t \in [0,1]$. Let us deal with the case $x \neq y$. If for all $k \in \{1,\dots,m\}$ $y \notin A_k(x)$, Theorem B.3 is a consequence of Corollary B.43.

Let us now assume that there exists $k \in \{1,\dots,m\}$ such that $y \in A_k(x)$. From Lemma B.46, there exist $N \in \mathbb{N}$ and a sequence $(b_j)_{j\in\{0,\dots,N+1\}} \subset \overline{\Omega}^{N+2}$ such that $b_0 = x$, $b_{N+1} = y$, $(b_j)_{j\in\{1,\dots,N\}} \subset \{x_1,\dots,x_m\}^N$ (with the convention $\{x_1,\dots,x_m\}^0 = \emptyset$) and for all $k \in \{0,\dots,N\}$, $b_k \neq b_{k+1}$ and

$$d_a(x,y) = \sum_{k=0}^{N} d_a(b_k,b_{k+1}). \tag{B.101}$$

Let us deal with the case $N \geq 2$, the cases $N = 0$ and $N = 1$ are treated similarly. Let $k \in \{1,\dots,N-1\}$ and let us consider the term $d_a(b_k,b_{k+1})$ in (B.101) (the first term $d_a(x,b_1)$ and the last term $d_a(b_N,y)$ in the sum are treated in a similar way). One can label the points $\{x_1,\dots,x_m\}$ such that $b_k = x_1$ and $b_{k+1} = x_2$. Point 2 in Lemma B.46 implies that $x_2 \notin A_j(x_1)$ for all $j \in \{3,\dots,m\}$. From Lemma B.45, for any $\delta > 0$ there exists $z_1 \in \partial B_a(x_1,\delta)$ such that $d_a(x_1,x_2) = d_a(x_1,z_1) + d_a(z_1,x_2)$ (where B_a is defined by (B.99)). By taking δ small enough, this implies that $z_1 \notin A_1(x_2)$ and $z_1 \notin \{x_1,\dots,x_m\}$. Likewise, from Lemma B.45, for any $\delta > 0$ there exists $z_2 \in \partial B_a(x_2,\delta)$ such that $d_a(z_1,x_2) = d_a(z_1,z_2) + d_a(z_2,x_2)$ and by taking δ small enough, this implies that $z_2 \notin A_2(z_1)$ and $z_2 \notin \{x_1,\dots,x_m\}$. Therefore one gets

$$d_a(b_k,b_{k+1}) = d_a(x_1,x_2) = d_a(x_1,z_1) + d_a(z_1,z_2) + d_a(z_2,x_2).$$

Taking δ small enough and using Lemma B.44, there exists a continuous and piecewise C^∞ curve γ_1 defined on $(-\infty, 0]$ such that $d_a(x_1, z_1) = L(\gamma_1, (-\infty, 0])$, $\lim_{t\to-\infty} \gamma_1(t) = x_1$, $\gamma_1(0) = z_1$, and $\partial\{t \in (-\infty, 0],\ \gamma_1(t) \in \partial\Omega\}$ is either empty or a single point. Similarly, there exists a continuous and piecewise C^∞ curve γ_2 defined on $[0, +\infty)$ such that $d_a(z_2, x_2) = L(\gamma_2, [0, +\infty))$, $\gamma_2(0) = z_2$, $\lim_{t\to+\infty} \gamma_2(t) = x_2$ and $\partial\{t \in [0, +\infty),\ \gamma_2(t) \in \partial\Omega\}$ is either empty or a single point. Let us show by contradiction that $z_2 \notin A_j(z_1)$ for all $j \in \{3, \dots, m\}$. On the one hand, if $z_2 \in A_j(z_1)$ for some $j \in \{3, \dots, m\}$, one has

$$d_a(x_1, x_2) = d_a(x_1, z_1) + d_a(z_1, x_j) + d_a(x_j, z_2) + d_a(z_2, x_2).$$

On the other hand, $x_1 \notin A_j(x_2)$, and thus

$$d_a(x_1, x_2) < d_a(x_1, x_j) + d_a(x_j, x_2) \le d_a(x_1, z_1) + d_a(z_1, x_j) + d_a(x_j, z_2) + d_a(z_2, x_2).$$

This leads to a contradiction. Therefore $z_2 \notin A_j(z_1)$ for all $j \in \{3, \dots, m\}$. One also has by a similar reasoning that $z_2 \notin A_1(z_1)$. Indeed, If $z_2 \in A_1(z_1)$, then one has on the one hand

$$d_a(z_1, x_2) = d_a(z_1, z_2) + d_a(z_2, x_2) = d_a(z_1, x_1) + d_a(x_1, z_2) + d_a(z_2, x_2).$$

On the other hand, since $z_1 \notin A_1(x_2)$, one has

$$d_a(z_1, x_2) < d_a(z_1, x_1) + d_a(x_1, x_2) \le d_a(z_1, x_1) + d_a(x_1, z_2) + d_a(z_2, x_2).$$

This leads to a contradiction. In conclusion $z_2 \notin A_j(z_1)$ for all $j \in \{1, \dots, m\}$. Therefore, from Corollary B.43, there exists a curve $\gamma \in A(z_1, z_2)$ such that $d_a(z_1, z_2) = L(\gamma, (0, 1))$. In conclusion, we have built three curves γ, γ_1 and γ_2 such that

$$d_a(b_k, b_{k+1}) = L(\gamma_1, (-\infty, 0]) + L(\gamma, (0, 1)) + L(\gamma_2, [0, +\infty)).$$

A similar reasoning for all the terms in the sum in (B.101) concludes the proof of Theorem B.3. ∎

A consequence of Theorem B.3 is the following.

Lemma B.47. *Let us assume that **[H1]** and **[H3]** hold. Let $(x, y) \in \overline{\Omega}$. Let us denote by $((\gamma_1, I_1), \dots, (\gamma_N, I_N))$ the curves given by Theorem B.3 ordered such that*

$$\lim_{t\to(\inf I_1)^+} \gamma_1(t) = x, \qquad \lim_{t\to(\sup I_N)^-} \gamma_N(t) = y,$$

and which realize the Agmon distance between x and y. Let $k_1 \le k_2$ with $(k_1, k_2) \in \{1, \dots, N\}^2$ and let $t_1 \in \overline{I_{k_1}}$ and $t_2 \in \overline{I_{k_2}}$. If $k_1 = k_2$, t_1 and t_2 are chosen such that $t_1 \le t_2$. Then one has

$$d_a(\gamma_{k_1}(t_1), \gamma_{k_2}(t_2)) = \begin{cases} L(\gamma_{k_1}, (t_1, \sup I_{k_1})) + \displaystyle\sum_{k=k_1+1}^{k_2-1} L(\gamma_k, I_k) + L(\gamma_{k_2}, (\inf I_{k_2}, t_2)) \text{ if } k_1 < k_2, \\ L(\gamma_{k_1}, (t_1, t_2)) \text{ if } k_1 = k_2, \end{cases}$$

where by convention, if $k_2 = k_1 + 1$, $\sum_{k=k_1+1}^{k_2-1} L(\gamma_k, I_k) = 0$. In addition the following equality holds

$$d_a(x, y) = d_a(x, \gamma_{k_1}(t_1)) + d_a(\gamma_{k_1}(t_1), \gamma_{k_2}(t_2)) + d_a(\gamma_{k_2}(t_2), y).$$

Proof. Let us make the proof for $k_1 < k_2$ (the case $k_1 = k_2$ is treated in a similar way). One has using the triangular inequality for the Agmon distance and Lemma B.32,

$$d_a\left(\gamma_{k_1}(t_1), \gamma_{k_2}(t_2)\right) \leq L\left(\gamma_{k_1}, (t_1, \sup I_{k_1})\right) + \sum_{k=k_1+1}^{k_2-1} L\left(\gamma_k, I_k\right) + L\left(\gamma_{k_2}, (\inf I_{k_2}, t_2)\right).$$

Let us now conclude the proof by contradiction. Assume that

$$d_a(\gamma_{k_1}(t_1), \gamma_{k_2}(t_2)) < L(\gamma_{k_1}, (t_1, \sup I_{k_1})) + \sum_{k=k_1+1}^{k_2-1} L(\gamma_k, I_k) + L(\gamma_{k_2}, (\inf I_{k_2}, t_2)).$$

Using the triangular inequality, one has

$$\begin{aligned} d_a\left(x, y\right) &\leq d_a(x, \gamma_{k_1}(t_1)) + d_a(\gamma_{k_1}(t_1), \gamma_{k_2}(t_2)) + d_a(\gamma_{k_2}(t_2), y) \\ &< \sum_{k=1}^{k_1-1} L(\gamma_k, I_k) + L(\gamma_{k_1}, (\inf I_{k_1}, t_1)) + L(\gamma_{k_1}, (t_1, \sup I_{k_1})) \\ &\quad + \sum_{k=k_1+1}^{k_2-1} L(\gamma_k, I_k) + L(\gamma_{k_2}, (\inf I_{k_2}, t_2)) + L(\gamma_{k_2}, (t_2, \sup I_{k_2})) \\ &\quad + \sum_{k=k_2+1}^{N} L(\gamma_k, I_k) = d_a\left(x, y\right), \end{aligned}$$

where by convention, if $k_1 = 1$, $\sum_{k=1}^{k_1-1} L(\gamma_k, I_k) = 0$ and if $k_2 = N$, $\sum_{k=k_2+1}^{N} L(\gamma_k, I_k) = 0$. The last inequality is impossible and all the previous inequalities have to be equalities. This proves Lemma B.47. ∎

B.3.4.3 On the equality in (B.79)

We end up this section with some results in case of equality in the inequality (B.79). We will prove in particular Proposition B.49 which has been used in Section B.3.2.2 above to give lower bounds on the Agmon distance.

Corollary B.48. *Let us assume that **[H1]** and **[H3]** hold. Let $x, y \in \overline{\Omega}$ with $f(x) \leq f(y)$. Let us denote by $((\gamma_1, I_1), \ldots, (\gamma_N, I_N))$ the curves given by Theorem B.3 ordered such that*

$$\lim_{t \to (\inf I_1)^+} \gamma_1(t) = x, \qquad \lim_{t \to (\sup I_N)^-} \gamma_N(t) = y,$$

and which realize the Agmon distance between x and y. If it holds:

$$d_a\left(x, y\right) = f(y) - f(x),$$

then for all $i \in \{1, \ldots, N\}$, there exist measurable functions $\lambda_i : I_i \to \mathbb{R}_+$ such that for almost every t in $\{t \in I_i,\ \gamma_i(t) \in \Omega\}$

$$\gamma_i'(t) = \lambda_i(t) \nabla f\left(\gamma_i(t)\right),$$

and such that for almost every t in $\operatorname{int}\{t \in I_i,\ \gamma_i(t) \in \partial\Omega\}$

$$\gamma_i'(t) = \lambda_i(t)\nabla_T f\left(\gamma_i(t)\right).$$

Moreover, if I_i is not bounded (namely $I_i = (-\infty, 0]$ or $I_i = [0, +\infty)$), $\lambda_i(t)$=1 for almost every $t \in I_i$, and if $I_i = [0,1]$, $\lambda_i \in L^\infty([0,1], \mathbb{R}_+)$.

Proof. Using Lemma B.25, one gets using first the triangular inequality and then the Cauchy-Schwarz inequality

$$\begin{aligned} f(y) - f(x) &= \sum_{k=1}^{N} \left(\int_{\{t\in I_k,\ \gamma_k(t)\in\Omega\}} (\nabla f)(\gamma_k)\cdot\gamma_k' + \int_{\operatorname{int}\{t\in I_k,\ \gamma_k(t)\in\partial\Omega\}} (\nabla_T f)(\gamma_k)\cdot\gamma_k' \right) \\ &\leq \sum_{k=1}^{N} \left(\int_{\{t\in I_k,\ \gamma_k(t)\in\Omega\}} |\nabla f(\gamma_k)||\gamma_k'| + \int_{\operatorname{int}\{t\in I_k,\ \gamma_k(t)\in\partial\Omega\}} |\nabla_T f(\gamma_k)||\gamma_k'| \right) \\ &= \sum_{k=1}^{N} L\left(\gamma_k, I_k\right) = d_a\left(x, y\right). \end{aligned}$$

If $d_a\left(x,y\right) = f(y) - f(x)$, then the previous inequality is necessarily an equality. This leads to the desired result applying the cases of equality in both the triangular inequality and the Cauchy-Schwarz inequalities. In particular, this gives, for $k \in \{1, \ldots, N\}$, the existence of the nonnegative functions $\lambda_k : I_k \to \mathbb{R}_+$.

Assume now that I_i is not bounded. Using the construction of the curves $(\gamma_k)_{k=1,\ldots,N}$, this implies that I_i is either $(-\infty, 0]$ or $[0, +\infty)$ and γ_i is constructed using the gradient flow of the eikonal solution near a critical point x^* of f or of $f|_{\partial\Omega}$ (see Lemma B.44 and Remarks B.7 and B.9). Let us assume that x^* is a critical point of $f|_{\partial\Omega}$ and $I_i = [0, +\infty)$ (the other cases are treated similarly). Let Φ be the solution of (B.93) on the neighoborood V^* of x^* (see Proposition B.38). By considering if necessary a smaller neighborhood V^*, one can assume that $V^* \cap \partial\Omega \subset U^*$, where U^* is the neighborhood of x^* in $\partial\Omega$ introduced in Proposition B.37, so that from (B.93) and (B.92), it holds on $V^* \cap \partial\Omega$: $|\nabla_T \Phi| = |\nabla_T f|$. The curve γ_i satisfies by construction $\lim_{t\to\infty} \gamma_i(t) = x^*$ and

$$\gamma_i' = \begin{cases} -\nabla\Phi(\gamma_i) \text{ in } \Omega, \\ -\nabla_T\Phi(\gamma_i) \text{ on } \partial\Omega. \end{cases}$$

In addition, by the previous reasoning, one also has

$$\gamma_i' = \begin{cases} \lambda_i \nabla f(\gamma_i) \text{ in } \Omega, \\ \lambda_i \nabla_T f(\gamma_i) \text{ on } \partial\Omega, \end{cases}$$

for some function $\lambda_i : I_i \to \mathbb{R}_+$. Taking the norm in the two previous equalities, using the fact that Φ solves (B.93) together with the equality (B.92), one obtains that $\lambda_i = 1$. Let us finally consider the case $I_i = [0,1]$. Then, by construction, the curve γ_i does not meet any critical points of the functions f and $f|_{\partial\Omega}$. This implies that $\inf_{I_i} |\nabla f(\gamma_i)| > 0$ and $\inf_{I_i} |\nabla_T f(\gamma_i)| > 0$, and thus, since $\|\gamma_i'\|_{L^\infty} < \infty$, one concludes that $\lambda_i \in L^\infty([0,1], \mathbb{R}_+)$. ∎

Let us define the notion of generalized integral curves.

Definition B.8. *Let $D \subset \overline{\Omega}$ be a C^∞ domain and $X \in C^\infty(D, \mathbb{R})$. Let $N \in \mathbb{N}^*$ and for $i \in \{1, ..., N\}$, let $I_i \subset \mathbb{R}$ be an interval and $\gamma_i : I_i \to D$ be Lipschitz and which satisfy*

$$\lim_{t \to (\inf I_1)^+} \gamma_1(t) \in \overline{\Omega}, \qquad \lim_{t \to (\sup I_N)^-} \gamma_N(t) \in \overline{\Omega},$$

and for all $k \in \{1, \ldots, N-1\}$,

$$\lim_{t \to (\sup I_k)^-} \gamma_k(t) = \lim_{t \to (\inf I_{k+1})^+} \gamma_{k+1}(t).$$

The set of curves $\{\gamma_1, \ldots, \gamma_N\}$ is a generalized integral curve of $\begin{cases} \nabla X \text{ in } D \cap \Omega, \\ \nabla_T X \text{ on } D \cap \partial\Omega \end{cases}$ if for all $i \in \{1, \ldots, N\}$, there exist measurable functions $\lambda_i : I_i \to \mathbb{R}_+$ such that for almost every t in $\{t \in I_i,\ \gamma_i(t) \in D \cap \Omega\}$: $\gamma_i'(t) = \lambda_i(t) \nabla X(\gamma_i(t))$, and such that for almost every t in $\operatorname{int}\{t \in I_i,\ \gamma_i(t) \in \partial\Omega \cap D\}$: $\gamma_i'(t) = \lambda_i(t) \nabla_T X(\gamma_i(t))$.

The notion of generalized integral curve has been introduced in the case of manifolds without boundary in [38]. As introduced in Definition B.8, the set of curves $\{\gamma_1, \ldots, \gamma_N\}$ given by Corollary B.48 is a generalized integral curve of the vector field $\begin{cases} \nabla f \text{ in } \Omega, \\ \nabla_T f \text{ on } \partial\Omega \end{cases}$. Let us mention that in the case when Ω is a manifold without boundary, Corollary B.48 is exactly [38, Lemma A2.2].

Proposition B.49. *Let us assume that **[H1]** and **[H3]** hold. Let us denote by $\{z_1, \ldots, z_n\}$ the local minima of $f|_{\partial\Omega}$ ordered such that $f(z_1) \leq f(z_2) \leq \ldots \leq f(z_n)$. Then, for all $i < j$, $(i, j) \in \{1, \ldots, n\}^2$, one has*

$$d_a(z_i, z_j) > f(z_j) - f(z_i).$$

Proof. From the inequality (B.79), one has $d_a(z_i, z_j) \geq f(z_j) - f(z_i)$. Let us prove Proposition B.49 by contradiction. Assume that $d_a(z_i, z_j) = f(z_j) - f(z_i)$ for some $i < j$. Denote by $((\gamma_1, I_1), \ldots, (\gamma_m, I_m))$ the curves given by Theorem B.3 ordered such that

$$\lim_{t \to (\inf I_1)^+} \gamma_1(t) = z_i, \qquad \lim_{t \to (\sup I_m)^-} \gamma_m(t) = z_j,$$

and which realize the Agmon distance between z_i and z_j. Since $d_a(z_i, z_j) = f(z_j) - f(z_i)$, from Corollary B.48, for all $i \in \{1, \ldots, m\}$, there exist measurable functions $\lambda_i : I_i \to \mathbb{R}_+$ such that for almost every t in $\{t \in I_i,\ \gamma_i(t) \in \Omega\}$, $\gamma_i'(t) = \lambda_i(t) \nabla f(\gamma_i(t))$, and such that for almost every t in $\operatorname{int}\{t \in I_i,\ \gamma_i(t) \in \partial\Omega\}$, $\gamma_i'(t) = \lambda_i(t) \nabla_T f(\gamma_i(t))$ (the set of curves $\{\gamma_1, \ldots, \gamma_m\}$ is a generalized integral curve of the vector field $\begin{cases} \nabla f \text{ in } \Omega, \\ \nabla_T f \text{ on } \partial\Omega \end{cases}$, according to Definition B.8). Let us recall that from Remark B.9, $I_1 = (-\infty, 0]$ and $I_m = [0, +\infty)$ since z_i and z_j are critical points of $f|_{\partial\Omega}$.

Step 1. Let us show that for all $t \in (-\infty, 0]$, $\gamma_1(t) \in \partial\Omega$. On the one hand, from Remark B.9, $\lim_{t \to -\infty} \gamma_1(t) = z_i$ and

$$\gamma_1' = \begin{cases} \nabla\Phi(\gamma_1) \text{ in } \Omega \\ \nabla_T \Phi(\gamma_1) \text{ on } \partial\Omega, \end{cases}$$

where Φ solves (B.93). On the other hand, from Corollary B.48, one has

$$\gamma_1' = \begin{cases} \nabla f(\gamma_1) \text{ in } \Omega \\ \nabla_T f(\gamma_1) \text{ on } \partial\Omega. \end{cases}$$

Then, for all $t \geq 0$, one has $\frac{d}{dt}\left(f(\gamma_1)(t) - \Phi(\gamma_1(t))\right) = 0$. Therefore there exists $C > 0$ such that for all $t \in (-\infty, 0]$, $\gamma_1(t) \in \{x,\, f(x) - \Phi(x) = C\}$. Since $\lim_{t\to-\infty} \gamma_1(t) = z_i$ and $(f - \Phi)(z_i) = f(z_i)$, one gets that $C = f(z_i)$ and thus for all $t \in (-\infty, 0]$, $\gamma_1(t) \in \{x,\, f(x) - \Phi(x) = f(z_i)\}$. From Corollary B.39 and Proposition B.40, γ_1 lives in a neighborhood U^* of z_i such that (see Equation (B.95)):

$$\{x,\, f(x) - \Phi(x) = f(z_i)\} \subset \partial\Omega.$$

We thus get that for all $t \geq 0$, $\gamma_1(t) \in \partial\Omega$, and then $\gamma_1'(t) = \nabla_T f(\gamma_1(t)) = \nabla_T \Phi(\gamma_1(t))$. Step 1 is proved.

Step 2. We are going to show that for all $t \in I_k$, $\gamma_k(t) \in \partial\Omega$. If it is not the case, from Step 1, there exist $k \in \{2, \ldots, m\}$ and $t_k \in I_k$ such that $\gamma_k(t_k) \in \Omega$. Let us define the first time, denoted by t^*, for which the curves $((\gamma_2, I_2), \ldots, (\gamma_m, I_m))$ leave $\partial\Omega$. By construction of the curves $\gamma_1, ..., \gamma_m$, there are two cases: either t^* is finite (and thus belongs to $\text{int}(I_k)$ for $k \in \{1, ..., m\}$) or, there exist $j \in \{1, ..., m-1\}$, $s < 0$ and $z \in \partial\Omega$ such that $g(z) = 0$, $\lim_{t\to+\infty} \gamma_j(t) = z$, $\lim_{t\to-\infty} \gamma_{j+1}(t) = z$ and $\gamma_{j+1}(-\infty, s) \subset \Omega$ for which we set $t^* = -\infty$. Let us assume that t^* is finite and belongs to $\text{int}(I_k)$ (the other case is treated similarly).

As in Step 1 of the proof of Proposition B.26, let us now introduce a smooth tangential and normal system of coordinates around $\gamma_k(t^*)$ in $\overline{\Omega}$, denoted by $\phi(x) = (x_T, x_N)$. The function ϕ is defined from a neighborhood of $\gamma_k(t^*)$ in $\overline{\Omega}$ to $\mathbb{R}^d$. Moreover, one has $x_N \geq 0$ and $x_N(x) = 0$ if and only if $x \in \partial\Omega$. We may assume that the neighborhood $V_\alpha \subset \mathbb{R}^d$ on which ϕ is defined is such that $\phi(V_\alpha) = U \times [0, \alpha]$ for $\alpha > 0$ and $U \subset \mathbb{R}^{d-1}$. Since $\partial_n f > 0$ on $\partial\Omega$, $\alpha > 0$ can be chosen small enough such that $\nabla f(x) \cdot n(x) > 0$ for all $x \in V_\alpha$ where $n(x) = -\frac{\nabla x_N(x)}{|\nabla x_N(x)|}$. Indeed, for $x \in \partial\Omega$, $n(x)$ is nothing but the unit outward normal to $\partial\Omega$.

Now, by continuity of the curve γ_k, there exists $\varepsilon > 0$ such that $[t^*, t^* + \varepsilon] \subset I_k$ and for all $t \in [t^*, t^* + \varepsilon]$, $\gamma_k(t) \in V_\alpha$. The mapping $t \in [t^*, t^* + \varepsilon] \mapsto x_N(\gamma_k(t))$ is Lipschitz and satisfies: for almost every $s \in (t^*, t^* + \varepsilon)$,

$$\frac{d}{ds} x_N(\gamma_k(s)) = -|\nabla x_N(\gamma_k(s))|\, \gamma_k'(s) \cdot n(\gamma_k(s)).$$

Then, for all $t \in [t^*, t^* + \varepsilon]$, one has:

$$\frac{d}{ds} x_N(\gamma_k(s)) = \begin{cases} 0 \text{ for a.e. } s \in \text{int}\,\{u \in (t^*, t),\ \gamma_k(u) \in \partial\Omega\} \\ -|\nabla x_N(\gamma_k(s))|\, \lambda_k(s)\, \nabla f(\gamma_k(s)) \cdot n(\gamma_k(s)) \text{ for a.e. } s \in \{u \in (t^*, t),\ \gamma_k(u) \in \Omega\}. \end{cases}$$

Since $\partial\{u \in (t^*, t),\ \gamma_k(u) \in \partial\Omega\}$ is of Lebesgue measure zero (see Theorem B.3) and since $\nabla f \cdot n > 0$ in V_α, one has from Lemma B.25, for all $t \in [t^*, t^* + \varepsilon]$

$$x_N(\gamma_k(t)) = x_N(\gamma_k(t)) - x_N(\gamma_k(t^*)) = \int_{t^*}^{t} \frac{d}{ds} x_N(\gamma_k(s))\, ds \leq 0.$$

This implies that for all $t \in [t^*, t^* + \varepsilon]$, $x_N(\gamma_k(t)) = 0$ and thus $\gamma_k(t) \in \partial\Omega$ for all $t \in [t^*, t^* + \varepsilon]$. This contradicts the definition of t^*. Step 2 is proved.

Step 3. From the last two steps, for all $t \in [0, +\infty)$, $\gamma_m(t) \in \partial\Omega$. From Corollary B.48, one has $\gamma_m'(t) = \nabla_T f(\gamma_m(t))$ for all $t \in [0, +\infty)$ and therefore, the map $t \in [0, +\infty) \mapsto f(\gamma_m(t))$ is increasing (indeed, one has $\frac{d}{dt} f(\gamma_m(t)) = |\nabla_T f(\gamma_m(t))|^2$). This is impossible since z_j is a local minimum of $f|_{\partial\Omega}$. This concludes the proof of Proposition B.49 by contradiction. ∎

B.3.5 Agmon distance in a neighborhood of the basin of attraction of a local minimum of $f|_{\partial\Omega}$ and eikonal equation

The aim of this section is to generalize the results of Section B.3.3 to relate the Agmon distance and the solution to an eikonal equation on a neighborhood of a basin of attraction B_z (see Definition B.4) of a local minimum z of $f|_{\partial\Omega}$. Let first introduce a solution to the eikonal equation $|\nabla\phi|^2 = |\nabla f|^2$ defined globally on a neighborhood of the boundary $\partial\Omega$.

Proposition B.50. *Let us assume that **[H3]** holds. There exists a neighborhood of $\partial\Omega$ in $\overline{\Omega}$, denoted $V_{\partial\Omega}$, such that there exists $\Phi \in C^\infty(V_{\partial\Omega}, \mathbb{R})$ satisfying*

$$\begin{cases} |\nabla\Phi|^2 = |\nabla f|^2 \text{ in } \Omega \cap V_{\partial\Omega} \\ \Phi = f \text{ on } \partial\Omega \\ \partial_n \Phi = -\partial_n f \text{ on } \partial\Omega. \end{cases} \tag{B.102}$$

Moreover, one has the following uniqueness results: if $\tilde{\Phi}$ is a C^∞ real valued function defined on a neighborhood $\tilde{V}$ of $\partial\Omega$ satisfying (B.102)*, then $\tilde{\Phi} = \Phi$ on $\tilde{V} \cap V_{\partial\Omega}$.*

Proof. Let $z \in \partial\Omega$. Using [19] or [22], thanks to **[H3]**, there exists a neighborhood of z in $\overline{\Omega}$, denoted by $\mathcal{V}_z$, such that there exists $\Phi \in C^\infty(\mathcal{V}_z, \mathbb{R})$ satisfying

$$\begin{cases} |\nabla\Phi|^2 = |\nabla f|^2 \text{ in } \Omega \cap \mathcal{V}_z \\ \Phi = f \text{ on } \partial\Omega \cap \mathcal{V}_z \\ \partial_n \Phi = -\partial_n f \text{ on } \partial\Omega \cap \mathcal{V}_z. \end{cases}$$

Moreover, $\mathcal{V}_z$ can be chosen such that the following uniqueness result holds: if a function $\tilde{\Phi} \in C^\infty(\mathcal{V}_z, \mathbb{R})$ satisfies the previous equalities, then $\tilde{\Phi} = \Phi$ on $\mathcal{V}_z$. Now, one concludes using the fact that $\partial\Omega$ is compact and can thus be covered by a finite number of these neighborhoods $(\mathcal{V}_z)_{z \in \partial\Omega}$. ∎

Remark B.10. *Let us mention another standard approach to prove Proposition B.50, using the notion of viscosity solutions. Let us recall some results from [49, Theorem 5.1]. For $(x, y) \in \overline{\Omega}^2$, one defines*

$$\tilde{d}(x, y) := \inf_{T>0, \gamma} \int_0^T |\nabla f(\gamma(t))| \, dt,$$

where the infimum is taken over $T > 0$ and over Lipschitz curves $\gamma : [0,T] \to \overline{\Omega}$ which satisfy $\gamma(0) = x$, $\gamma(T) = y$, $|\gamma'| \leq 1$. Then $v(x) := \inf\left\{f(y) + \tilde{d}(x,y)\,,\ y \in \partial\Omega\right\}$ is Lipschitz and is a viscosity solution of

$$\begin{cases} |\nabla v| = |\nabla f| \text{ in } \Omega \\ \quad v = f \text{ on } \partial\Omega. \end{cases}$$

Let us notice that this implies $|\partial_n v| = |\partial_n f|$. To prove Proposition B.50 using this result, one has to show that v is C^∞ near $\partial\Omega$ and $\partial_n v = -\partial_n f$. This is a consequence of the characteristic method, see [49, Section 1.2].

Remark B.11. *Let x^* be a local minimum of $f|_{\partial\Omega}$ and let us denote by $\tilde{\Phi}$ the solution to the eikonal equation* (B.94) *introduced in Corollary B.39, defined on a neighborhood V^* of x^*. Then, one has on $V^* \cap V_{\partial\Omega}$:*

$$\tilde{\Phi} = \Phi - f(x^*)$$

where Φ is the solution to (B.102).

Let us now introduce the function f_- which will be used in the sequel.

Proposition B.51. *Assume that **[H3]** holds. Let $\Phi \in C^\infty(V_{\partial\Omega}, \mathbb{R})$ be the function introduced in Proposition B.50. Let us define the function $f_- \in C^\infty(V_{\partial\Omega}, \mathbb{R})$ by*

$$f_- = \frac{\Phi - f}{2}. \tag{B.103}$$

Then, $f_- = 0$ on $\partial\Omega$, and up to choosing a smaller neighborhood $V_{\partial\Omega}$ of $\partial\Omega$, the function f_- is positive in $V_{\partial\Omega} \setminus \partial\Omega$ and $|\nabla f_-| > 0$ on $V_{\partial\Omega}$.

Proof. Since $\partial_n(\Phi - f) = -2\partial_n f < 0$ and $\Phi = f$ on $\partial\Omega$, then, up to choosing a smaller neighborhood $V_{\partial\Omega}$ of $\partial\Omega$, one has $\Phi > f$ on $V_{\partial\Omega} \setminus \partial\Omega$ and $|\nabla(\Phi - f)| > 0$ on $V_{\partial\Omega}$. ∎

We are now in position to prove the main result of this section.

Proposition B.52. *Let us assume that **[H1]** and **[H3]** hold. Let Φ be the function given by Proposition B.50. Denote by z a local minimum of $f|_{\partial\Omega}$ and denote by $B_z \subset \partial\Omega$ the associated basin of attraction (see Definition B.4). Besides, let $\Gamma_z \subset \partial\Omega$ be an open domain such that $\overline{\Gamma_z} \subset B_z$ and $z \in \Gamma_z$. Then there exists a neighborhood of $\overline{\Gamma_z}$ in $\overline{\Omega}$, denoted by V_{Γ_z}, such that $\overline{\partial V_{\Gamma_z} \cap \partial\Omega} \subset B_z$ and for all $x \in V_{\Gamma_z}$,*

$$d_a(x,z) = \Phi(x) - f(z).$$

Notice that in this proposition, Γ_z can be chosen as large as we want in B_z.

Proof. Let Φ be the function given by Proposition B.50. The proof is divided into three steps.

Step 1. Let us first define V_{Γ_z}. To this end let us denote by f_- and $V_{\partial\Omega}$ respectively the function and the neighborhood of $\partial\Omega$ given by Proposition B.51. For $\varepsilon > 0$ small enough one defines

$$V_\varepsilon = \{y \in \Omega,\ 0 \leq f_-(y) \leq \varepsilon\} \subset V_{\partial\Omega}. \tag{B.104}$$

The parameter $\varepsilon > 0$ can be chosen such that there is no critical point of f on $\partial V_\varepsilon \cap \Omega = \{y \in \Omega,\ f_-(y) = \varepsilon\}$. The set V_ε is a neighborhood of $\partial\Omega$ in $\overline{\Omega}$ (see Figure B.7 for a schematic representation). Let us now fix such a $\varepsilon > 0$. Assumption **[H3]** together with the fact that $\partial_n \Phi < 0$ on $\partial\Omega$, imply that there exists a neighborhood V_{Γ_z} of $\overline{\Gamma_z}$ in $\overline{\Omega}$, such that $V_{\Gamma_z} \subset V_\varepsilon$, $\overline{\partial V_{\Gamma_z} \cap \partial\Omega} \subset B_z$ and

$$\partial_n \Phi > 0, \text{ on } \partial V_{\Gamma_z} \cap \Omega.$$

The set V_{Γ_z} is schematically represented on Figure B.8.

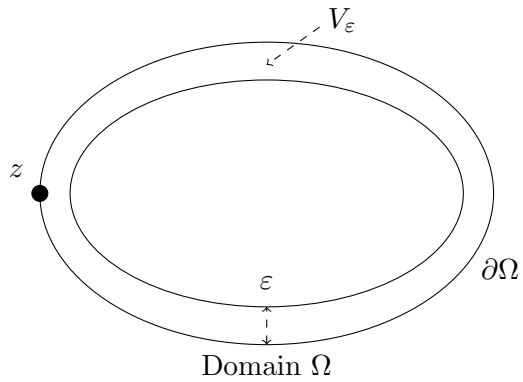

Figure B.7: The set V_ε.

Step 2. Let us first prove that for all $x \in V_{\Gamma_z}$, $d_a(x, z) \geq \Phi(x) - f(z)$. For $x \in V_{\Gamma_z}$, denote by $((\gamma_1, I_1), \ldots, (\gamma_N, I_N))$ the curves given by Theorem B.3 ordered such that

$$\lim_{t \to (\inf I_1)^+} \gamma_1(t) = z, \qquad \lim_{t \to (\sup I_N)^-} \gamma_N(t) = x,$$

and which realize the Agmon distance between x and z. One has to deal with the two following cases:

1. either $\forall\ k \in \{1, \ldots, N\}$, $\forall t \in I_k$, $\gamma_k(t) \in V_\varepsilon$,
2. or $\exists\ k \in \{1, \ldots, N\}$ and $\exists\ t \in I_k$, $\gamma_k(t) \in \overline{\Omega} \setminus V_\varepsilon$.

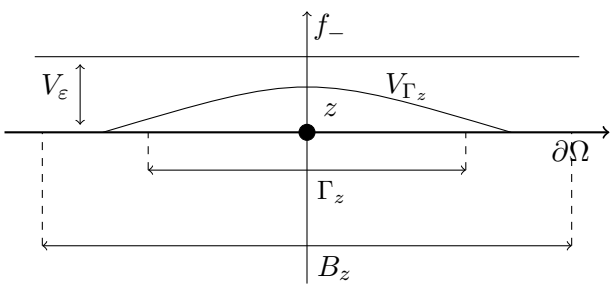

Figure B.8: The set V_{Γ_z}.

In the first case, since Φ is defined on V_ε, it holds

$$\Phi(x) - f(z) = \Phi(x) - \Phi(z) = \sum_{j=1}^{N} \int_{I_j} \frac{d}{dt} \Phi \circ \gamma_j(t)\, dt.$$

Using Lemma B.25 and the fact that $|\nabla \Phi| = g$ on $\Omega \cap V_{\partial\Omega}$ and $|\nabla_T \Phi| = g$ on $\partial\Omega$, it holds, for all $j \in \{1, \dots, N\}$,

$$\int_{I_j} \frac{d}{dt} \Phi \circ \gamma_j(t)\, dt \leq L(\gamma_j, I_j)$$

and thus

$$\Phi(x) - f(z) \leq \sum_{j=1}^{N} L(\gamma_j, I_j) = d_a(x, z).$$

Let us now consider the second case. Let us introduce $k_1 \in \{1, \dots, N\}$ and $t_1 \in I_{k_1}$ such that for all $t < t_1$, $\gamma_{k_1}(t) \in V_\varepsilon$, for all $k \in \{1, \dots, k_1 - 1\}$, for all $t \in I_k$, $\gamma_k(t) \in V_\varepsilon$ and such that there exists $\beta > 0$ such that for all $t \in (t_1, t_1 + \beta]$, $\gamma_{k_1}(t) \notin V_\varepsilon$. The couple (k_1, t_1) thus represents the "first time" the curves $\gamma_1, \dots, \gamma_N$ leave V_ε. Likewise, let us introduce $k_2 \in \{1, \dots, N\}$ and $t_2 \in I_{k_2}$ such that for all $t > t_2$, $\gamma_{k_2}(t) \in V_\varepsilon$, for all $k \in \{k_2 + 1, \dots, N\}$, for all $t \in I_k$, $\gamma_k(t) \in V_\varepsilon$ and such that there exists $\beta > 0$ such that for all $t \in [t_2 - \beta, t_2)$, $\gamma_{k_2}(t) \notin V_\varepsilon$. The couple (k_2, t_2) thus represents the "last time" the curves $\gamma_1, \dots, \gamma_N$ leave $\overline{\Omega} \setminus V_\varepsilon$. From Step 1, there is no critical point of f on $\partial V_\varepsilon \cap \Omega = \{y \in \Omega,\ f_-(y) = \varepsilon\}$. Therefore, by construction of the curves $(\gamma_k)_{k=1,\dots,N}$, the times t_1 and t_2 are finite and belong respectively to $\operatorname{int} I_{k_1}$ and $\operatorname{int} I_{k_2}$. One has by continuity of γ_{k_1} and γ_{k_2}, $f_-(\gamma_{k_1}(t_1)) = f_-(\gamma_{k_2}(t_2)) = \varepsilon$. Since Φ is defined on V_ε, using again Lemma B.25 and the fact that $|\nabla \Phi| = g$ on Ω and $|\nabla_T \Phi| = g$, one has

$$|\Phi(\gamma_{k_1}(t_1)) - \Phi(z)| \leq \sum_{j=1}^{k_1 - 1} L(\gamma_j, I_j) + L(\gamma_{k_1}, (\inf I_{k_1}, t_1)).$$

In addition, using Lemma B.47,

$$\sum_{j=1}^{k_1 - 1} L(\gamma_j, I_j) + L(\gamma_{k_1}, (\inf I_{k_1}, t_1)) = d_a(z, \gamma_{k_1}(t_1)).$$

Thus $|\Phi(\gamma_{k_1}(t_1)) - \Phi(z)| \leq d_a(z, \gamma_{k_1}(t_1))$. By similar arguments, one obtains $|\Phi(x) - \Phi(\gamma_{k_2}(t_2))| \leq d_a(\gamma_{k_2}(t_2), x)$. Thanks to the definition (B.103) of f_- and using the fact that $f_-(\gamma_{k_1}(t_1)) = f_-(\gamma_{k_2}(t_2)) = \varepsilon$, one has $|f(\gamma_{k_2}(t_2)) - f(\gamma_{k_1}(t_1))| = |\Phi(\gamma_{k_2}(t_2)) - \Phi(\gamma_{k_1}(t_1))|$. In addition, using (B.79) one obtains $d_a(\gamma_{k_1}(t_1), \gamma_{k_2}(t_2)) \geq |f(\gamma_{k_2}(t_2)) - f(\gamma_{k_1}(t_1))| = |\Phi(\gamma_{k_2}(t_2)) - \Phi(\gamma_{k_1}(t_1))|$. Using Lemma B.47 and gathering these three last inequalities, one gets

$$\begin{aligned} d_a(x, z) &= d_a(z, \gamma_{k_1}(t_1)) + d_a(\gamma_{k_1}(t_1), \gamma_{k_2}(t_2)) + d_a(\gamma_{k_2}(t_2), x) \\ &\geq |\Phi(z) - \Phi(\gamma_{k_1}(t_1))| + |\Phi(\gamma_{k_2}(t_2)) - \Phi(\gamma_{k_1}(t_1))| + |\Phi(x) - \Phi(\gamma_{k_2}(t_2))| \\ &\geq |\Phi(z) - \Phi(x)| \geq \Phi(x) - \Phi(z) = \Phi(x) - f(z). \end{aligned}$$

Step 3. Let us now show that for all $x \in V_{\Gamma_z}$, $d_a(x,z) \leq \Phi(x) - f(z)$. The proof of this inequality is very similar to the second step in the proof of Proposition B.40. For $x \in V_{\Gamma_z}$, let γ be defined by (B.96)–(B.97) (where Φ is defined by (B.102)), with $\gamma(0) = x$. The function γ is with values in V_{Γ_z} since $\partial_n \Phi > 0$ on $\partial V_{\Gamma_z} \cap \Omega$ and $\partial V_{\Gamma_z} \cap \partial\Omega \subset B_z$. Thus γ is defined on $\mathbb{R}_+$. Thanks to the definition (B.96) of the vector field X, if there exists a time $t_{\partial\Omega}$ such that $\gamma(t_{\partial\Omega})$ is in $\partial\Omega$, then, for all $t \geq t_{\partial\Omega}$, $\gamma(t) \in \partial\Omega$. The function $t \in \mathbb{R}_+ \mapsto \gamma(t)$ is continuous, piecewise C^∞ and satisfies

$$\lim_{t \to +\infty} \gamma(t) = z.$$

Then, as in the second step of the proof of Proposition B.40, one has

$$\Phi(x) - f(z) = L\left(\gamma, (0, \infty)\right).$$

Using Lemma B.32, one obtains that $d_a(x,z) \leq L(\gamma, (0,\infty)) = \Phi(x) - f(z)$. This proves the inequality: for all $x \in V_{\Gamma_z}$, $d_a(x,z) \leq \Phi(x) - f(z)$. This concludes the proof of Proposition B.52. ∎

The following corollary is similar to Corollary B.48 in the sense that is deals with the case of equality between the Agmon distance and the function Φ introduced in Proposition B.50. Corollary B.53 will be needed in the proof of Proposition B.65.

Corollary B.53. *Let us assume that **[H1]** and **[H3]** hold. Let Φ be the function introduced in Proposition B.50 and, let f_- and $V_{\partial\Omega}$ be respectively the function and the neighborhood of $\partial\Omega$ given by Proposition B.51. Let V_α be defined by* (B.104) *and where the parameter $\alpha > 0$ is chosen such $V_\alpha \subset V_{\partial\Omega}$, there is no critical point of f on $\partial V_\alpha \cap \Omega = \{w \in \Omega,\ f_-(w) = \alpha\}$, $\partial_n f > 0$ on $\partial V_\alpha \cap \Omega$, $\partial_n f^- < 0$ on $\partial V_\alpha \cap \Omega$ and $|\nabla\Phi| \neq 0$ in V_α (it is possible to choose such an $\alpha > 0$ since $\partial_n f^- = \partial_n \Phi = -\partial_n f < 0$ on $\partial\Omega = V_0$). Let $x, y \in V_\alpha$ and denote by $((\gamma_1, I_1), \ldots, (\gamma_N, I_N))$ the curves given by Theorem B.3 ordered such that $\lim_{t \to (\inf I_1)^+} \gamma_1(t) = x$, $\lim_{t \to (\sup I_N)^-} \gamma_N(t) = y$ and which realize the Agmon distance between x and y. Let us assume that*

$$\Phi(x) - \Phi(y) = d_a(x,y).$$

Then, for all $i \in \{1, \ldots, N\}$, $\operatorname{Im} \gamma_i \subset V_\alpha$ and there exist measurable functions $\lambda_i : I_i \to \mathbb{R}_+$ such that for almost every t in $\{t \in I_i,\ \gamma_i(t) \in \Omega\}$, one has $\gamma_i'(t) = -\lambda_i(t) \nabla\Phi\left(\gamma_i(t)\right)$, and such that for almost every t in $\operatorname{int}\{t \in I_i,\ \gamma_i(t) \in \partial\Omega\}$, one has $\gamma_i'(t) = -\lambda_i(t) \nabla_T\Phi\left(\gamma_i(t)\right)$. Moreover, if I_i is not bounded (namely $I_i = (-\infty, 0]$ or $I_i = [0, +\infty)$), $\lambda_i(t)$=1 for almost every $t \in I_i$, and if $I_i = [0,1]$, $\lambda_i \in L^\infty([0,1], \mathbb{R}_+)$.

According to Definition B.8, the set of curves $\{\gamma_1, \ldots, \gamma_N\}$ introduced in Corollary B.53 is a generalized integral curve of the vector field $\begin{cases} -\nabla\Phi \text{ in } V_\alpha \cap \Omega, \\ -\nabla_T\Phi \text{ on } \partial\Omega \end{cases}$.

Proof. The proof of this statement is similar to the proof of Proposition B.52.

Let us first prove that for all $i \in \{1, \ldots, N\}$, $\operatorname{Im} \gamma_i \subset V_\alpha$. If it is not the case, then there exist $k \in \{1, \ldots, N\}$ and $t \in I_k$ such that $\gamma_k(t) \in \overline{\Omega} \setminus V_\alpha$. Let the couples (t_1, k_1) and (t_2, k_2) be defined as in Step 2 of the proof of Proposition B.52. Then, one has (see

the second step of the proof of Proposition B.52), $d_a(x, \gamma_{k_1}(t_1)) \geq \Phi(x) - \Phi(\gamma_{k_1}(t_1))$, $d_a(\gamma_{k_1}(t_1), \gamma_{k_2}(t_2)) \geq \Phi(\gamma_{k_1}(t_1)) - \Phi(\gamma_{k_2}(t_2))$ and $d_a(\gamma_{k_2}(t_2), y) \geq \Phi(\gamma_{k_2}(t_2)) - \Phi(y)$. Since one has by assumption and from Lemma B.47:

$$\Phi(x) - \Phi(y) = d_a(x, y) = d_a(x, \gamma_{k_1}(t_1)) + d_a(\gamma_{k_1}(t_1), \gamma_{k_2}(t_2)) + d_a(\gamma_{k_2}(t_2), y),$$

all the previous inequalities are equalities and in particular, it holds:

$$d_a(\gamma_{k_1}(t_1), \gamma_{k_2}(t_2)) = \Phi(\gamma_{k_1}(t_1)) - \Phi(\gamma_{k_2}(t_2)) = f(\gamma_{k_2}(t_2)) - f(\gamma_{k_1}(t_1)) \geq 0.$$

Using Corollary B.48, this implies that when restricting γ_{k_1} to $I_{k_2} \cap [t_1, \infty)$ and γ_{k_2} to $I_{k_1} \cap (-\infty, t_2]$ the set of curves $\{\gamma_{k_1}, ..., \gamma_{k_2}\}$ is a generalized integral curve of $\begin{cases} \nabla f \text{ in } \Omega, \\ \nabla_T f \text{ on } \partial\Omega \end{cases}$ (see Definition B.8). Let $D = \Omega \setminus V_\alpha$ ($\partial D = \Omega \cap V_\alpha = \{w \in \Omega, f_-(w) = \alpha\}$ is C^∞ since f^- is C^∞ and $\partial_n f^- < 0$ on $\partial V_\alpha \cap \Omega = \partial D$ which imply that there is no critical point of f_- on ∂D). Then, from Corollary B.48 and by definition of (t_1, k_1) (see the second step of the proof of Proposition B.52), there exists $\varepsilon > 0$ and a measurable function λ: $[t_1, t_1 + \varepsilon] \to \mathbb{R}^+$ such that for all $t \in [t_1, t_1 + \varepsilon]$:

$$\gamma'_{k_1}(t) = \lambda(t) \nabla f\left(\gamma_{k_1}(t)\right)$$

and for all $t \in (t_1, t_1 + \varepsilon]$:

$$\gamma_{k_1}(t) \in D. \tag{B.105}$$

As in Step 2 of the proof of Proposition B.49, let us introduce a smooth tangential and normal system of coordinates around $\gamma_{k_1}(t_1) \in \partial D$ in $\overline{D}$, denoted by $\phi(x) = (x_T, x_N)$. The function ϕ is defined from a neighborhood of $\gamma_{k_1}(t_1)$ in $\overline{D}$ to $\mathbb{R}^d$. Moreover, one has $x_N \geq 0$ and $x_N(x) = 0$ if and only if $x \in \partial D$. We may assume that the neighborhood $U_\beta \subset \overline{D}$ on which ϕ is defined is such that $\phi(U_\beta) = U \times [0, \beta]$ for $\beta > 0$ and $U \subset \mathbb{R}^{d-1}$. Since $\partial_n f > 0$ on ∂D, $\beta > 0$ can be chosen small enough such that $\nabla f(x) \cdot n(x) > 0$ for all $x \in U_\beta$ where $n(x) = -\frac{\nabla x_N(x)}{|\nabla x_N(x)|}$. Indeed, for $x \in \partial D$, $n(x)$ is nothing but the unit outward normal to ∂D. Now, by continuity of the curve γ_{k_1}, there exists $\mu > 0$ such that for all $t \in (t_1, t_1 + \mu]$, $\gamma_{k_1}(t) \in U_\beta$. The same considerations as in Step 2 of the proof of Proposition B.49 can then be used to show that:

$$x_N(\gamma(t)) \leq 0,$$

for all $t \in [t_1, t_1 + \mu]$ and thus $\gamma_{k_1}(t) \notin D$ for all $t \in [t_1, t_1 + \mu]$. This contradicts (B.105). Thus, for all $i \in \{1, \ldots, N\}$, $\operatorname{Im} \gamma_i \subset V_\alpha$.

Then, the announced result follows by the same arguments as those used in the proof of Corollary B.48 with f replaced by Φ together with the fact that Φ satisfies (B.102) on V_α and for all $i \in \{1, \ldots, N\}$, $\operatorname{Im} \gamma_i \subset V_\alpha$. ∎

B.4 Construction of the quasi-modes and proof of Theorem B.1

The aim of this section is to build the quasi-modes $\tilde{u}$ and $(\tilde{\phi}_i)_{i=1,\ldots n}$ satisfying the conditions stated in Section B.2.2.2. Let us recall that $\operatorname{span}(\tilde{u})$ (resp. $\operatorname{span}(\tilde{\phi}_i, i = 1, \ldots, n)$)

is intended to be a good approximation (in the sense made precise in items 1 and 2 in Proposition B.17) of $\mathrm{Ran}\left(\pi_{[0,\sqrt{h})}\left(L^{D,(0)}_{f,h}(\Omega)\right)\right)$ (resp. $\mathrm{Ran}\left(\pi_{[0,h^{\frac{3}{2}})}\left(\Delta^{D,(1)}_{f,h}(\Omega)\right)\right)$).

As recalled in Proposition B.16, it is known that the dimension of $\mathrm{Ran}\left(\pi_{[0,h^{\frac{3}{2}})}\left(\Delta^{D,(1)}_{f,h}(\Omega)\right)\right)$ is equal to the number of generalized critical points of index 1 (see [34, Section 3]) which are in our setting, thanks to assumptions **[H1]**, **[H2]** and **[H3]**, the local minima $(z_i)_{i=1,\dots,n}$ of $f|_{\partial\Omega}$. In addition, it is known that the 1-forms in $\mathrm{Ran}\left(\pi_{[0,h^{\frac{3}{2}})}\left(\Delta^{D,(1)}_{f,h}(\Omega)\right)\right)$ are localized in the limit $h \to 0$ in small neighborhoods of the local minima $(z_i)_{i=1,\dots,n}$.

For each local minimum z_i, we construct an associated quasi-mode $\tilde{\phi}_i$, using an auxiliary Witten Laplacian on 1-forms with mixed tangential-normal boundary conditions. This Witten Laplacian is defined on a domain $\dot{\Omega}_i \subset \Omega$ with suitable boundary conditions, so that its only small eigenvalue (namely in the interval $[0, h^{\frac{3}{2}})$) is 0, thanks to a complex property (see [34,47]). The associated eigenform is localized near z_i, which can be proven thanks to Agmon estimates. Moreover, a precise estimate of this eigenform can be obtained thanks to a WKB expansion. The quasi-mode $\tilde{\phi}_i$ is then this eigenform multiplied by a suitable cut-off function.

This section is organized as follows. In Section B.4.1, we define a Witten Laplacian with mixed boundary conditions on a open domain $\dot{\Omega}_i \subset \Omega$ associated to each z_i, $i \in \{1, \dots, n\}$, and we study its spectrum. Section B.4.2 is dedicated to the construction of the quasi-modes $((\tilde{\phi}_i)_{i=1,\dots,n}, \tilde{u})$. In Section B.4.3, we prove Agmon estimates on the eigenform associated with the smallest eigenvalue of the Witten Laplacian with mixed boundary conditions on $\dot{\Omega}_i$ and in Section B.4.4 we compare this eigenform with a WKB approximation. We finally use this construction and these estimates to prove Theorem B.1 in Section B.4.5.

B.4.1 Geometric setting and definition of the Witten Laplacians with mixed boundary conditions

This section is organized as follows. In Section B.4.1.1, we discuss some general results on traces of differential forms and we introduce the Witten Laplacians with mixed tangential Dirichlet boundary conditions and normal Dirichlet boundary conditions on manifolds with boundary. In Section B.4.1.2, the domain $\dot{\Omega}_i \subset \Omega$ associated with each z_i, $i \in \{1, \dots, n\}$, is defined. Finally, Section B.4.1.3 is dedicated to the study of the spectrum of the Witten Laplacian with mixed tangential Dirichlet boundary conditions and normal Dirichlet boundary conditions on $\dot{\Omega}_i$.

B.4.1.1 Trace estimates for differential forms and Witten Laplacians with mixed boundary conditions

In this section, we first discuss some general results on traces of differential forms. This is crucial to then build the Witten Laplacians with mixed boundary conditions. In the following, $\dot{\Omega}$ refers to any submanifold $\dot{\Omega}$ of Ω with Lipschitz boundary. We will call such a submanifold a Lipschitz domain.

We first recall that for any Lipschitz domain $\dot{\Omega}$, the trace application

$$\begin{cases} \Lambda^{p+1}H^1(\dot{\Omega}) \to \Lambda^{p+1}H^{\frac{1}{2}}(\partial\dot{\Omega}) \\ \qquad G \mapsto G|_{\partial\Omega} \end{cases}$$

is a linear continuous and surjective application. We would like to present extensions of this result to less regular forms.

<u>Weak definition of traces</u>

For a Lipschitz domain $\dot{\Omega}$, let us introduce the functional spaces

$$\Lambda^p H_d(\dot{\Omega}) := \left\{ u \in \Lambda^p L^2(\dot{\Omega}),\ du \in \Lambda^{p+1} L^2(\dot{\Omega}) \right\} \tag{B.106}$$

and

$$\Lambda^p H_{d^*}(\dot{\Omega}) \ := \ \left\{ u \in \Lambda^p L^2(\dot{\Omega}),\ d^* u \in \Lambda^{p-1} L^2(\dot{\Omega}) \right\} \tag{B.107}$$

equipped with their natural graph norms. One recalls that for a differential form f in $L^2(\partial\dot{\Omega})$, the tangential and normal components are defined as follows:

$$f = \mathbf{t} f + \mathbf{n} f \quad \text{with} \quad \mathbf{t} f = \mathbf{i}_n (n^\flat \wedge f) \quad \text{and} \quad \mathbf{n} f = n^\flat \wedge (\mathbf{i}_n f), \tag{B.108}$$

where the superscript $\flat$ stands for the usual musical isomorphism: $n^\flat$ is the 1-form associated with the outgoing unit normal vector n. Moreover,

$$\|f\|^2_{L^2(\partial\dot{\Omega})} = \|\mathbf{t} f\|^2_{L^2(\partial\dot{\Omega})} + \|\mathbf{n} f\|^2_{L^2(\partial\dot{\Omega})} = \|n^\flat \wedge f\|^2_{L^2(\partial\dot{\Omega})} + \|\mathbf{i}_n f\|^2_{L^2(\partial\dot{\Omega})}.$$

The Green formula for differential forms $(u, v) \in \Lambda^p H^1(\dot{\Omega}) \times \Lambda^{p+1} H^1(\dot{\Omega})$ writes

$$\begin{aligned} \langle du, v \rangle_{L^2(\dot{\Omega})} - \langle u, d^* v \rangle_{L^2(\dot{\Omega})} &= \int_{\partial\dot{\Omega}} \langle n^\flat \wedge u, v \rangle_{T^*_\sigma \dot{\Omega}} d\sigma = \int_{\partial\dot{\Omega}} \langle n^\flat \wedge u, \mathbf{n} v \rangle_{T^*_\sigma \dot{\Omega}} d\sigma \\ &= \int_{\partial\dot{\Omega}} \langle u, \mathbf{i}_n v \rangle_{T^*_\sigma \dot{\Omega}} d\sigma = \int_{\partial\dot{\Omega}} \langle \mathbf{t} u, \mathbf{i}_n v \rangle_{T^*_\sigma \dot{\Omega}} d\sigma, \end{aligned} \tag{B.109}$$

where we used the standard relation $(n^\flat \wedge)^* = \mathbf{i}_n$.

Using this Green formula, the tangential (resp. normal) traces can be defined for forms in $\Lambda H_d(\dot{\Omega})$ (resp. $\Lambda H_{d^*}(\dot{\Omega})$) by duality. Indeed, for any $u \in \Lambda^p H_d(\dot{\Omega})$, $n^\flat \wedge u \in \Lambda^{p+1} H^{-\frac{1}{2}}(\partial\dot{\Omega})$ is defined by

$$\forall g \in \Lambda^{p+1} H^{\frac{1}{2}}(\partial\dot{\Omega}),\ \langle n^\flat \wedge u, g \rangle_{H^{-\frac{1}{2}}(\partial\dot{\Omega}), H^{\frac{1}{2}}(\partial\dot{\Omega})} = \langle du, G \rangle_{L^2(\dot{\Omega})} - \langle u, d^* G \rangle_{L^2(\dot{\Omega})}, \tag{B.110}$$

where G is any form in $\Lambda^{p+1} H^1(\dot{\Omega})$ whose trace in $\Lambda^{p+1} H^{\frac{1}{2}}(\partial\dot{\Omega})$ is g. This definition is independent of the chosen extension G. Similarly, for any $u \in \Lambda^p H_{d^*}(\dot{\Omega})$, $\mathbf{i}_n u \in \Lambda^{p-1} H^{-\frac{1}{2}}(\partial\dot{\Omega})$ is defined by

$$\forall g \in \Lambda^{p-1} H^{\frac{1}{2}}(\partial\dot{\Omega}),\ \langle \mathbf{i}_n u, g \rangle_{H^{-\frac{1}{2}}(\partial\dot{\Omega}), H^{\frac{1}{2}}(\partial\dot{\Omega})} = \langle u, dG \rangle_{L^2(\dot{\Omega})} - \langle d^* u, G \rangle_{L^2(\dot{\Omega})}, \tag{B.111}$$

where G is any extension of g in $\Lambda^{p-1} H^1(\dot{\Omega})$.

Let Γ be any subset of $\partial\dot{\Omega}$. For $u \in \Lambda^p H_d(\dot{\Omega})$, we will write $\mathbf{t} u|_\Gamma = 0$ if $n^\flat \wedge u|_\Gamma = 0$. If $u \in \Lambda^p H_d(\dot{\Omega})$ and $n^\flat \wedge u|_\Gamma \in \Lambda^{p+1} L^2(\Gamma)$, the tangential trace on Γ is defined by

$$\mathbf{t} u|_\Gamma := \mathbf{i}_n (n^\flat \wedge u) \in \Lambda^p L^2(\Gamma)\ ,\ \text{so that } \|\mathbf{t} u\|_{L^2(\Gamma)} = \|n^\flat \wedge u\|_{L^2(\Gamma)}. \tag{B.112}$$

Similarly, for $u \in \Lambda^p H_{d^*}(\dot{\Omega})$, we will write $\mathbf{n} u|_\Gamma = 0$ if $\mathbf{i}_n u|_\Gamma = 0$. If $u \in \Lambda^p H_{d^*}(\dot{\Omega})$ and $\mathbf{i}_n u|_\Gamma \in \Lambda^{p-1} L^2(\Gamma)$, the normal trace on Γ is defined by

$$\mathbf{n} u|_\Gamma := n^\flat \wedge (\mathbf{i}_n u) \in \Lambda^p L^2(\Gamma)\ ,\ \text{so that } \|\mathbf{n} u\|_{L^2(\Gamma)} = \|\mathbf{i}_n u\|_{L^2(\Gamma)}. \tag{B.113}$$

Lastly, if $u \in \Lambda^p H_d(\dot{\Omega}) \cap \Lambda^p H_{d^*}(\dot{\Omega})$ is such that $n^\flat \wedge u|_\Gamma \in \Gamma^{p+1} L^2(\Gamma)$ and $\mathbf{i}_n u \in \Gamma^{p-1} L^2(\Gamma)$ then u admits a trace $u|_\Gamma$ in $L^2(\Gamma)$ defined by

$$u|_\Gamma := \mathbf{t}u|_\Gamma + \mathbf{n}u|_\Gamma. \tag{B.114}$$

This definition is compatible with (B.108) and such a differential form satisfies

$$\|u|_\Gamma\|^2_{L^2(\Gamma)} = \|\mathbf{t}u|_\Gamma\|^2_{L^2(\Gamma)} + \|\mathbf{n}u|_\Gamma\|^2_{L^2(\Gamma)} = \|n^\flat \wedge u\|_{L^2(\Gamma)} + \|\mathbf{i}_n u\|_{L^2(\Gamma)}.$$

All the above definitions coincide moreover with the usual ones when u belongs to $\Lambda^\ell H^1(\dot{\Omega})$.

Let us finally note for further references that if traces are in $L^2(\partial\dot{\Omega})$, a direct consequence of the Green formula (B.109) is the following: for every $u, v \in \Lambda L^2(\dot{\Omega})^2$ such that $du, d^*u, d^*du, dd^*u, dv, d^*v \in \Lambda L^2(\dot{\Omega})$ and $n^\flat \wedge d^*_{f,h}u$, $\mathbf{i}_n d_{f,h}u$, $n^\flat \wedge v$, $\mathbf{i}_n v \in \Lambda L^2(\partial\dot{\Omega})$,

$$\begin{aligned}\langle (d_{f,h}d^*_{f,h} + d^*_{f,h}d_{f,h})u, v\rangle_{L^2(\dot{\Omega})} &= \langle d_{f,h}u, d_{f,h}v\rangle_{L^2(\dot{\Omega})} + \langle d^*_{f,h}u, d^*_{f,h}v\rangle_{L^2(\dot{\Omega})} \\ &+ h\int_{\partial\dot{\Omega}} \langle n^\flat \wedge d^*_{f,h}u, n^\flat \wedge (\mathbf{i}_n v)\rangle_{T^*_\sigma\dot{\Omega}} d\sigma - h\int_{\partial\dot{\Omega}} \langle n^\flat \wedge v, n^\flat \wedge (\mathbf{i}_n d_{f,h}u)\rangle_{T^*_\sigma\dot{\Omega}} d\sigma.\end{aligned} \tag{B.115}$$

<u>The Gaffney's inequality</u>

The following extension of Gaffney's inequality (see [65]) will be useful in the sequel (we refer to Section B.2.1.1 for the definitions of the Hilbert space $\Lambda^p H^1_T(\dot{\Omega})$ and $\Lambda^p H^1_N(\dot{\Omega})$).

Lemma B.54. *Let $\dot{\Omega}$ be a smooth domain. The equality*

$$\left\{u \in \Lambda^p L^2(\dot{\Omega}) \text{ s.t. } du, d^*u \in L^2(\dot{\Omega}) \text{ and } \mathbf{t}u = 0 \text{ on } \partial\dot{\Omega}\right\} = \Lambda^p H^1_T(\dot{\Omega})$$

holds algebraically and topologically, the functional space in the left-hand side being equipped with the norm associated with the scalar product

$$Q(u, v) := \langle u, v\rangle_{L^2(\dot{\Omega})} + \langle du, dv\rangle_{L^2(\dot{\Omega})} + \langle d^*u, d^*v\rangle_{L^2(\dot{\Omega})}.$$

In a similar way, the following equality holds algebraically and topologically:

$$\left\{u \in \Lambda^p L^2(\dot{\Omega}) \text{ s.t. } du, d^*u \in L^2(\dot{\Omega}) \text{ and } \mathbf{n}u = 0 \text{ on } \partial\dot{\Omega}\right\} = \Lambda^p H^1_N(\dot{\Omega}).$$

Notice that in the definition of the functional spaces above, the equalities $\mathbf{t}u = 0$ and $\mathbf{n}u = 0$ hold in the weak sense defined above (see (B.112) and (B.113)). A direct consequence of this lemma is that a differential form in $\Lambda H_d(\dot{\Omega}) \cap \Lambda H_{d^*}(\dot{\Omega})$ such that $\mathbf{t}u = 0$ or $\mathbf{n}u = 0$ on $\partial\dot{\Omega}$ admits a trace in $\Lambda L^2(\partial\dot{\Omega})$.

Remark B.12. *The statement of Gaffney's inequality in [65] reads as follows (see indeed Corollary 2.1.6 and Theorem 2.1.7 there):*

$$\exists C > 0,\ \forall u \in \Lambda^p H^1_T(\dot{\Omega}) \cup \Lambda^p H^1_N(\dot{\Omega}),\ \|u\|^2_{H^1(\dot{\Omega})} \le CQ(u, u). \tag{B.116}$$

Since it also holds that, for some $C' > 0$ and any $u \in \Lambda^p H^1(\dot{\Omega})$, $Q(u, u) \le C'\|u\|^2_{H^1(\dot{\Omega})}$, the scalar products $\langle\cdot,\cdot\rangle_{H^1}$ and $Q(\cdot,\cdot)$ are then equivalent on both $\Lambda^p H^1_T(\dot{\Omega})$ and $\Lambda^p H^1_N(\dot{\Omega})$. The above lemma can be seen as a generalization of this result.

Proof. We only prove the first equality in Lemma B.54, the second one being similar. Let us define

$$H := \left\{ u \in \Lambda^p L^2(\dot{\Omega}) \text{ s.t. } du, d^*u \in \Lambda L^2(\dot{\Omega}) \quad \text{and} \quad n^\flat \wedge u = 0 \text{ on } \partial\dot{\Omega} \right\}$$

which is a Hilbert space once equipped with the scalar product Q. From Gaffney's inequality (B.116), $\Lambda^p H^1_T(\dot{\Omega})$ is a closed subset of H and to conclude, we just have to show that $\left(\Lambda^p H^1_T(\dot{\Omega})\right)^\perp = \{0\}$, the orthogonal complement of H being taken with respect to the norm inherited from Q. Consider then $u \in H$ such that for any $v \in \Lambda^p H^1_T(\dot{\Omega})$,

$$0 = Q(u,v) = \langle u, v\rangle_{L^2(\dot{\Omega})} + \langle du, dv\rangle_{L^2(\dot{\Omega})} + \langle d^*u, d^*v\rangle_{L^2(\dot{\Omega})}.$$

The above equality holds in particular for every $v \in D$ where

$$D = \{v \in \Lambda^p H^2(\dot{\Omega}),\ \mathbf{t}v|_{\partial\dot{\Omega}} = \mathbf{t}d^*v|_{\partial\dot{\Omega}} = 0\}. \tag{B.117}$$

Fix such a v. Since $n^\flat \wedge u = 0$ on $\partial\dot{\Omega}$, applying (B.110) to u and $dv \in \Lambda^{p+1}H^1(\dot{\Omega})$ then leads to

$$\langle du, dv\rangle_{L^2(\dot{\Omega})} = \langle u, d^*dv\rangle_{L^2(\dot{\Omega})}.$$

Applying also (B.111) to u and $d^*v \in \Lambda^{p-1}H^1(\dot{\Omega})$ gives

$$\langle d^*u, d^*v\rangle_{L^2(\dot{\Omega})} = \langle u, dd^*v\rangle_{L^2(\dot{\Omega})} - \langle \mathbf{i}_n u, d^*v|_{\partial\dot{\Omega}}\rangle_{H^{-\frac{1}{2}}(\partial\dot{\Omega}), H^{\frac{1}{2}}(\partial\dot{\Omega})}.$$

Since $\Lambda^p\mathcal{C}^\infty\left(\overline{\dot{\Omega}}\right)$ is densely embedded in both $\Lambda^p H_d(\dot{\Omega})$ and $\Lambda^p H_{d^*}(\dot{\Omega})$ (see for example [41, Proposition 3.1]), we have moreover for some sequence $(u_k)_{k\in\mathbb{N}}$ of $\Lambda^p\mathcal{C}^\infty\left(\overline{\dot{\Omega}}\right)$ forms:

$$\begin{aligned}
\langle \mathbf{i}_n u, d^*v|_{\partial\dot{\Omega}}\rangle_{H^{-\frac{1}{2}}(\partial\dot{\Omega}), H^{\frac{1}{2}}(\partial\dot{\Omega})} &= \lim_{k\to+\infty} \int_{\partial\dot{\Omega}} \langle \mathbf{i}_n u_k, d^*v\rangle_{T^*_\sigma\dot{\Omega}} d\sigma \\
&= \lim_{k\to+\infty} \int_{\partial\dot{\Omega}} \langle \mathbf{i}_n u_k, n^\flat \wedge (\mathbf{i}_n d^*v)\rangle_{T^*_\sigma\dot{\Omega}} d\sigma \\
&= 0,
\end{aligned}$$

where the second equality is a consequence of $\mathbf{t}d^*v|_{\partial\dot{\Omega}} = 0$. It consequently follows

$$0 = \langle u, v\rangle_{L^2(\dot{\Omega})} + \langle u, d^*dv\rangle_{L^2(\dot{\Omega})} + \langle u, dd^*v\rangle_{L^2(\dot{\Omega})} = \langle u, (I + \Delta^{(p)}_H)v\rangle_{L^2(\dot{\Omega})}, \tag{B.118}$$

where $\Delta^{(p)}_H$ denotes the Hodge Laplacian on $\dot{\Omega}$ with domain D defined by (B.117). Since the unbounded operator $(\Delta^{(p)}_H, D)$ is selfadjoint and nonnegative on $\Lambda^p L^2(\dot{\Omega})$, we have in particular $\mathbb{R}an(I + \Delta^{(p)}_H) = \Lambda^p L^2(\dot{\Omega})$ and we deduce from (C.152) that $u = 0$, which completes the proof. ∎

The case of mixed normal-tangential Dirichlet boundary conditions

Let Γ_T and Γ_N be two disjoint open subsets of $\partial\dot{\Omega}$ such that $\overline{\Gamma_T} \cup \overline{\Gamma_N} = \partial\dot{\Omega}$. The objective of this section is to consider differential forms such that $\mathbf{t}u = 0$ on Γ_T and $\mathbf{n}u = 0$ on Γ_N, and to state results on the existence of a trace in $L^2(\partial\dot{\Omega})$ for such differential forms, as well as subelliptic estimates.

In general, a trace in $L^2(\partial\dot{\Omega})$ does not exist in such a setting [8, 41]: one needs a geometric assumption, namley that Γ_T and Γ_N meet at an angle strictly smaller than π. This means that the angle between Γ_T and Γ_N measured in $\dot{\Omega}$ is smaller than π. More precisely, see [8, 41], locally around any point $x_0 \in \overline{\Gamma_T} \cap \overline{\Gamma_N}$, one requires that there exists a local system of coordinates $(x_1, x'', x_n) \in \mathbb{R} \times \mathbb{R}^{d-2} \times \mathbb{R}$ on a neighborhood V_0 of x_0, and two Lipschitz functions $\varphi : \mathbb{R}^{n-1} \to \mathbb{R}$ and $\psi : \mathbb{R}^{n-2} \to \mathbb{R}$ such that $\dot{\Omega} \cap V_0 = \{x_n > \varphi(x_1, x'')\}$, $\Gamma_T \cap V_0 = \{x_n = \varphi(x_1, x'')$ and $x_1 > \psi(x'')\}$ and $\Gamma_N \cap V_0 = \{x_n = \varphi(x_1, x'')$ and $x_1 < \psi(x'')\}$ and

$$\begin{aligned} \partial_{x_1}\varphi(x_1, x'') \geq \kappa \text{ on } x_1 > \psi(x'') \\ \partial_{x_1}\varphi(x_1, x'') \leq -\kappa \text{ on } x_1 < \psi(x'') \end{aligned} \tag{B.119}$$

for some positive κ. This is equivalent to the existence of a smooth vector field θ on $\partial\dot{\Omega}$ such that $\langle \theta, n\rangle < 0$ on Γ_T and $\langle \theta, n\rangle > 0$ on Γ_N, which is one of the key ingredient of the proofs used in [8, 41].

Let Γ be any subset of $\partial\dot{\Omega}$. According to [41, Proposition 3.1], the space

$$\left\{u \in \Lambda^p \mathcal{C}^\infty\left(\overline{\dot{\Omega}}\right),\ u \equiv 0 \text{ in a neighborhood of } \partial\dot{\Omega} \setminus \Gamma\right\}$$

is densely embedded in both

$$\Lambda^p H_{d,\Gamma}(\dot{\Omega}) := \left\{u \in \Lambda^p H_d(\dot{\Omega}),\ \operatorname{supp}(n^\flat \wedge u) \subset \overline{\Gamma}\right\}$$

and

$$\Lambda^p H_{d^*,\Gamma}(\dot{\Omega}) := \left\{u \in \Lambda^p H_{d^*}(\dot{\Omega}),\ \operatorname{supp}(\mathbf{i}_n u) \subset \overline{\Gamma}\right\}.$$

In addition, according to [41, Theorem 3.4], for $(u, v) \in \Lambda^p H_d(\dot{\Omega}) \times \Lambda^{p+1} H_{d^*}(\dot{\Omega})$ satisfying the trace conditions

$$\mathbf{i}_n v \in \Lambda^p L^2(\partial\dot{\Omega}),\ \operatorname{supp} \mathbf{i}_n v \subset \Gamma \quad \text{and} \quad n^\flat \wedge u \in \Lambda^{p+1} L^2(\Gamma),$$

or

$$n^\flat \wedge u \in \Lambda^{p+1} L^2(\partial\dot{\Omega}),\ \operatorname{supp}(n^\flat \wedge u) \subset \Gamma \quad \text{and} \quad \mathbf{i}_n v \in \Lambda^p L^2(\Gamma),$$

one has the following Green formula (compare with (B.109)):

$$\begin{aligned} \langle du, v\rangle_{L^2(\dot{\Omega})} - \langle u, d^* v\rangle_{L^2(\dot{\Omega})} &= \int_\Gamma \langle n^\flat \wedge u, n^\flat \wedge (\mathbf{i}_n v)\rangle_{T^*_\sigma \dot{\Omega}} d\sigma \\ &= \int_\Gamma \langle \mathbf{i}_n(n^\flat \wedge u), \mathbf{i}_n v\rangle_{T^*_\sigma \dot{\Omega}} d\sigma. \end{aligned} \tag{B.120}$$

One is now ready to state the following proposition implied by Theorems 1.1 and 1.2 of [41] (see also Theorems 4.1 and 4.2 of [28]).

Proposition B.55. *Let us assume that $\dot{\Omega}$ is a Lipschitz domain. Let Γ_T and Γ_N be two disjoint Lipschitz open subsets of $\partial\dot{\Omega}$ such that $\overline{\Gamma_T} \cup \overline{\Gamma_N} = \partial\dot{\Omega}$ and such that Γ_T and Γ_N meet at an angle strictly smaller than π. Then, the following results hold:*
(i) Let u be a differential form such that

$$u \in \Lambda^p L^2(\dot{\Omega}),\ du \in L^2(\dot{\Omega}), d^* u \in L^2(\dot{\Omega}),\ \mathbf{t}u|_{\Gamma_T} = 0 \text{ and } \mathbf{n}u|_{\Gamma_N} = 0.$$

Then u satisfies

$$u \in \Lambda^p H^{\frac{1}{2}}(\dot{\Omega}) \quad \textit{and} \quad \mathbf{i}_n u,\ n^\flat \wedge u \in \Lambda^p L^2(\partial\dot{\Omega})$$

as well as the subelliptic estimate:

$$\|u\|_{H^{\frac{1}{2}}(\dot{\Omega})} + \|u|_{\partial\dot{\Omega}}\|_{L^2(\partial\dot{\Omega})} \ \leq\ C\left(\|u\|_{L^2(\dot{\Omega})} + \|du\|_{L^2(\dot{\Omega})} + \|d^*u\|_{L^2(\dot{\Omega})}\right), \tag{B.121}$$

where $u|_{\partial\dot{\Omega}}$ is defined by (B.114).

(ii) The unbounded operators $d_T^{(p)}(\dot{\Omega})$ and $\delta_N^{(p)}(\dot{\Omega})$ on $\Lambda^p L^2(\dot{\Omega})$ defined by

$$d_T^{(p)}(\dot{\Omega}) = d_{f,h}^{(p)} \textit{ with domain } D\left(d_T^{(p)}(\dot{\Omega})\right) = \left\{u \in \Lambda^p L^2(\dot{\Omega}),\ d_{f,h}u \in \Lambda^{p+1}L^2(\dot{\Omega}),\ \mathbf{t}u|_{\Gamma_T} = 0\right\},$$

and

$$\delta_N^{(p)}(\dot{\Omega}) = \left(d_{f,h}^{(p)}\right)^* \textit{ with domain } D\left(\delta_N^{(p)}(\dot{\Omega})\right) = \left\{u \in \Lambda^p L^2(\dot{\Omega}),\ d_{f,h}^*u \in \Lambda^{p-1}L^2(\dot{\Omega}),\ \mathbf{n}u|_{\Gamma_N} = 0\right\},$$

are closed, densely defined, and adjoint one of each other.

Note that in the point *(i)* of Proposition B.55, d and d^* can be replaced by $d_{f,h}$ and $d_{f,h}^*$ owing to the relations $d_{f,h} = hd + df\wedge$ and $d_{f,h}^* = hd^* + \mathbf{i}_{\nabla f}$. Moreover, the point *(ii)* is actually proven in [28, 41] for d and d^* but remains true for $d_{f,h}$ and $d_{f,h}^*$ since $(df\wedge)^* = \mathbf{i}_{\nabla f}$ on $L^2(\dot{\Omega})$.

The mixed Witten Laplacian $\Delta_{f,h}^M(\dot{\Omega})$

We are now in position to define the mixed Witten Laplacian $\Delta_{f,h}^M(\dot{\Omega})$ (the upperscript M stands for mixed boundary conditions) with tangential Dirichlet boundary conditions on Γ_T and normal Dirichlet boundary conditions on Γ_N (see [28,41] for more results on such operators). The operator $\Delta_{f,h}^{M,(p)}(\dot{\Omega})$ on $L^2(\dot{\Omega})$ is defined by

$$\Delta_{f,h}^{M,(p)}(\dot{\Omega}) := d_T^{(p-1)}(\dot{\Omega}) \circ \delta_N^{(p)}(\dot{\Omega}) + \delta_N^{(p+1)}(\dot{\Omega}) \circ d_T^{(p)}(\dot{\Omega}), \tag{B.122}$$

in the sense of composition of unbounded operators, where d_T and δ_N have been introduced in Proposition B.55. Noticing that for any $u \in \Lambda^p H_d(\dot{\Omega})$ such that $\mathbf{t}u|_{\Gamma_T} = 0$, one has $\mathbf{t}du|_{\Gamma_T} = 0$, which is well known for $u \in \Lambda^p H^1(\dot{\Omega})$ and can be checked here using (B.110). Likewise, one has $\mathbf{t}d_{f,h}u|_{\Gamma_T} = 0$ for $u \in \Lambda^p H_d(\dot{\Omega})$ such that $\mathbf{t}u|_{\Gamma_T} = 0$. This implies in particular

$$\begin{cases} \overline{\mathrm{Im}\ d_T} \subset \ \mathrm{Ker}\ d_T \quad \text{and} \quad d_T^2 = 0 \\ \overline{\mathrm{Im}\ \delta_N} \subset \ \mathrm{Ker}\ \delta_N \quad \text{and} \quad \delta_N^2 = 0 \end{cases} \tag{B.123}$$

(since $d_{f,h}d_{f,h} = 0$ in the distributional sense). Owing to this last relation and to Proposition B.55, a result due to Gaffney (see e.g. the proof of [28, Propositions 2.3 and 2.4]) states that $\Delta_{f,h}^{M,(p)}(\dot{\Omega})$ is a densely defined nonnegative selfadjoint operator on $L^2(\dot{\Omega})$ (with domain (B.124)-see below).

The domain $D\left(\mathcal{Q}_{f,h}^{M,(p)}(\dot{\Omega})\right)$ of the closed quadratic form $\mathcal{Q}_{f,h}^{M,(p)}(\dot{\Omega})$ associated with $\Delta_{f,h}^{M,(p)}(\dot{\Omega})$ is given by

$$\begin{aligned} D\left(\mathcal{Q}_{f,h}^{M,(p)}(\dot{\Omega})\right) &= D\left(d_T^{(p)}(\dot{\Omega})\right) \cap D\left(\delta_N^{(p)}(\dot{\Omega})\right) \\ &= \left\{v \in \Lambda^p L^2(\dot{\Omega}),\ dv \in L^2(\dot{\Omega}), d^*v \in L^2(\dot{\Omega}),\ \mathbf{t}v|_{\Gamma_T} = 0 \text{ and } \mathbf{n}v|_{\Gamma_N} = 0\right\} \end{aligned}$$

and for any $u, v \in D\left(\mathcal{Q}_{f,h}^{M,(p)}(\dot{\Omega})\right)$,

$$\mathcal{Q}_{f,h}^{M,(p)}(\dot{\Omega})(u,v) = \langle d_T u, d_T v\rangle_{L^2} + \langle \delta_N u, \delta_N v\rangle_{L^2}.$$

This is proven in [28, Theorem 2.8].

The domain $D\left(\Delta_{f,h}^{M,(p)}(\dot{\Omega})\right)$ is explicitly given by:

$$\begin{aligned} D\left(\Delta_{f,h}^{M,(p)}(\dot{\Omega})\right) = \Big\{ & u \in L^2(\dot{\Omega}) \text{ s.t. } d_{f,h}u,\ d_{f,h}^* u,\ d_{f,h}^* d_{f,h} u,\ d_{f,h} d_{f,h}^* u \in L^2(\dot{\Omega}) \\ & \text{and } \mathbf{t}u|_{\Gamma_T} = 0,\ \mathbf{t}d_{f,h}^* u|_{\Gamma_T} = 0,\ \mathbf{n}u|_{\Gamma_N} = 0,\ \mathbf{n}d_{f,h}u|_{\Gamma_N} = 0 \Big\}. \end{aligned} \tag{B.124}$$

The traces $\mathbf{t}d_{f,h}^* u$ and $\mathbf{n}d_{f,h}u$ are a priori defined in $H^{-\frac{1}{2}}(\dot{\Omega})$ but actually belong to $L^2(\dot{\Omega})$. Indeed, we have $\mathbf{n}d_{f,h}u|_{\Gamma_N} = 0$ by definition of $D\left(\Delta_{f,h}^{M,(p)}(\dot{\Omega})\right)$ and $\mathbf{t}d_{f,h}u|_{\Gamma_T} = 0$ by (B.110), so $d_{f,h}u$ is in $D\left(\mathcal{Q}_{f,h}^{M,(p+1)}(\dot{\Omega})\right)$ and therefore has a trace in $L^2(\dot{\Omega})$ according to Proposition B.55. This argument also holds for $d_{f,h}^* u \in D\left(\mathcal{Q}_{f,h}^{M,(p-1)}(\dot{\Omega})\right)$.

We end up this section with the following lemma which will be frequently used in the sequel.

Lemma B.56. *Under the assumptions of Proposition B.55 and if Γ_T and Γ_N are C^∞, the following formula holds: for any $u \in D\left(\mathcal{Q}_{f,h}^{M,(p)}(\dot{\Omega})\right)$,*

$$\begin{aligned} \mathcal{Q}_{f,h}^{M,(p)}(\dot{\Omega})(u,u) &= \|d_{f,h}u\|_{L^2(\dot{\Omega})}^2 + \left\|d_{f,h}^* u\right\|_{L^2(\dot{\Omega})}^2 \\ &= h^2 \|du\|_{L^2(\dot{\Omega})}^2 + h^2 \|d^* u\|_{L^2(\dot{\Omega})}^2 \\ &\quad + \||\nabla f|\, u\|_{L^2(\dot{\Omega})}^2 + h\langle(\mathcal{L}_{\nabla f} + \mathcal{L}_{\nabla f}^*)u, u\rangle_{L^2(\dot{\Omega})} \\ &\quad - h\left(\int_{\Gamma_T} - \int_{\Gamma_N}\right) \langle u, u\rangle_{T_\sigma^*\dot{\Omega}} \partial_n f \, d\sigma, \end{aligned} \tag{B.125}$$

where $\mathcal{L}$ stands for the Lie derivative.

Notice that the boundary integral terms are well defined since $u|_{\partial\dot{\Omega}} \in L^2(\dot{\Omega})$ thanks to point *(i)* in Proposition B.55.

Proof. For $u \in D\left(\mathcal{Q}_{f,h}^{M,(p)}(\dot{\Omega})\right)$, one first gets by straightforward computations,

$$\begin{aligned} \|d_{f,h}u\|_{L^2(\dot{\Omega})}^2 + \left\|d_{f,h}^* u\right\|_{L^2(\dot{\Omega})}^2 &= h^2 \|du\|_{L^2(\dot{\Omega})}^2 + h^2 \|d^* u\|_{L^2(\dot{\Omega})}^2 + \|df \wedge u\|_{L^2(\dot{\Omega})}^2 \\ &\quad + \|\mathbf{i}_{\nabla f} u\|_{L^2(\dot{\Omega})}^2 + \ h(\langle df \wedge u, du\rangle_{L^2(\dot{\Omega})} + \langle du, df \wedge u\rangle \\ &\quad + \langle d^* u, \mathbf{i}_{\nabla f} u\rangle_{L^2(\dot{\Omega})} + \langle \mathbf{i}_{\nabla f} u, d^* u\rangle) \\ &= h^2 \|du\|_{L^2(\dot{\Omega})}^2 + h^2 \|d^* u\|_{L^2(\dot{\Omega})}^2 + \||\nabla f|\, u\|_{L^2(\dot{\Omega})}^2 \\ &\quad + h\langle(\mathcal{L}_{\nabla f} + \mathcal{L}_{\nabla f}^*)u, u\rangle_{L^2(\dot{\Omega})} + h(\langle df \wedge u, du\rangle_{L^2(\dot{\Omega})} \\ &\quad - \langle d^*(df \wedge u), u\rangle_{L^2(\dot{\Omega})} - \langle d\mathbf{i}_{\nabla f} u, u\rangle_{L^2(\dot{\Omega})} + \langle \mathbf{i}_{\nabla f} u, d^* u\rangle_{L^2(\dot{\Omega})}), \end{aligned}$$

where the last equality holds thanks to the the relations $(d\varphi\wedge)^* = \mathbf{i}_{\nabla\varphi}$,

$$\mathcal{L}_{\nabla f} = d \circ \mathbf{i}_{\nabla\varphi} + \mathbf{i}_{\nabla\varphi} \circ d \quad \text{and} \quad \mathbf{i}_{\nabla\varphi}(d\varphi \wedge u) + d\varphi \wedge (\mathbf{i}_{\nabla\varphi} u) = |\nabla\varphi|^2 u.$$

To get the boundary integral terms in (B.125) one uses (B.120), which gives here, since $u \in D\left(\mathcal{Q}_{f,h}^{M,(p)}(\dot{\Omega})\right)$ and $df \wedge u$, $\mathbf{i}_{\nabla f} u \in \Lambda H_d(\dot{\Omega}) \cap \Lambda H_{d^*}(\dot{\Omega})$:

$$\langle df \wedge u, du\rangle_{L^2(\dot{\Omega})} - \langle d^*(df \wedge u), u\rangle_{L^2(\dot{\Omega})} = \int_{\Gamma_N} \langle n^\flat \wedge u, n^\flat \wedge \mathbf{i}_n(df \wedge u)\rangle_{T^*_\sigma \dot{\Omega}} d\sigma \quad \text{(B.126)}$$

and

$$\langle \mathbf{i}_{\nabla f} u, d^* u\rangle_{L^2(\dot{\Omega})} - \langle d\mathbf{i}_{\nabla f} u, u\rangle_{L^2(\dot{\Omega})} = -\int_{\Gamma_T} \langle n^\flat \wedge \mathbf{i}_{\nabla f} u, n^\flat \wedge \mathbf{i}_n u\rangle_{T^*_\sigma \dot{\Omega}} d\sigma. \quad \text{(B.127)}$$

Now, note that by Lemma B.54, u is a $\Lambda^p H^1$ form outside $\overline{\Gamma_T} \cap \overline{\Gamma_N}$ and then admits a boundary trace defined a.e. on $\partial\dot{\Omega}$ which belongs to $L^2_{\text{loc}}(\partial\dot{\Omega} \setminus (\overline{\Gamma_T} \cap \overline{\Gamma_N}))$. But this trace has to be $u|_{\partial\dot{\Omega}}$ as defined by (B.114) and is hence a $L^2(\partial\dot{\Omega})$ form owing to the first point of Proposition B.55. The proof follows easily: looking at (B.126) for example, one gets, defining $\Gamma_N^\varepsilon := \{x \in \Gamma_N,\ d^{\partial\dot{\Omega}}(x, \partial\Gamma_N) > \varepsilon\}$,

$$\begin{aligned}
\int_{\Gamma_N} \langle n^\flat \wedge u, n^\flat \wedge \mathbf{i}_n(df \wedge u)\rangle_{T^*_\sigma \dot{\Omega}} d\sigma &= \lim_{\varepsilon \to 0^+} \int_{\Gamma_N^\varepsilon} \langle n^\flat \wedge u, n^\flat \wedge \mathbf{i}_n(df \wedge u)\rangle_{T^*_\sigma \dot{\Omega}} d\sigma \\
&= \lim_{\varepsilon \to 0^+} \int_{\Gamma_N^\varepsilon} \langle u, \mathbf{i}_n(n^\flat \wedge \mathbf{i}_n(df \wedge u))\rangle_{T^*_\sigma \dot{\Omega}} d\sigma \\
&= \lim_{\varepsilon \to 0^+} \int_{\Gamma_N^\varepsilon} \langle u, \mathbf{i}_n(df \wedge u)\rangle_{T^*_\sigma \dot{\Omega}} d\sigma \\
&= \lim_{\varepsilon \to 0^+} \int_{\Gamma_N^\varepsilon} (\partial_n f \langle u, u\rangle_{T^*_\sigma \dot{\Omega}} - \langle u, df \wedge \mathbf{i}_n u\rangle_{T^*_\sigma \dot{\Omega}}) d\sigma \\
&= \int_{\Gamma_N} \partial_n f \langle u, u\rangle_{T^*_\sigma \dot{\Omega}} d\sigma,
\end{aligned}$$

where we used the usual trace properties for H^1 forms on Γ_N^ε, the fact that $\mathbf{i}_n u = 0$ at the second to last line and the Lebesgue dominated convergence theorem at the last line. ∎

Remark B.13. *Lemma B.56 will be applied several times to the set $\dot{\Omega}$ constructed in Proposition B.58 below. Actually, the set Γ_N which is constructed in Proposition B.58 (see indeed $\Gamma_{2,i}$ there) is not C^∞ and is equal to $\Gamma_N = \Gamma_{N,1} \cup \Gamma_{N,2} \cup \left(\partial\Gamma_{N,1} \cap \partial\Gamma_{N,2}\right)$ where $\Gamma_{N,1}$ and $\Gamma_{N,2}$ are two C^∞ open subsets of $\partial\dot{\Omega}$ which intersect at an angle $\frac{3}{2}\pi$ (see Figures B.10 and B.11). However, Lemma B.56 is still valid for the set $\dot{\Omega}$ constructed in Proposition B.58. Indeed, in the proof Lemma B.56, it is sufficient to change the definition of Γ_N^ε as follows: $\Gamma_N^\varepsilon = \{x \in \Gamma_{N,1},\ d^{\partial\dot{\Omega}}(x, \partial\Gamma_{N,1}) > \varepsilon\} \cup \{x \in \Gamma_{N,2},\ d^{\partial\dot{\Omega}}(x, \partial\Gamma_{N,2}) > \varepsilon\}$.*

B.4.1.2 Construction of the domain $\dot{\Omega}_i$

In this section weassumes **[H1]**, **[H2]** and **[H3]**. Let us consider $z_i \in \{z_1, \ldots, z_n\}$ a local minimum of $f|_{\partial\Omega}$. The objective of this section is to build the domain $\dot{\Omega}_i$ on which the Witten Laplacian with mixed tangential-normal boundary conditions will be defined.

This auxiliary operator will be a Witten Laplacian associated with tangential and normal Dirichlet boundary conditions, such that z_i remains the only generalized critical point. Let us recall that $x_0 \in \Omega$ is the minimum of f on $\overline{\Omega}$. Let Ω_0 be a small smooth open neighborhood of x_0 such that the $\partial_n f < 0$ on $\Gamma_0 = \partial\Omega_0$, n being the outward normal derivative to $\Omega \setminus \Omega_0$. Let $\Gamma_{1,i}$ denote a subset of B_{z_i}, as large as we want in B_{z_i}. The basic idea is to define $\dot{\Omega} = \Omega \setminus \overline{\Omega_0}$ and to consider a Witten Laplacian on $\dot{\Omega}$, with tangential zero boundary conditions on $\Gamma_0 \cup \Gamma_{1,i}$ and with normal zero boundary conditions on $\partial\Omega \setminus \overline{\Gamma_{1,i}}$. This would indeed yield an operator on a domain $\dot{\Omega}$ with a single generalized critical point, namely z_i. There is however a technical difficulty in this approach, related to the fact that differential forms with mixed normal and tangential Dirichlet boundary conditions are singular at the boundary between the domains where tangential and normal boundary conditions are applied, as explained in Section B.4.1.1. With the previous construction, $\Gamma_{1,i}$ and $\partial\Omega\setminus\overline{\Gamma_{1,i}}$ meet at an angle π. We therefore need to define a domain $\dot{\Omega}_i$ stricly included in $\Omega \setminus \overline{\Omega_0}$, with boundary $\partial\dot{\Omega}_i = \overline{\Gamma_0} \cup \overline{\Gamma_{1,i}} \cup \overline{\Gamma_{2,i}}$ where $\Gamma_0 = \partial\Omega_0$ as defined above, $\Gamma_{1,i} \cap \Gamma_{2,i} = \emptyset$, $\Gamma_{1,i} \subset B_{z_i}$ is as large as we want in B_{z_i} and $\Gamma_{2,i}$ meets $\Gamma_{1,i}$ at an angle strictly smaller than π (see (B.119) above for a proper definition). We will then consider a Witten Laplacian with tangential zero boundary conditions on $\Gamma_0 \cap \Gamma_{1,i}$ and normal zero boundary conditions on $\Gamma_{2,i}$. Moreover, in order not to introduce new generalized critical point on $\Gamma_{2,i}$, we would like to keep the property $\partial_n f > 0$ on $\Gamma_{2,i}$ (where n denotes the outward normal derivative to $\dot{\Omega}_i$). The aim of this section is indeed to define such a domain $\dot{\Omega}_i$.

A system of coordinates on a neighborhood of $\partial\Omega$.

Let us consider the function f_- defined on a neighborhood $V_{\partial\Omega}$ of $\partial\Omega$, as introduced in Proposition B.51. Recall that $f_-(x) = 0$ for $x \in \partial\Omega$ and that $V_{\partial\Omega}$ can be chosen such that $f_- > 0$ on $V_{\partial\Omega} \setminus \partial\Omega$ and $|\nabla f_-| \neq 0$ on $V_{\partial\Omega}$. Let us now consider $\varepsilon > 0$ such that

$$V_\varepsilon = \{y \in \Omega,\, 0 \leq f_-(y) \leq \varepsilon\} \subset V_{\partial\Omega}.$$

For any $x \in V_\varepsilon$, the dynamics

$$\begin{cases} \gamma_x'(t) = -\dfrac{\nabla f_-}{|\nabla f_-|^2}(\gamma_x(t)) \\ \gamma_x(0) = x \end{cases} \tag{B.128}$$

is such that $\gamma_x(t_x) \in \partial\Omega$, where

$$t_x = \inf\{t,\, \gamma_x(t) \notin \operatorname{int} V_\varepsilon\}.$$

This is indeed a consequence of the fact that $\frac{d}{dt} f_-(\gamma_x(t)) = -1 < 0$ on $[0, t_x)$.

The application

$$\Gamma : \begin{cases} V_\varepsilon \to \partial\Omega \times [-\varepsilon, 0] \\ x \mapsto (\gamma_x(t_x), -t_x) \end{cases}$$

defines a C^∞ diffeomorphism. The inverse application of Γ is $(x', x_d) \in \partial\Omega \times [-\varepsilon, 0] \mapsto \gamma_{x'}(x_d)$.

Definition B.9. *Let us assume that the hypothesis **[H3]** holds. Let us define the following system of coordinates for $x \in V_\varepsilon$:*

$$\forall x \in V_\varepsilon,\, (x'(x), x_d(x)) = (\gamma_x(t_x), -t_x) \in \partial\Omega \times [-\varepsilon, 0]. \tag{B.129}$$

Notice that, by construction (since $\frac{d}{dt} f_-(\gamma_x(t)) = -1$),

$$x_d(x) = -f_-(x).$$

Thus, in this system of coordinates, $\{x_d = 0\} = \partial\Omega$ and $\{x_d < 0\} = \Omega \cap V_\varepsilon$.

We will sometimes need to use a local system of coordinates in $\partial\Omega$, that we will then denote by the same notation x'. By using the same procedure as above, (x', x_d) then defines a local system of coordinates. Let us make this precise. For $y \in \partial\Omega$, let us consider $x' : V_y \to \mathbb{R}^{d-1}$ a smooth local system of coordinates in $\partial\Omega$, in a neighborhood $V_y \subset \partial\Omega$ of y. These coordinates are then extended in a neighborhood of V_y in Ω, as constant along the integral curves of $\gamma'(t) = \frac{\nabla f_-}{|\nabla f_-|^2}(\gamma(t))$, for $t \in [0, \varepsilon]$. The function $x \mapsto (x', x_d)$ (where, we recall, $x_d(x) = -f_-(x)$) thus defines a smooth system of coordinates in a neighborhood W_y of y in $\overline{\Omega}$. In this system of coordinates, the tensor metric G writes:

$$G(x', x_d) = G_{dd}(x', x_d)\, dx_d^2 + \sum_{i,j=1}^{d-1} G_{ij}(x', x_d)\, dx_i dx_j.$$

where $x' = (x_1, \ldots, x_{d-1})$. In particular if $\psi : V_y \to \mathbb{R}$ is a Lipschitz function which only depends on x', it holds a.e. on V_y:

$$|\nabla\psi(x', x_d)| = |\nabla(\psi|_{\Sigma_{x_d}})(x')|, \tag{B.130}$$

where $\forall a > 0$, $\Sigma_a := \{x \in V_\eta,\, x_d(x) = a\}$ is endowed with the Riemannian structure induced by the Riemannian structure in Ω.

<u>Definitions of the functions Ψ_i, $f_{+,i}$ and $f_{-,i}$.</u>

Definition B.10. *Let us assume that the hypotheses **[H1]** and **[H3]** hold. Let us consider z_i a local minimum of $f|_{\partial\Omega}$ as introduced in hypothesis **[H2]**. Let us define on Ω the following Lipschitz functions*

$$\Psi_i(x) := d_a(x, z_i), \quad f_{+,i} := \frac{\Psi_i + f - f(z_i)}{2} \text{ and } f_{-,i} := \frac{\Psi_i - (f - f(z_i))}{2}.$$

Owing to $\Psi_i(x) = d_a(x, z_i) \geq |f(x) - f(z_i)|$ for all $x \in \Omega$, the functions $f_{\pm,i}$ are non negative and

$$f = f(z_i) + f_{+,i} - f_{-,i} \text{ and } \Psi_i = f_{+,i} + f_{-,i} \text{ on } \Omega.$$

Let $\Gamma_{1,i} \subset B_{z_i}$ be an open smooth $d-1$ dimensional manifold with boundary such that $z_i \in \Gamma_{1,i}$ and $\overline{\Gamma_{1,i}} \subset B_{z_i}$. From Proposition B.52, there exists a neighborhood of $\overline{\Gamma_{1,i}}$ in $\overline{\Omega}$, denoted $V_{\Gamma_{1,i}}$, such that $\overline{\partial V_{\Gamma_{1,i}} \cap \partial\Omega} \subset B_{z_i}$ and for all $x \in V_{\Gamma_{1,i}}$,

$$\Psi_i(x) = \Phi(x) - f(z_i).$$

where Φ is the solution to the eikonal equation in a neighborhood of the boundary (see Proposition B.50). Notice that it implies that on $V_{\Gamma_{1,i}}$ the function $f_{-,i}$ coincides with the function f_- defined in Proposition B.51 on $V_{\partial\Omega} \cap V_{\Gamma_{1,i}}$. Moreover, it implies that the functions $f_{\pm,i}$ are C^∞ on $V_{\Gamma_{1,i}}$ and one has:

$$\text{on } V_{\Gamma_{1,i}} \cap \partial\Omega, \quad f_{+,i} = f - f(z_i), \quad f_{-,i} = 0, \quad \partial_n f_{+,i} = 0, \text{ and } \partial_n f_{-,i} = -\partial_n f,$$

where n is the unit outward normal to Ω. Therefore, as in Proposition B.51, up to choosing a smaller neighborhood $V_{\Gamma_{1,i}}$ of $\overline{\Gamma_{1,i}}$ in $\overline{\Omega}$, the function $f_{-,i}$ is positive on $V_{\Gamma_{1,i}} \setminus \partial\Omega$ and such that

$$|\nabla f_{-,i}| \neq 0 \text{ in } V_{\Gamma_{1,i}}. \tag{B.131}$$

Besides, since $|\nabla \Psi_i| = |\nabla f|$ in $V_{\Gamma_{1,i}}$, one has

$$\nabla f_{+,i} \cdot \nabla f_{-,i} = 0 \text{ in } V_{\Gamma_{1,i}}, \tag{B.132}$$

and thus

$$|\nabla \Psi_i|^2 = |\nabla f|^2 = |\nabla f_{+,i}|^2 + |\nabla f_{-,i}|^2 \text{ in } V_{\Gamma_{1,i}}.$$

In the following, we will assume in addition that $V_{\Gamma_{1,i}}$ is sufficiently small so that the system of coordinates (x', x_d) introduced in Definition B.9 is well defined on $V_{\Gamma_{1,i}}$. A consequence of (B.132) is that $\frac{d}{dt} f_{+,i}(\gamma_x(t)) = 0$, where γ_x satisfies (B.128). Thus, in the system of coordinates (x', x_d), the functions $f_{+,i}$, Ψ_i and f write:

$$\begin{aligned} &f_{+,i}(x', x_d) = f_{+,i}(x', 0),\ \Psi_i(x', x_d) = f_{+,i}(x', 0) - x_d \\ &\text{and } f(x', x_d) = f(z_i) + f_{+,i}(x', 0) + x_d. \end{aligned}$$

Notice that by construction

$$\forall x \in V_{\Gamma_{1,i}},\ |\nabla f_{+,i}|(x) = 0 \iff x'(x) = x'(z_i). \tag{B.133}$$

Indeed, $f_{+,i}(x', x_d) = f_{+,i}(x', 0)$ and $x' \mapsto f_{+,i}(x', 0) = f(x', 0) - f(z_i)$ has a single critical point at $x'(z_i)$.

Strongly stable domain in B_{z_i}. In order to build an appropriate domain $\dot{\Omega}_i$, we will need to define $\Gamma_{1,i} \subset B_{z_i}$ as a strongly stable domain, as defined now.

Definition B.11. *A smooth open set $A \subset \partial\Omega$ is called strongly stable if*

$$\forall \sigma \in \partial A, \quad \langle \nabla f|_{\partial\Omega}(\sigma), n_\sigma(A) \rangle_{T_\sigma \partial\Omega} > 0,$$

where $n_\sigma(A) \in T_\sigma \partial\Omega$ denotes the outward normal to A at $\sigma \in \partial A$.

Notice that $\nabla f|_{\partial\Omega} = \nabla_T f = \nabla f_{+,i}$ (this is due to the fact that on B_{z_i}, one has $f - f(z_i) = \Psi_i$ and thus $\nabla_T f = \nabla_T \Psi_i$). Thus, the strong stability condition appearing in Definition B.11 is equivalent to

$$\forall \sigma \in \partial A, \quad \partial_{n_\sigma(A)} f_{+,i}(\sigma) > 0.$$

The name "stable" is justified by the following: if $A \subset \partial\Omega$ is strongly stable, then for any curve satisfying for all $t > 0$, $\gamma'(t) = -\nabla f|_{\partial\Omega}(\gamma(t))$ with $\gamma(0) \in \overline{A}$, one has for all $t \geq 0$, $\gamma(t) \in \overline{A}$.

The following proposition will be needed to get the existence of an arbitrary large and strongly stable domain in B_{z_i}.

Proposition B.57. *Let us assume that the hypotheses **[H1]** and **[H2]** hold. For all compact sets $K \subset B_{z_i}$ there exists a C^∞ open domain A which is strongly stable in the sense of Definition B.11, simply connected and such that $K \subset A$ and $\overline{A} \subset B_{z_i}$.*

Proof. For the ease of notation, we drop the subscript i in the proof. One will first construct the set A. Then it will be proven that A has the stated properties. For $a > 0$, let us define

$$L_a := f|_{\partial\Omega}^{-1}\big([f(z), f(z) + a)\big) \cap B_z.$$

For a fixed $a > 0$ small enough L_a is a C^∞ simply connected open set (which contains z) with boundary the level set $f|_{\partial\Omega}^{-1}(\{f(z) + a\})$. The domain L_a is C^∞ since f is C^∞.

Let us define for $x \in B_z$ the curves γ_x by

$$\gamma_x'(t) = \nabla f|_{\partial\Omega}(\gamma_x(t)), \quad \gamma_x(0) = x.$$

For any $x \in \partial L_a$, for all $t > 0$, $\gamma_x(-t) \in L_a$ since $t \geq 0 \mapsto f|_{\partial\Omega}(\gamma_x(-t))$ is decreasing ($\frac{d}{dt} f|_{\partial\Omega}(\gamma_x(-t)) = -|\nabla f|_{\partial\Omega}(\gamma_x(-t))|^2$ and $f|_{\partial\Omega}(\gamma_x(0)) = a$). Let us now define for $T > 0$

$$A_T := \{\gamma_x(t),\ x \in \partial L_a, t \in [0, T)\} \cup L_a \subset B_z.$$

One clearly has $A_T \subset A_{T'}$ if $T < T'$. One claims that A_T is a C^∞ simply connected open set which satisfies

$$\forall \sigma \in \partial A_T, \quad \partial_{n_\sigma(A_T)} f|_{\partial\Omega}(\sigma) > \ 0.$$

Let us first prove that A_T is C^∞. One has $\partial A_T = \{\gamma_x(T),\ x \in \partial L_a\}$. The boundary of A_T is thus a C^∞ homotopy of ∂L_a where the homotopy function is

$$H(t, x) = \gamma_x(t).$$

Additionally since this homotopy is with values in B_z and since L_a is simply connected (because L_a can be asymptotically retracted on z in the sense that for all $x \in L_a$, $\lim_{t\to-\infty} H(t, x) = z$), A_T is simply connected. Let us prove that A_T is open. Let us denote by $d_{\partial\Omega}$ the geodesic distance in $\partial\Omega$. Let $x_0 \in A_T \setminus \overline{L}_a$. There exists a time $t_0 \in (0, T)$ such that $\gamma_{x_0}(-t_0) \in L_a$. Let us define $\varepsilon_0 = d_{\partial\Omega}(\gamma_{x_0}(-t_0), \partial L_a)/2 > 0$. Since the mapping $y \mapsto \gamma_y(-t_0)$ is C^∞, there exists $\varepsilon_1 > 0$ such that if $d_{\partial\Omega}(x, y) \leq \varepsilon_1$ then $d_{\partial\Omega}(\gamma_y(-t_0), \gamma_{x_0}(-t_0)) \leq \varepsilon_0/2$ and thus $\gamma_y(-t_0) \in L_a$. Moreover, since $B_z \setminus \overline{L}_a$ is open, it can be assumed, taking maybe $\varepsilon_1 > 0t$ smaller, that $B_{\partial\Omega}(x_0, \varepsilon_1) \subset B_z \setminus \overline{L}_a$. Then, by continuity $\forall y \in B_{\partial\Omega}(x_0, \varepsilon_1)$, there exists $t_0(y) \in (0, t_0) \subset (0, T)$ such that $\gamma_y(-t_0(y)) \in \partial L_a$, which implies that $y \in A_T \setminus \overline{L}_a$. Thus $A_T \setminus \overline{L}_a$ is open. In addition, since L_a is open and since $\overline{L}_a \subset A_T$, one has that int $(A_T) =$ int $(A_T \setminus \overline{L}_a) \cup \overline{L}_a = (A_T \setminus \overline{L}_a) \cup \overline{L}_a = A_T$. Therefore the set A_T is open.

Let us now prove that A_T is strongly stable (see Definition B.11). By construction, A_T is stable for the dynamics $\gamma' = -\nabla f|_{\partial\Omega}(\gamma)$ and thus one has

$$\forall \sigma \in \partial A_T, \quad \partial_{n_\sigma(A_T)} f|_{\partial\Omega}(\sigma) \geq \ 0.$$

Let us defined now the function

$$\Upsilon : x \in B_z \setminus \overline{L}_a \mapsto (x', t) \in \partial L_a \times \mathbb{R}_+ \text{ s.t } \gamma_{x'}(t) = x.$$

Notice that Υ is a C^∞ diffeomorphism from B_z onto its range, and let us denote $F := \Upsilon^{-1}$ its inverse function ($F(x', t) = \gamma_{x'}(t)$). Assume that there exists $x \in A_T$ such that $\partial_{n_x(A_T)} f|_{\partial\Omega}(x) = 0$ and let $(x', T) = \Upsilon(x)$. This implies that $\nabla f|_{\partial\Omega}(x) \in T_x\partial A_T$ and thus $\partial_t F(x', T) \in T_x\partial A_T$. Furthermore $\mathbb{R}an\,(d_{x'}F(., T)) = T_x\partial A_T$ and thus $d_{(x',T)}F$ is

not invertible which contradicts the fact that F is a diffeomorphism.
It remains to prove that for any compact set $K \subset B_z$, there exists $T > 0$ such that $K \subset A_T$. One has

$$B_z = \bigcup_{T>0} A_T.$$

Indeed, if $x \in \overline{L}_a$, $x \in A_T$ for all $T > 0$ and if $x \in B_z \setminus \overline{L}_a$, $\lim_{t\to\infty} \gamma_x(-t) = z$ and thus there exists $s > 0$ such that $\gamma_x(-s) \in \partial L_a$ which implies that $x \in A_s$. Let $K \subset B_z$ be a compact set. Then $K \subset \bigcup_{T>0} A_T$ and thus by compactness there exists a sequence $(T_j)_{j=1,\dots,N} \subset \mathbb{R}^N$, with $0 < T_1 < \dots < T_m$ such that $K \subset \bigcup_{j=1}^m A_{T_j} = A_{T_m}$. This concludes the proof. ∎

Construction of the domain $\dot{\Omega}_i$. In this section, we introduce the domain $\dot{\Omega}_i$ (associated with z_i) on which the auxiliary Witten Laplacian with mixed tangential-normal Dirichlet boundary conditions is constructed.

Proposition B.58. *Let us assume that the hypotheses **[H1]**, **[H2]** and **[H3]** hold. Let us fix a neighborhood Ω_0 of x_0 (the global minimum of f in Ω) such that*

$$\partial_n f < 0 \text{ on } \Gamma_0 := \partial\Omega_0$$

where n denotes the outward normal to $\Omega \setminus \Omega_0$ on Γ_0. Let us consider a critical point z_i of $f|_{\partial\Omega}$. Then there exists a smooth open subset $\Gamma_{1,i}$ of B_{z_i} containing z_i and arbitrarily large in B_{z_i}, a neighborhood $V_{\Gamma_{1,i}}$ of $\overline{\Gamma_{1,i}}$ in $\overline{\Omega}$ such that $\overline{V_{\Gamma_{1,i}} \cap \partial\Omega} \subset B_{z_i}$ and a Lipschitz subset $\dot{\Omega}_i$ of $\Omega \setminus \Omega_0$ which are such that the following properties are satisfied:

1. *Following Proposition B.52,*

$$\forall x \in V_{\Gamma_{1,i}},\ d_a(x, z_i) = \Phi(x) - f(z_i)$$

   where Φ is the solution of the eikonal equation (B.102) *;*

2. *The system of coordinates (x', x_d) is defined on $V_{\Gamma_{1,i}}$, see Definition B.9 ;*

3. *$\partial\dot{\Omega}_i$ is composed of two connected components: Γ_0 and $\overline{\Gamma_{1,i}} \cup \overline{\Gamma_{2,i}}$;*

4. *$\Gamma_{1,i}$ and $\Gamma_{2,i}$ meet at an angle smaller than π, see* (B.119) *for a precise definition ;*

5. $$\forall x \in \partial\dot{\Omega}_i \setminus \Gamma_0,\ \partial_n f(x) > 0 \tag{B.134}$$

   where n is the outward normal derivative of $\dot{\Omega}_i$;

6. *and*

$$\forall x \in \Gamma_{2,i} \cap V_{\Gamma_{1,i}},\ \partial_n f_+(x) > 0. \tag{B.135}$$

7. *Moreover, for all $\delta > 0$, $\dot{\Omega}_i$ (and Ω_0) can be chosen such that*

$$\sup\{d_e(x, y),\ x \in \Gamma_{2,i},\ y \in B_{z_i}^c\} \le \delta \tag{B.136}$$

   and

$$\sup\{d_e(x_0, x),\ x \in \Gamma_0\} \le \delta \tag{B.137}$$

   where, we recall, d_e denotes the geodesic distance for the Euclidean metric on $\overline{\Omega}$.

We refer to Figure B.9 for a schematic representation of $\dot{\Omega}_i$.

Proof. The domain $\dot{\Omega}_i \subset \Omega$ is built as follows. First, let us fix a neighborhood Ω_0 of x_0 such that (B.137) is satisfied and

$$\partial_n f < 0 \text{ on } \Gamma_0 = \partial\Omega_0$$

where n denotes the outward normal to $\Omega \setminus \Omega_0$ on Γ_0 (this can be done for example by considering $\Omega_0 = \{x,\, f(x) < f(x_0) + \eta\}$ for some positive η). Second, let us consider a smooth subset $\Gamma_{1,i}$ of B_{z_i} which may be as large as we want in B_{z_i}, and which is strongly stable (see Proposition B.57 for the existence of such a set):

$$\langle \nabla f|_{\partial\Omega}, n(\Gamma_{1,i})\rangle_{T\partial\Omega} > 0 \text{ on } \partial\Gamma_{1,i}, \tag{B.138}$$

where $n(\Gamma_{1,i})$ denotes the outward normal derivative of $\Gamma_{1,i}$.

Once $\Gamma_{1,i}$ is fixed, the existence of a neighborhood $V_{\Gamma_{1,i}}$ of $\overline{\Gamma_{1,i}}$ in $\overline{\Omega}$ such that $\overline{V_{\Gamma_{1,i}} \cap \partial\Omega} \subset B_{z_i}$ and such that items 1 and 2 are fulfilled is a direct consequences of Proposition B.52.

Let us now consider the system of coordinates (x', x_d) introduced in Definition B.9. Let $V_{\partial\Gamma_{1,i}} \subset \partial\Omega$ denotes a neighborhood of $\partial\Gamma_{1,i}$ in $\partial\Omega$ and

$$V^+_{\partial\Gamma_{1,i}} = \overline{V_{\partial\Gamma_{1,i}} \cap \Gamma^c_{1,i}}.$$

The domain $\dot{\Omega}_i$ is then defined as follows:

$$\dot{\Omega}_i = \Omega \setminus (\overline{\Omega_0} \cup \{x' \in V^+_{\partial\Gamma_{1,i}} \text{ such that } x_d(x) \in [-\varphi(x'), 0]\})$$

where $\varphi : V^+_{\partial\Gamma_{1,i}} \to \mathbb{R}_+$ is a smooth function such that

$$\exists \varepsilon > 0,\, \forall x' \in \partial\Gamma_{1,i},\, \varphi(x') \geq \varepsilon$$

and $\dot{\Omega}_i$ is a connected Lipschitz subset of Ω. In the following, we denote by $\Gamma_{2,i} = \partial\dot{\Omega}_i \setminus (\overline{\Gamma_{1,i}} \cup \Gamma_0)$ (so that item 3 is true), see Figure B.10 for a schematic representation. For each point $z \in \partial\Gamma_{1,i}$, there is a small neighborhood $\mathcal{V}$ of z such that

$$\mathcal{V} \cap \Gamma_{2,i} \subset \{x = (x', x_d), x' \in \partial\Gamma_{1,i} \text{ and } x_d(x) \in (-\eta, 0]\}, \tag{B.139}$$

for some $\eta \in (0, \varepsilon)$. By choosing $\Gamma_{1,i}$ sufficiently large in B_{z_i}, and φ such that $\max\varphi$ is sufficiently small, (B.136) is satisfied. This concludes the verification of item 7.

For each point $y \in \partial\Gamma_{1,i}$, it is possible to construct locally a normal system of coodinate $x' = x_T = (x_{T,1}, x_{T,2}, \ldots, x_{T,d-1})$ in a neighborhood V_y of y in $\partial\Omega$, such that $\Gamma_{1,i} \cap V_y = \{x \in V_y, x_{T,1}(x) \leq 0\}$, $V^+_{\partial\Gamma_{1,i}} \cap V_y = \{x \in V_y, x_{T,1}(x) \geq 0\}$ and $\partial\Gamma_{1,i} \cap V_y = \{x \in V_y, x_{T,1}(x) = 0\}$. As explained after Definition B.9, by extending this system of coordinate inside Ω as constant along the curve associated with the vector field $\frac{\nabla f_-}{|\nabla f_-|^2}$, $x \mapsto (x'(x), x_d(x))$ then defines a local system of coordinates in a neighborhood W_y of y in $\overline{\Omega}$. For all $x \in \partial\Gamma_{1,i}$, the vector $n_z(\Gamma_1) = \frac{\nabla x_{T,1}(x)}{|\nabla x_{T,1}(x)|}$ is the outward normal vector to $\Gamma_{1,i}$ on $\partial\Gamma_{1,i}$. By a compactness argument, one gets that $\partial\Gamma_{1,i} \subset \sup_{k=1}^{K} \mathcal{V}_{y_k}$ for a finite number of points $y_k \in \partial\Gamma_{1,i}$. See Figure B.11 for a schematic representation of the function φ in this system of coordinates.

Let us now look at the boundary of $\dot{\Omega}_i$ in a neighborhood of $\partial\Gamma_{1,i}$ (see Figure B.10). For $\sigma \in \partial\dot{\Omega}_i$, let us denote by $n_\sigma(\dot{\Omega}_i)$ the unit outward normal to $\dot{\Omega}_i$. Let us show that for all $z \in \partial\Gamma_{1,i}$,

$$\lim_{\sigma \to z} n_\sigma(\dot{\Omega}_i) = n_z(\Gamma_{1,i}) \tag{B.140}$$

where the limit is taken for $\sigma \in \Gamma_{2,i}$. Let us prove (B.140). For any point $z \in \partial\Gamma_{1,i}$, there is a small neighborhood $\mathcal{V}$ of z in $\overline{\Omega}$ such that the system of coordinates (x_T, x_d) introduced above is well defined. In this system of coordinates,

$$\partial\dot{\Omega}_i \cap \mathcal{V} \cap \Gamma_{2,i} \subset \{x \in \mathcal{V},\, x_{T,1}(x) = 0 \text{ and } x_d(x) \in [-\varphi(x'(x_T(x))), 0]\}.$$

Moreover, the outward normal to $\dot{\Omega}_i$ on this subset is $n(\dot{\Omega}_i) = \frac{\nabla x_{T,1}}{|\nabla x_{T,1}|}$ and thus, by construction, for all $z \in \partial\Gamma_{1,i}$, (B.140) holds.

As a consequence of (B.140), the two submanifolds $\Gamma_{1,i}$ and $\Gamma_{2,i}$ meet at an angle smaller than π (see (B.119) and Figure B.12). This shows that item 4 is satisfied. Moreover, using (B.138) and the fact that $\nabla f|_{\partial\Omega} = \nabla f_+$ on $\partial\Omega$, one has: for all $z \in \partial\Gamma_{1,i}$,

$$\lim_{\sigma \to z} \nabla f_+(\sigma) \cdot n_\sigma(\dot{\Omega}_i) = \lim_{\sigma \to z} \nabla f(\sigma) \cdot n_\sigma(\dot{\Omega}_i) = \nabla f(z) \cdot n_z(\Gamma_{1,i}) > 0$$

where the limits are taken for $\sigma \in \Gamma_{2,i}$. Thus, up to choosing φ with $\max\varphi$ sufficiently small, it is possible to build $\dot{\Omega}_i$ such that (see Figure B.10)

$$\forall x \in \Gamma_{2,i} \text{ such that } x'(x) \in \partial\Gamma_{1,i},\, \partial_n f_+(x) > 0$$

where n here denotes the outward normal to $\dot{\Omega}_i$. This implies item 6. It also implies (since $\forall x \in \Gamma_{2,i}$ such that $x'(x) \in \partial\Gamma_{1,i}, \partial_n f(x) = \partial_n f_{+,i}(x) - \partial_n f_{-,i}(x) = \partial_n f_{+,i}(x)$):

$$\forall x \in \Gamma_{2,i} \text{ such that } x'(x) \in \partial\Gamma_{1,i},\, \partial_n f(x) > 0. \tag{B.141}$$

Finally, by using (B.141) and since $\partial_n f > 0$ on $\partial\Omega$, up to choosing φ with $\max\varphi$ sufficiently small, it is possible to build $\dot{\Omega}_i$ such that (see Figure B.10)

$$\forall x \in \partial\dot{\Omega}_i,\, \partial_n f(x) > 0$$

where n again denotes the outward normal to $\dot{\Omega}_i$. This is item 5, and this concludes the proof of Proposition B.58.

∎

Definition B.12. *Let us assume that the hypotheses **[H1]**, **[H2]** and **[H3]** hold. Let us consider a critical point z_i of $f|_{\partial\Omega}$. In the following, we denote by $\mathcal{S}_{M,i} := \{\dot{\Omega}_i, \Gamma_0, \Gamma_{1,i}, \Gamma_{2,i}, V_{\Gamma_{1,i}}\}$ an ensemble of sets satisfying the requirements of Proposition B.58.*

In the following, in order to reduce the amount of notation, the index i will sometimes be omitted. Thus, we will denote

$$z = z_i,\ \Gamma_1 = \Gamma_{1,i},\ \Gamma_2 = \Gamma_{2,i},\ \dot{\Omega} = \dot{\Omega}_i,\ V_{\Gamma_1} = V_{\Gamma_{1,i}},\ \Psi = \Psi_i,\ f_+ = f_{+,i} \text{ and } f_- = f_{-,i}.$$

We shall warn the reader whenerver the index i is dropped.

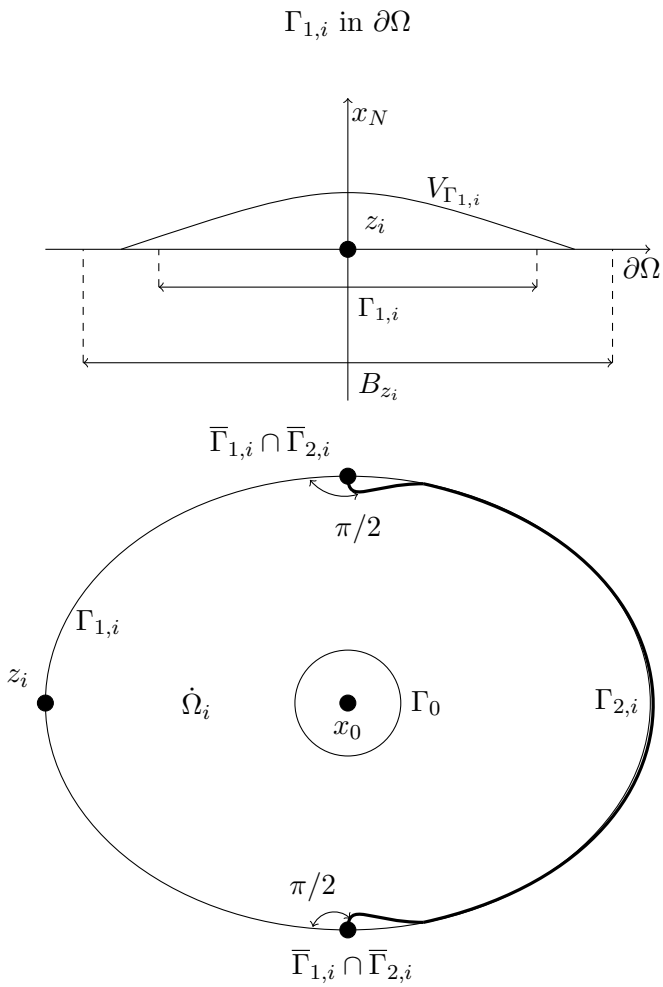

Figure B.9: The ensemble of sets $\mathcal{S}_{M,i} = \{\dot{\Omega}_i, \Gamma_0, \Gamma_{1,i}, \Gamma_{2,i}, V_{\Gamma_{1,i}}\}$ associated with a critical point z_i of $f|_{\partial\Omega}$.

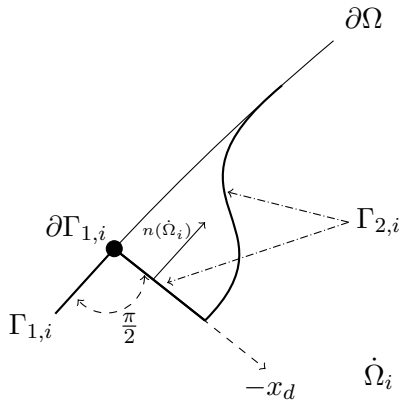

Figure B.10: $\dot{\Omega}_i$ near $\partial\Gamma_{1,i}$.

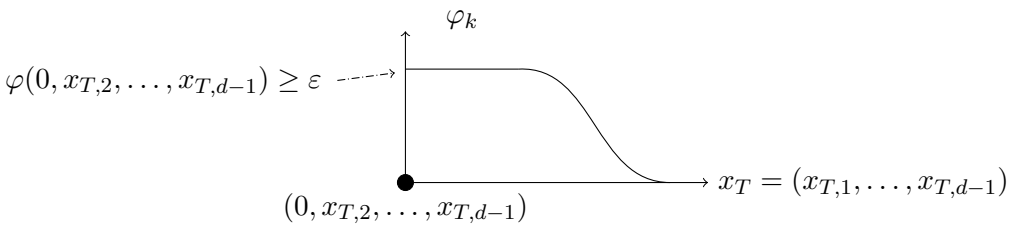

Figure B.11: The functions $x_T \in \mathbb{R}^{d-1} \mapsto \varphi(x_T)$.

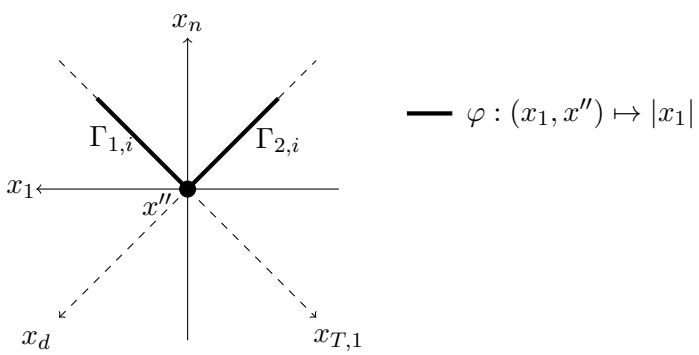

Figure B.12: The sets $\Gamma_{1,i}$ and $\Gamma_{2,i}$ meet at an angle smaller than π, according to (B.119): take $x_1 = \frac{x_d - x_{T,1}}{2}$, $x_n = -\frac{x_d + x_{T,1}}{2}$, $x'' = (x_{T,2}, \ldots, x_{T,d-1})$ and $\varphi(x_1, x'') = |x_1|$.

B.4.1.3 On the spectrum of the Witten Laplacian $\Delta^M_{f,h}(\dot{\Omega}_i)$

Troughout this section, one assumes **[H1]**, **[H2]** and **[H3]**. In this section, we introduce a Witten Laplacian with mixed tangential and normal Dirichlet boundary conditions, associated with the critical point z_i. Let $\mathcal{S}_{M,i} := \{\dot{\Omega}_i, \Gamma_0, \Gamma_{1,i}, \Gamma_{2,i}, V_{\Gamma_{1,i}}\}$ be an ensemble of sets associated with z_i, see Definition B.12.

Let us now consider the Witten Laplacian $\Delta^M_{f,h}$ on $\dot{\Omega}_i$ with zero tangential boundary

conditions on

$$\Gamma_T = \Gamma_0 \cup \Gamma_{1,i}$$

and zero normal boundary conditions on

$$\Gamma_N = \Gamma_{2,i}$$

as defined at the end of Section B.4.1.1 (see (B.122)–(B.124)). The main result of this section concerns the spectrum of the operator $\Delta_{f,h}^{M,(p)}(\dot{\Omega}_i)$.

Proposition B.59. *Let us assume that the hypotheses **[H1]**, **[H2]** and **[H3]** hold. Let $\Delta_{f,h}^{M,(p)}(\dot{\Omega}_i)$ be the unbounded nonnegative selfadjoint operator on $L^2(\dot{\Omega}_i)$ defined by* (B.122) *and with domain* (B.124) *with $\Gamma_T = \Gamma_1 \cup \Gamma_0$ and $\Gamma_N = \Gamma_2$. One has:*

(i) The operator $\Delta_{f,h}^{M,(p)}(\dot{\Omega}_i)$ has compact resolvent.

(ii) For any eigenvalue λ_p of $\Delta_{f,h}^{M,(p)}(\dot{\Omega}_i)$ and associated eigenform $u_p \in D\left(\Delta_{f,h}^{M,(p)}(\dot{\Omega}_i)\right)$, one has $d_{f,h}u_p \in D\left(\Delta_{f,h}^{M,(p+1)}\right)$ and $d_{f,h}^* u_p \in D\left(\Delta_{f,h}^{M,(p-1)}\right)$, with

$$d_{f,h}\Delta_{f,h}^{M,(p)}u_p = \Delta_{f,h}^{M,(p+1)}d_{f,h}u_p = \lambda_p d_{f,h}u_p$$

and

$$d_{f,h}^*\Delta_{f,h}^{M,(p)}(\dot{\Omega}_i)u_p = \Delta_{f,h}^{M,(p-1)}(\dot{\Omega}_i)d_{f,h}^*u_p = \lambda_p d_{f,h}^*u_p.$$

If in addition $\lambda_p \neq 0$, either $d_{f,h}u_p$ or $d_{f,h}^*u_p$ is nonzero.

(iii) There exist $c > 0$ and $h_0 > 0$ such that for any $p \in \{0, \dots, n\}$ and $h \in (0, h_0)$,

$$\dim \mathbb{R}an\ \pi_{[0,ch^{\frac{3}{2}})}\left(\Delta_{f,h}^{M,(p)}(\dot{\Omega}_i)\right) = \delta_{1,p} \quad \text{and} \quad \mathrm{Sp}\left(\Delta_{f,h}^{M,(1)}(\dot{\Omega}_i)\right) \cap [0, ch^{\frac{3}{2}}) = \{0\}.$$

Proof. Since the criticial point z_i is fixed, for the ease of notation, we drop the subscript i in the proof.

The point (i) follows from the compactness of the embedding $H^{\frac{1}{2}}(\dot{\Omega}) \hookrightarrow L^2(\dot{\Omega})$ (since additionally $D\left(\mathcal{Q}_{f,h}^M(\dot{\Omega})\right) \hookrightarrow H^{\frac{1}{2}}(\dot{\Omega})$ is continuous according to Proposition B.55). The point (ii) is then a straightforward consequence of the characterization of the domain of $\Delta_{f,h}^{M,(p)}(\dot{\Omega})$ together with (B.123). The statement in the case $\lambda_p \neq 0$ follows from

$$0 \neq \lambda_p\langle u_p, u_p\rangle_{L^2(\dot{\Omega})} = \langle \Delta_{f,h}^{M,(p)}(\dot{\Omega})u_p, u_p\rangle_{L^2(\dot{\Omega})} = \langle d_{f,h}u, d_{f,h}u_p\rangle_{L^2(\dot{\Omega})} + \langle d_{f,h}^*u_p, d_{f,h}^*u_p\rangle_{L^2(\dot{\Omega})}.$$

Let us now give the proof of the last point (iii), which is a consequence of (ii) together with ideas from [34, 47], since z_i is the only generalized critical point of f in $\overline{\dot{\Omega}}$ for $\Delta_{f,h}^{D,(1)}(\dot{\Omega})$. According to the last part of (ii), it suffices to prove that for some $c > 0$, one has for any $p \in \{0, \dots, n\}$ and h small enough,

$$\dim \mathbb{R}an\ \pi_{[0,ch^{\frac{3}{2}})}\left(\Delta_{f,h}^{M,(p)}(\dot{\Omega})\right) = \delta_{1,p}.$$

Pick up $u \in D\left(\mathcal{Q}_{f,h}^{M,(p)}(\dot{\Omega})\right)$. From the Green formula (B.125) and from the fact that $\mathcal{L}_{\nabla f} + \mathcal{L}_{\nabla f}^*$ is a 0th order differential operator, one has that there exists $C_0 > 0$ such

that for all $u \in D\left(\mathcal{Q}_{f,h}^{M,(p)}(\dot{\Omega})\right)$ and all smooth cut-off function χ supported in $\dot{\Omega}$ (whose support avoids $\partial\dot{\Omega}$):

$$\|d_{f,h}\chi u\|^2_{L^2(\dot{\Omega})} + \left\|d^*_{f,h}\chi u\right\|^2_{L^2(\dot{\Omega})} \geq \left(\inf_{\mathrm{supp}\chi} |\nabla f|^2 - hC_0\right)\|\chi u\|^2.$$

Thus, since f has no critical point in $\dot{\Omega}$, there exists some $C > 0$ independent of $u \in D\left(\mathcal{Q}_{f,h}^{M,(p)}(\dot{\Omega})\right)$ such that for any smooth cut-off function χ supported in $\dot{\Omega}$ (whose support avoids $\partial\dot{\Omega}$) and h small enough,

$$\mathcal{Q}_{f,h}^{M,(p)}(\dot{\Omega})(\chi u) \ \geq \ C\|\chi u\|^2.$$

Note in addition that owing to $\partial_n f > 0$ on Γ_2 and $\partial_n f < 0$ on Γ_0, the boundary terms in the Green formula (B.125) are non negative, for any smooth cut-off function χ supported in a neighborhood of any point in $\Gamma_2 \cup \Gamma_0$ (whose support avoids some neighborhood of Γ_1). Thus, the same considerations show that for h small enough, for such functions χ, taking maybe C smaller, $\forall u \in D\left(\mathcal{Q}_{f,h}^{M,(p)}(\dot{\Omega})\right)$

$$\mathcal{Q}_{f,h}^{M,(p)}(\dot{\Omega})(\chi u) \ \geq \ C\|\chi u\|^2.$$

According to the analysis done in [34, Section 3.4], the same estimate also holds for χ supported in a sufficiently small neighborhood of some point $x \neq z$, $x \in \Gamma_1$ (whose support avoids a neighborhood of $\{z\} \cup \partial\Gamma_1$). This is related to the fact that Γ_1 does not contain any generalized critical point of f in the tangential sense except z. Let us now show that such an estimate is also valid near $\partial\Gamma_1$. In order to prove it, one recalls that

$$f = f(z) + f_+ - f_- \text{ a.e on } \Omega \text{ and } |\nabla f|^2 = |\nabla f_-|^2 + |\nabla f_+|^2 \text{ a.e near } \partial\Gamma_1,$$

where $f_\pm$ are smooth and satisfy the following relations on B_z:

$$f_+ = f - f(z),\ f_- = 0,\ \partial_n f_+ = 0 \text{ and } \partial_n f_- = -\partial_n f.$$

Hence, for any χ supported in a sufficiently small neighborhood of $\partial\Gamma_1$, one deduces from the relation $\mathcal{Q}_{-f_-,h}^{M,(p)}(\dot{\Omega})(\chi u) \geq 0$, the Green formula (B.125), and the fact that $\mathcal{L}_{-\nabla f_-} + \mathcal{L}^*_{-\nabla f_-}$ is a 0th order differential operator, that there exists $C_1 > 0$ independent of $u \in D\left(\mathcal{Q}_{f,h}^{M,(p)}(\dot{\Omega})\right)$ such that:

$$\begin{aligned} h\left(\int_{\Gamma_1} - \int_{\Gamma_2}\right)\langle \chi u, \chi u\rangle_{T^*_\sigma\dot{\Omega}}\partial_n f_-\, d\sigma \geq & -h^2\|d\chi u\|^2_{L^2(\dot{\Omega})} - h^2\|d^*\chi u\|^2_{L^2(\dot{\Omega})} \\ & - \||\nabla f_-|\,\chi u\|^2_{L^2(\dot{\Omega})} - C_1 h\|\chi u\|^2_{L^2(\dot{\Omega})}. \end{aligned}$$

Using again the Green formula (B.125), the relation $f - f(z) = f_+ - f_-$ with $\partial_n f_+ = 0$ on Γ_1, and the fact that $\mathcal{L}_{\nabla f} + \mathcal{L}^*_{\nabla f}$ is a 0th order differential operator then leads to the existence of $C_2 > 0$ independent of $u \in D\left(\mathcal{Q}_{f,h}^{M,(p)}(\dot{\Omega})\right)$ s.t.

$$\mathcal{Q}_{f,h}^{M,(p)}(\dot{\Omega})(\chi u) \geq \||\nabla f_+|\,\chi u\|^2_{L^2(\dot{\Omega})} - C_2 h\|\chi u\|^2_{L^2(\dot{\Omega})} + h\int_{\Gamma_2}\langle \chi u|\chi u\rangle_{T^*_\sigma\dot{\Omega}}\partial_n f_+\, d\sigma.$$

Since f_+ has no critical point around $\partial\Gamma_1$ (see (B.133)), one has then for h small enough, taking maybe C smaller:

$$\mathcal{Q}_{f,h}^{M,(p)}(\dot{\Omega})(\chi u) \geq C\|\chi u\|^2_{L^2(\dot{\Omega})} + h\int_{\Gamma_2} \langle \chi u|\chi u\rangle_{T^*_\sigma\dot{\Omega}} \partial_n f_+ \, d\sigma. \tag{B.142}$$

Let us recall that due to our construction of Γ_2 near $\partial\Gamma_1$, one has (see (B.135) in Proposition B.58):

$$\partial_n f_+(\sigma) > 0 \text{ for } \sigma \in \Gamma_2 \text{ sufficiently close to } \partial\Gamma_1.$$

This implies that for χ supported near $\partial\Gamma_1$ with sufficiently small support and h small enough:

$$\mathcal{Q}_{f,h}^{M,(p)}(\dot{\Omega})(\chi u) \geq C\|\chi u\|^2_{L^2(\dot{\Omega})}.$$

Lastly, since z is a generalized critical point with index 1 in the tangential sense, it follows from [34, Proposition 4.3.2] that for χ supported in a neighborhood of z and h small enough, the spectrum of the Friedrichs extension associated with the quadratic form

$$\left\{v \in \Lambda^p H^1(\operatorname{supp}\chi);\ \mathbf{t}v|_{\Gamma_1} = v|_{\partial\operatorname{supp}\chi\setminus\overline{\Gamma}_1} = 0\right\} \ni v \mapsto \|d_{f,h}v\|^2_{L^2} + \left\|d^*_{f,h}v\right\|^2_{L^2}$$

does not meet $[0, h^{\frac{3}{2}})$ if $p \neq 1$, and consists of exactly one eigenvalue in $[0, h^{\frac{3}{2}})$ which is actually exponentially small – i.e. of the form $O(e^{-\frac{C_3}{h}})$ – if $p = 1$. Denote by ψ_1 some normalized eigenvalue associated with this exponentially small eigenvalue in this last case.

Using the IMS localization formula (see for example [12] for a proof)

$$\begin{aligned}
&\forall (\chi_k)_{k\in\{1,\dots,K\}} \in \left(C^\infty\left(\overline{\dot{\Omega}}\right)\right)^K \text{ s.t. } \sum_{k=1}^K \chi_k^2 = 1 \\
&\mathcal{Q}_{f,h}^{M,(p)}\left(\dot{\Omega}\right)(u) = \sum_{k=1}^K \left(\mathcal{Q}_{f,h}^{M,(p)}(\dot{\Omega})(\chi_k u) - h^2\left\||\nabla\chi_k|u\right\|^2_{L^2(\dot{\Omega})}\right)
\end{aligned} \tag{B.143}$$

and the previous analysis then shows that choosing $\chi_1 \in C^\infty\left(\overline{\dot{\Omega}}\right)$ supported in a neighborhood of z with $\chi_1 = 1$ near z, one gets for some $C, C' > 0$ independent of $u \in D\left(\mathcal{Q}_{f,h}^{M,(p)}(\dot{\Omega})\right)$ and h small enough:

$$\mathcal{Q}_{f,h}^{M,(p)}(\dot{\Omega})(u) \geq \mathcal{Q}_{f,h}^{M,(p)}(\dot{\Omega})(\chi_1 u) + C\|(1-\chi_1^2)^{\frac{1}{2}}u\|^2_{L^2(\dot{\Omega})} - C'h^2\left\|u\right\|^2_{L^2(\dot{\Omega})}. \tag{B.144}$$

If $p \neq 1$, one deduces immediately from (B.144) that for h small enough,

$$\mathcal{Q}_{f,h}^{M,(p)}(\dot{\Omega})(u) \geq h^{\frac{3}{2}}\left\|\chi_1 u\right\|^2_{L^2(\dot{\Omega})} + C\|(1-\chi_1^2)^{\frac{1}{2}}u\|^2_{L^2(\dot{\Omega})} - C'h^2\left\|u\right\|^2_{L^2(\dot{\Omega})},$$

and then that for some $c > 0$ and h small enough:

$$\mathcal{Q}_{f,h}^{M,(p)}(\dot{\Omega})(u) \ \geq\ ch^{\frac{3}{2}}\left\|u\right\|^2_{L^2(\dot{\Omega})}.$$

If $p=1$, one obtains from (B.144) the same conclusion for any u such that $\int_{\dot\Omega} u\chi_1\psi_1 = 0$ and therefore $\Delta_{f,h}^{M,(p)}(\dot\Omega)$ has no eigenvalue in $[0, ch^{\frac{3}{2}})$ if $p \neq 1$ and at most one if $p=1$. To end up the proof, it is sufficient to remark that $\tilde\psi_1$, the extension of ψ_1 to $\dot\Omega$ by 0 outside $\operatorname{supp}\chi_1$, belongs to $D\left(\mathcal{Q}_{f,h}^{M,(1)}(\dot\Omega)\right)$ and satisfies for h small:

$$\mathcal{Q}_{f,h}^{M,(1)}(\dot\Omega)(\tilde\psi_1) = \|d_{f,h}\psi_1\|_{L^2(\dot\Omega)} + \|d_{f,h}^*\psi_1\|_{L^2(\dot\Omega)} = O(e^{-\frac{C_3}{h}}) \ < \ ch^{\frac{3}{2}}.$$

∎

Following Proposition B.59, let us introduce an L^2-normalized eigenform $u_{h,i}^{(1)}$ of $\Delta_{f,h}^{M,(1)}(\dot\Omega_i)$ associated with the eigenvalue 0:

$$\Delta_{f,h}^{M,(1)}(\dot\Omega_i)\, u_{h,i}^{(1)} = 0 \text{ in } \dot\Omega_i \text{ and } \left\|u_{h,i}^{(1)}\right\|_{L^2(\dot\Omega_i)} = 1. \tag{B.145}$$

The quasi-mode $\tilde\phi_i$ will be built using a suitable truncation of $u_{h,i}^{(1)}$. Notice that thanks to item (iii) in Proposition B.59, $u_{h,i}^{(1)}$ is unique up to a multiplication by ± 1: this multiplicative constant will be fixed in Proposition B.64 below.

B.4.2 Definition of the quasi-modes

Troughout this section, one assumes **[H1]**, **[H2]** and **[H3]**. In this section, we construct the function $\tilde u$ and a family of 1-forms $(\tilde\phi_i)_{i=1,\dots,n}$ which will satisfy the estimates stated in Section B.2.2.2. For each $i \in \{1,\dots,n\}$, the 1-form $\tilde\phi_i$ will be constructed by a suitable truncation of an eigenfunction $u_{h,i}$ associated with the eigenvalue 0 of the mixed Witten Laplacian attached with $z_i \in \{z_1,\dots,z_n\}$, as defined in Section B.4.1.3.

We recall that Σ_i is an open set included in $\partial\Omega$ containing z_i which is such that $\overline{\Sigma}_i \subset B_{z_i}$ (see Definition B.4).

B.4.2.1 Definition of the quasi-mode $\tilde u$

Definition B.13. *Let us consider the global minimum x_0 introduced in the hypothesis **[H2]**. Let $\chi \in C_c^\infty(\Omega)$ such that $\{x \in \Omega | \chi(x) = 1\}$ is a neighborhood of x_0 and such that $0 \le \chi \le 1$ (in particular $\chi(x_0) = 1$). The quasi-mode $\tilde u$ is defined by*

$$\tilde u := \frac{\chi}{\sqrt{\int_\Omega \chi^2 e^{-\frac{2f}{h}}}}.$$

The function $\tilde u$ belongs to $C_c^\infty(\Omega)$ and therefore $\tilde u \in H_0^1\left(e^{-\frac{2}{h}f(x)}dx\right)$. The function χ will be chosen such that $\operatorname{supp}(|\nabla\chi|)$ is as close as needed to $\partial\Omega$, as will be made precise in Section B.4.5.

Let us first prove that $\tilde u$ satisfies item $2(b)$ in Proposition B.17.

Lemma B.60. *Let us assume that the hypotheses **[H1]** and **[H2]** hold. Then, for any $\delta > 0$ there exist $h_0 > 0$, $C > 0$ and $\chi \in C_c^\infty(\Omega)$ such that the set $\{x \in \Omega | \chi(x) = 1\}$ is a neighborhood of x_0, $0 \leq \chi \leq 1$ and for all $h \in (0, h_0)$*

$$\int_\Omega |\nabla \tilde{u}|^2 e^{-\frac{2f}{h}} \leq C h^{-\frac{d}{2}} e^{-2\frac{(f(z_1)-f(x_0))-\delta}{h}},$$

where $\tilde{u}$ is defined in Definition B.13.

Proof. There exists a constant C such that

$$\int_\Omega |\nabla \tilde{u}(x)|^2 e^{-\frac{2f(x)}{h}} dx \leq C \frac{\int_{\text{supp}\nabla\chi} e^{-2\frac{f(x)}{h}} dx}{\int_\Omega \chi^2(y) e^{-2\frac{f(y)}{h}} dy}.$$

Since supp$\nabla\chi$ can be chosen arbitrarly close to $\partial\Omega$ and since z_1 is the minimum of V on$\partial\Omega$, by continuity of f, for any $\delta > 0$ there exists $\chi \in C^\infty(\Omega)$ such that $\{x \in \Omega | \chi(x) = 1\}$ is a neighborhood of x_0, $0 \leq \chi \leq 1$ and

$$\int_{\text{supp}\nabla\chi} e^{-2\frac{f(x)}{h}} dx \leq C e^{-2\frac{f(z_1)+2\delta}{h}}.$$

Moreover, since x_0 is the global minimum of f in Ω, one gets, using Laplace's method

$$\int_\Omega \chi^2(y) e^{-2\frac{f(y)}{h}} dy = \frac{(\pi\ h)^{\frac{d}{2}}}{\sqrt{\det \text{ Hess} f(x_0)}} e^{-2\frac{f(x_0)}{h}} (1 + O(h)).$$

This yields the desired estimate. ∎

Notice that item 2(b) in Proposition B.17 is a direct consequence of Lemma B.60.

B.4.2.2 Definition of the quasi-mode $\tilde{\phi}_i$ attached to z_i

Let z_i be a local minimum of $f|_{\partial\Omega}$. Let $\mathcal{S}_{M,i} := \{\dot{\Omega}_i, \Gamma_0, \Gamma_{1,i}, \Gamma_{2,i}, V_{\Gamma_{1,i}}\}$ be an ensemble of sets associated with z_i, see Definition B.12. Thanks to Propositions B.57 and B.58, the set $\Gamma_{1,i}$ can be taken such that $\overline{\Sigma}_i \subset \Gamma_{1,i}$. We recall that Section B.4.1 was dedicated to the construction of a domain $\dot{\Omega}_i \subset \Omega$ and a mixed Witten Laplacian $\Delta_{f,h}^{M,(1)}(\dot{\Omega}_i)$ (see (B.122)) associated with this ensemble of sets $\mathcal{S}_{M,i}$. Proposition B.59 gives the spectral properties of the operator $\Delta_{f,h}^{M}(\dot{\Omega}_i)$. In the following, we consider a normalized eigenform $u_{h,i}^{(1)} \in D\left(\Delta_{f,h}^{M,(1)}(\dot{\Omega}_i)\right)$ associated with the first eigenvalue 0, i.e. such that (B.145) holds

The quasi-mode $\tilde{\phi}_i$ is defined as the following truncation of $u_{h,i}^{(1)}$.

Definition B.14. *Let us assume that the hypotheses **[H1]**, **[H2]** and **[H3]** hold. Let $\chi_i \in C^\infty\left(\overline{\Omega}\right)$ be such that:*

1. *$\chi_i \in C_c^\infty\left(\dot{\Omega}_i \cup \Gamma_{1,i}\right)$ (and thus $\chi_i = 0$ on a neighborhood of $\Gamma_{2,i} \cup \Gamma_0$ and on a neighborhood of $\partial\Omega \setminus \Gamma_{1,i}$),*

2. *$\chi_i = 1$ on a neighborhood of $\overline{\Sigma}_i$ in $\overline{\dot{\Omega}_i}$,*

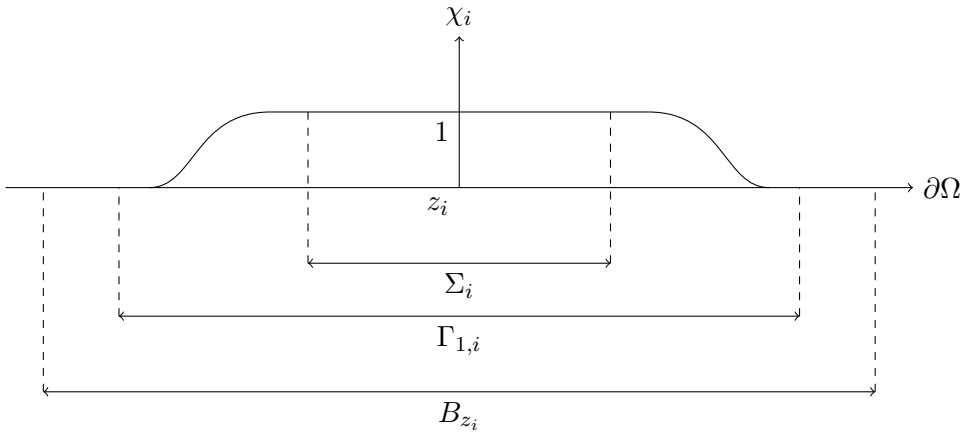

Figure B.13: The support of χ_i on $\partial\Omega$.

3. $0 \leq \chi_i \leq 1$.

One defines $\mathcal{V}_i := \{x \in \Omega | \chi_i(x) = 1\}$. *The quasi-mode* $\tilde{\phi}_i$ *is defined on* Ω *by:*

$$\tilde{\phi}_i := \frac{\chi_i u_{h,i}^{(1)}}{\sqrt{\int_\Omega \left|\chi_i(x) u_{h,i}^{(1)}(x)\right|^2 dx}}. \tag{B.146}$$

The support of χ_i on $\partial\Omega$ is represented on Figure B.13 and the support of χ_i in Ω is represented in Figure B.14. The function χ_i will be chosen such that the $\mathrm{supp}(|\nabla\chi_i|)$ is as close as needed from $B_{z_i}^c \subset \partial\Omega$ or from x_0, as will be made precise at the end of Section B.4.5. This is possible thanks to item 7 in Proposition B.58.

Using Lemma B.54 and the fact that $\mathbf{t}\chi_i u_{h,i}^{(1)} = 0$ (on $\partial\Omega$), one easily shows that

$$\tilde{\phi}_i \in \Lambda^1 H_T^1(\Omega).$$

Using now standard elliptic regularity results, one can check that $\tilde{\phi}_i$ is actually a $C_c^\infty(\Omega \cup \Gamma_{1,i})$ function.

We will show in Section B.4.5 that the family of forms $(\tilde{u}, \tilde{\phi}_1, \ldots, \tilde{\phi}_n)$ satisfy the estimates stated in Sections B.2.2.1 and B.2.2.2. This requires some preliminary results on the eigenforms $(u_{h,i}^{(1)})_{i\in\{1,\ldots n\}}$ that are provided in Section B.4.3 and B.4.4.

B.4.3 Agmon estimates on $u_{h,i}^{(1)}$

Throughout this section, one assumes **[H1]**, **[H2]** and **[H3]**. In all this section, we consider, for a fixed critical point z_i, an ensemble of sets $\mathcal{S}_{M,i}$ associated with z_i (see Definition B.12) and an L^2-normalized eigenform $u_{h,i}^{(1)}$ of $\Delta_{f,h}^{M,(1)}(\dot{\Omega}_i)$ associated with the eingevalue 0, as introduced at the end of Section B.4.1.3.

The aim of this section is to prove the following proposition.

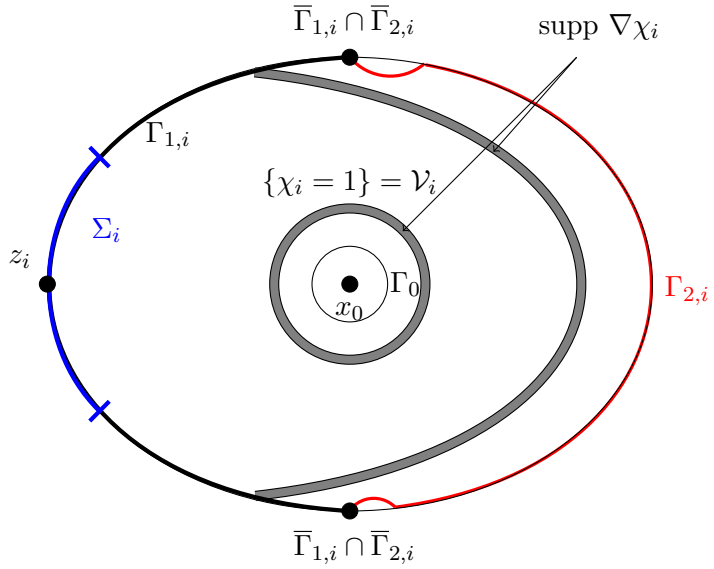

Figure B.14: The set $\mathcal{V}_i = \left\{x \in \Omega \middle| \chi_i(x) = 1\right\}$ and, in gray, the support of $\nabla\chi_i$.

Proposition B.61. *Let us assume that the hypotheses **[H1]**, **[H2]** and **[H3]** hold. Any L^2-normalized eigenform $u_{h,i}^{(1)}$ of $\Delta_{f,h}^{M,(1)}(\dot{\Omega}_i)$ associated with the eigenvalue 0 satisfies:*

$$\exists N \in \mathbb{N},\ \left\|e^{\frac{\Psi_i}{h}} u_{h,i}^{(1)}\right\|_{L^2(\dot{\Omega}_i)} + \left\|d\left(e^{\frac{\Psi_i}{h}} u_{h,i}^{(1)}\right)\right\|_{L^2(\dot{\Omega}_i)} + \left\|d^*\left(e^{\frac{\Psi_i}{h}} u_{h,i}^{(1)}\right)\right\|_{L^2(\dot{\Omega}_i)} = O(h^{-N}) \tag{B.147}$$

where, we recall, $\Psi_i(x) = d_a(x, z_i)$ (see Definition B.10).

For the ease of notation, we drop the subscript i in the remaining of this section.

The proof is inspired by the first part of the proof of [34, Proposition 4.3.2] where the authors consider a Witten Laplacian with mixed tangential – full Dirichlet boundary conditions in a local system of coordinates in a neighborhood of z. The proof actually only requires that $u_h^{(1)}$ is an eigenform of $\Delta_{f,h}^{M,(1)}(\dot{\Omega})$ associated with an eigenvalue $\lambda_h = O(h)$. It crucially relies on the following Agmon-type energy equality.

Lemma B.62. *Let us assume that the hypotheses **[H1]**, **[H2]** and **[H3]** hold. Let φ be a real-valued Lipschitz function on $\overline{\dot{\Omega}}$. Then, for any $u \in D\left(\mathcal{Q}_{f,h}^{M,(1)}(\dot{\Omega})\right)$, one has:*

$$\begin{aligned}\mathcal{Q}_{f,h}^{M,(1)}(\dot{\Omega})(u, e^{2\frac{\varphi}{h}}u) &= h^2 \left\|de^{\frac{\varphi}{h}}u\right\|^2_{L^2(\dot{\Omega})} + h^2 \left\|d^*e^{\frac{\varphi}{h}}u\right\|^2_{L^2(\dot{\Omega})} \\ &\quad + \langle(|\nabla f|^2 - |\nabla\varphi|^2 + h\mathcal{L}_{\nabla f} + h\mathcal{L}^*_{\nabla f})e^{\frac{\varphi}{h}}u, e^{\frac{\varphi}{h}}u\rangle_{L^2(\dot{\Omega})} \\ &\quad + h\left(-\int_{\Gamma_0\cup\Gamma_1} + \int_{\Gamma_2}\right)\langle u, u\rangle_{T^*_\sigma\dot{\Omega}}\, e^{\frac{2}{h}\varphi}\partial_n f\, d\sigma.\end{aligned} \tag{B.148}$$

Moreover, when $u \in D\left(\Delta_{f,h}^{M,(1)}(\dot{\Omega})\right)$*, the left-hand side equals* $\langle e^{2\frac{\varphi}{h}}\Delta_{f,h}^{M,(1)}(\dot{\Omega})u, u\rangle_{L^2(\dot{\Omega})}$.

Proof. This result is standard for manifolds without boundary or for bounded manifolds and quadratic forms with full normal or tangential boundary conditions (see e.g. [19, 34, 47]). We extend it here to our setting.

Note first that $u \in D\left(\mathcal{Q}_{f,h}^{M,(1)}(\dot{\Omega})\right)$ implies $e^{2\frac{\varphi}{h}}u \in D\left(\mathcal{Q}_{f,h}^{M,(1)}(\dot{\Omega})\right)$, since for $u \in D\left(\mathcal{Q}_{f,h}^{M,(1)}(\dot{\Omega})\right)$, $n^\flat \wedge e^{2\frac{\varphi}{h}}u = e^{2\frac{\varphi}{h}}n^\flat \wedge u$ and $\mathbf{i}_n e^{2\frac{\varphi}{h}}u = e^{2\frac{\varphi}{h}}\mathbf{i}_n u$. One then gets by straightforward computations:

$$\begin{aligned}
\mathcal{Q}_{f,h}^{M,(1)}(\dot{\Omega})(u, e^{2\frac{\varphi}{h}}u) &= \langle d_{f,h}u, d_{f,h}(e^{2\frac{\varphi}{h}}u)\rangle + \langle d_{f,h}^*u, d_{f,h}^*(e^{2\frac{\varphi}{h}}u)\rangle \\
&= \langle e^{\frac{\varphi}{h}}d_{f,h}u, d_{f,h}(e^{\frac{\varphi}{h}}u)\rangle + \langle e^{\frac{\varphi}{h}}d_{f,h}u, d\varphi \wedge (e^{\frac{\varphi}{h}}u)\rangle \\
&\quad + \langle e^{\frac{\varphi}{h}}d_{f,h}^*u, d_{f,h}^*(e^{\frac{\varphi}{h}}u)\rangle - \langle e^{\frac{\varphi}{h}}d_{f,h}^*u, \mathbf{i}_{\nabla\varphi}(e^{\frac{\varphi}{h}}u)\rangle \\
&= \langle d_{f,h}(e^{\frac{\varphi}{h}}u), d\varphi \wedge (e^{\frac{\varphi}{h}}u)\rangle - \langle d\varphi \wedge (e^{\frac{\varphi}{h}}u), d_{f,h}(e^{\frac{\varphi}{h}}u)\rangle \\
&\quad + \|d_{f,h}(e^{\frac{\varphi}{h}}u)\|^2 - \|d\varphi \wedge (e^{\frac{\varphi}{h}}u)\|^2 + \|d_{f,h}^*(e^{\frac{\varphi}{h}}u)\|^2 - \|\mathbf{i}_{\nabla\varphi}e^{\frac{\varphi}{h}}u\|^2 \\
&\quad + \langle \mathbf{i}_{\nabla\varphi}(e^{\frac{\varphi}{h}}u), d_{f,h}^*(e^{\frac{\varphi}{h}}u)\rangle - \langle d_{f,h}^*(e^{\frac{\varphi}{h}}u), \mathbf{i}_{\nabla\varphi}(e^{\frac{\varphi}{h}}u)\rangle \ .
\end{aligned}$$

Let us set $\tilde{u} := e^{\frac{\varphi}{h}}u \in D\left(Q_{f,h}^{M,(1)}(\dot{\Omega})\right)$. Using the same relations as in the proof of Lemma B.56 leads to

$$\begin{aligned}
\mathcal{Q}_{f,h}^{M,(1)}(\dot{\Omega})(u, e^{2\frac{\varphi}{h}}u) = \mathcal{Q}_{f,h}^{M,(1)}(\dot{\Omega})(\tilde{u}) &- \langle |\nabla\varphi|^2\,\tilde{u}, \tilde{u}\rangle - \langle d\varphi \wedge \tilde{u}, d_{f,h}\tilde{u}\rangle \\
&+ \langle d_{f,h}\tilde{u}, d\varphi \wedge \tilde{u}\rangle + \langle \mathbf{i}_{\nabla\varphi}\tilde{u}, d_{f,h}^*\tilde{u}\rangle - \langle d_{f,h}^*\tilde{u}, \mathbf{i}_{\nabla\varphi}\tilde{u}\rangle
\end{aligned}$$

and hence to

$$\mathcal{Q}_{f,h}^{M,(1)}(\dot{\Omega})(u, e^{2\frac{\varphi}{h}}u) = \mathcal{Q}_{f,h}^{M,(1)}(\dot{\Omega})(\tilde{u}) - \langle |\nabla\varphi|^2\,\tilde{u}, \tilde{u}\rangle \ .$$

One concludes by applying Lemma B.56. ∎

Proof. (of Proposition B.61)
Following the proof of [34, Proposition 4.3.2], one proves the result in two steps. First, the Agmon estimate along $\Gamma_1 \subset \partial\Omega$ is proven by applying Lemma B.62 with a function φ close to f_+ (recall that on Γ_1, $f_+ = \Psi$). The Agmon estimate in $\dot{\Omega}$ is then obtained using again Lemma B.62 with φ close to Ψ, and the Agmon estimate along Γ_1.

In order to separate the analysis along Γ_1 and elsewhere, one introduces two smooth cut-off functions χ_0 and χ_1 on $\overline{\Omega}$ such that:

$$\chi_1 := \sqrt{1-\chi_0^2}\ , \quad \chi_0 = 1 \text{ on } \overline{V_{\Gamma_1}} \text{ with } \operatorname{supp}\chi_0 \subset V'_{\Gamma_1},$$

for a set $V'_{\Gamma_1} \subset \overline{\Omega}$ such that for some $\varepsilon > 0$, (see Figure B.15)

(i) $(V_{\Gamma_1} + B(0,\varepsilon)) \cap \overline{\Omega} \subset V'_{\Gamma_1}$,

(ii) $\Gamma'_1 := V'_{\Gamma_1} \cap \partial\Omega$ is smooth and $(\Gamma_1 + B(0,\varepsilon)) \cap \partial\Omega \subset \Gamma'_1$ and $(\Gamma'_1 + B(0,\varepsilon)) \cap \partial\Omega \subset B_z$,

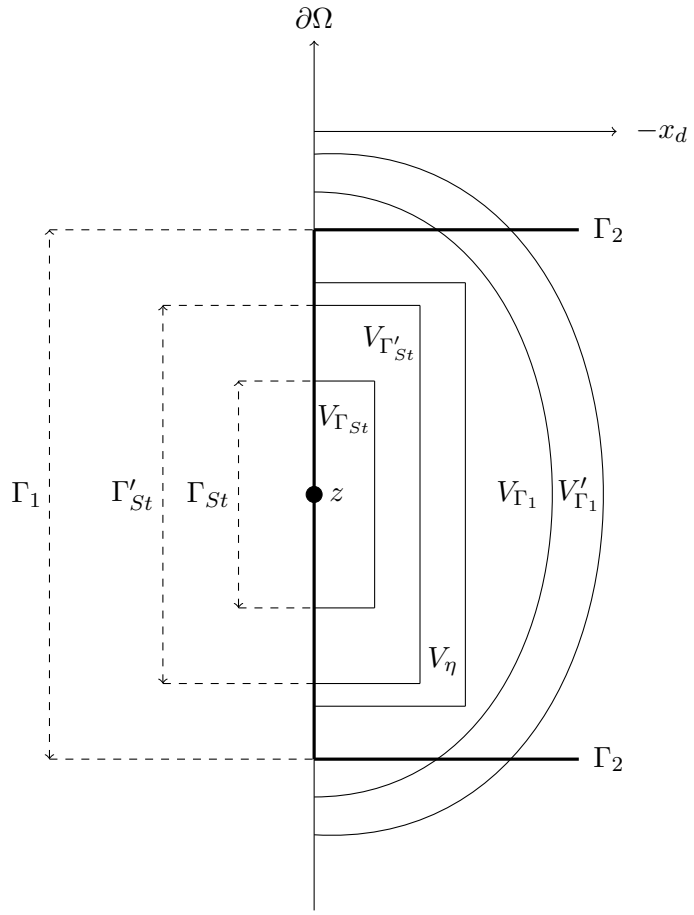

Figure B.15: Neighborhoods of z.

(iii) $\Psi = d_a(z, \cdot)$ is a smooth solution to the following eikonal equation in V'_{Γ_1} (see Proposition B.52):

$$\begin{cases} |\nabla\Psi|^2 = |\nabla f|^2 \text{ in } V'_{\Gamma_1} \\ \Psi = f - f(z) \text{ on } \Gamma'_1 \\ \partial_n\Psi = -\partial_n f \text{ on } \Gamma'_1 \ . \end{cases}$$

It is possible to choose V'_{Γ_1} such that all the properties stated previously on V_{Γ_1} also hold on V'_{Γ_1} (in particular (B.131), (B.132) and the properties stated in Proposition B.58). We recall that one has by (B.78):

$$|\nabla\Psi|^2 \leq |\nabla f|^2 \quad \text{a.e. in } \Omega.$$

Thus

$$|\nabla f_\pm| = \left|\nabla\left(\frac{\Psi \pm (f - f(z))}{2}\right)\right| \leq |\nabla f| \text{ a.e. in } \Omega.$$

Thanks to the relations $f - f(z) = f_+ - f_-$ and $\Psi = f_+ + f_-$, together with the equality $|\nabla\Psi|^2 = |\nabla f|^2$ a.e in V'_{Γ_1}, one has

$$\nabla f_- \cdot \nabla f_+ = 0 \quad \text{a.e in } V'_{\Gamma_1},\ |\nabla\Psi|^2 = |\nabla f|^2 = |\nabla f_+|^2 + |\nabla f_-|^2 \quad \text{a.e in } V'_{\Gamma_1}.$$

Let now $u_h^{(1)} \in D\left(\Delta_{f,h}^{M,(1)}(\dot{\Omega})\right)$ satisfy

$$\Delta_{f,h}^{M,(1)}(\dot{\Omega})\, u_h^{(1)} = 0 \text{ and } \left\|u_h^{(1)}\right\|_{L^2(\dot{\Omega})} = 1.$$

Step 1: Agmon estimate in Γ_1.

In this part, we are going to prove the estimate (B.147) with Ψ replaced by f_+ namely:

$$\|e^{\frac{f_+}{h}} u_h^{(1)}\|_{L^2(\dot{\Omega})} + \|d(e^{\frac{f_+}{h}} u_h^{(1)})\|_{L^2(\dot{\Omega})} + \|d^*(e^{\frac{f_+}{h}} u_h^{(1)})\|_{L^2(\dot{\Omega})} = O(h^{-N_0})$$

for some integer N_0. By the trace result (B.121), this will give the estimate $\left\|e^{\frac{f-f(z)}{h}} u_h^{(1)}\right\|_{L^2(\Gamma_1)} = O(h^{-N_0})$ which is the first step to prove (B.147).

To get these results, the idea is to apply Lemma B.62 to a convenient φ comparable with f_+ and such that $|\nabla\varphi| \leq |\nabla f_+|$. This kind of estimate is classic and the ideas behind the computations presented below, which follow [34, 47], originate from the article [35] where similar estimates were obtained in the case of manifolds without boundary. The presence of a boundary leads here to some technicalities which can somehow hide the reasoning and we refer for example to [19, 30] for a presentation of semi-classical Agmon estimates in manifolds without boundary. We recall from the work [35] that if one just wants to get an error of the form $O(e^{\frac{\varepsilon}{h}})$ with $\varepsilon > 0$ arbitrarily small, the choice $\varphi = (1-\varepsilon)f_+$ is sufficient, but it does not yield an error of the form $O(h^{-N})$. To get such an error term, a good choice for φ is (B.149).

Let $\varphi : \dot{\Omega} \to \mathbb{R}$ be the following Lipschitz function:

$$\varphi = \begin{cases} f_+ - Ch \ln \dfrac{f_+}{h} \text{ if } f_+ > Ch, \\ f_+ - Ch \ln C \text{ if } f_+ \leq Ch, \end{cases} \tag{B.149}$$

for some constant $C > 1$ that will be fixed at the end of this step. Define the associated level sets:

$$\Omega_- = \left\{x \in \dot{\Omega} \text{ s.t. } f_+(x) \leq Ch\right\} \quad \text{and} \quad \Omega_+ = \dot{\Omega} \setminus \Omega_-.$$

Then $\nabla\varphi = \nabla f_+$ a.e. in Ω_- and

$$\nabla\varphi = \nabla f_+ \left(1 - \frac{Ch}{f_+}\right) \quad \text{a.e. in } \Omega_+.$$

This implies in particular the two following inequalities valid a.e. on Ω_+ and that will be used in the sequel:

$$|\nabla f_+|^2 - |\nabla\varphi|^2 = |\nabla f_+|^2 \left(\frac{2Ch}{f_+} - \frac{C^2h^2}{f_+^2}\right) \geq Ch\frac{|\nabla f_+|^2}{f_+} \text{ on } \Omega_+ \tag{B.150}$$

$$|\nabla f|^2 - |\nabla\varphi|^2 \geq |\nabla f|^2 - |\nabla f_+|^2 \left(1 - \frac{Ch}{f_+}\right) \geq Ch\frac{|\nabla f|^2}{f_+} \text{ on } \Omega_+. \tag{B.151}$$

The last inequality in (B.151) is a consequence of the inequality $|\nabla f_+|^2 \leq |\nabla f|^2$. This implies in particular that $|\nabla\varphi| \leq |\nabla f|$ a.e. in $\dot{\Omega}$.

Note lastly that there exists a constant $K > 0$ depending on f_+ and f, such that

$$\frac{|\nabla f|^2}{f_+} \geq K \text{ in } \dot{\Omega} \text{ and } \frac{|\nabla f_+|^2}{f_+} \geq K \text{ in } V'_{\Gamma_1}\,, \tag{B.152}$$

the last inequality being a consequence of the facts that $f_+(x', x_d) = f_+(x', 0)$ and $x' \mapsto f(x', 0) = f(z) + f_+(x', 0)$ is a Morse function with z as only critical point.

Now, using the fact that $\Delta_{f,h}^{M,(1)}(\dot{\Omega})\, u_h^{(1)} = 0$ and the IMS localisation formula (B.143), one gets

$$\begin{aligned} 0 &= \mathcal{Q}_{f,h}^{M,(1)}(\dot{\Omega})(u_h^{(1)}, e^{2\frac{\varphi}{h}} u_h^{(1)}) \\ &= \sum_{k\in\{0,1\}} \left[\mathcal{Q}_{f,h}^{M,(1)}(\dot{\Omega})(\chi_k u_h^{(1)}, e^{2\frac{\varphi}{h}} \chi_k u_h^{(1)}) - h^2 \left\| |\nabla \chi_k| e^{\frac{\varphi}{h}} u_h^{(1)} \right\|^2_{L^2(\dot{\Omega})} \right]. \end{aligned}$$

Setting $\tilde{u}_h^{(1)} := e^{\frac{\varphi}{h}} u_h^{(1)}$ and applying (B.148) to $\chi_k u_h^{(1)}$, $k \in \{0,1\}$, one obtains:

$$\begin{aligned} &C_1 h^2 \sum_{k\in\{0,1\}} \left\| \chi_k \tilde{u}_h^{(1)} \right\|^2_{L^2(\dot{\Omega})} = C_1 h^2 \left\| \tilde{u}_h^{(1)} \right\|^2_{L^2(\dot{\Omega})} \\ &\geq \sum_{k\in\{0,1\}} \Big[\left\| h d\chi_k \tilde{u}_h^{(1)} \right\|^2_{L^2(\dot{\Omega})} + \left\| h d^* \chi_k \tilde{u}_h^{(1)} \right\|^2_{L^2(\dot{\Omega})} + \langle (|\nabla f|^2 - |\nabla \varphi|^2) \chi_k \tilde{u}_h^{(1)}, \chi_k \tilde{u}_h^{(1)} \rangle_{L^2(\dot{\Omega})} \\ &\quad + h \langle (\mathcal{L}_{\nabla f} + \mathcal{L}^*_{\nabla f}) \chi_k \tilde{u}_h^{(1)}, \chi_k \tilde{u}_h^{(1)} \rangle_{L^2(\dot{\Omega})} \Big] + h \left(\int_{\Gamma_2} - \int_{\Gamma_1} \right) \langle \chi_0 \tilde{u}_h^{(1)}, \chi_0 \tilde{u}_h^{(1)} \rangle \partial_n f \, d\sigma, \end{aligned}$$

where $C_1 = \max(\|\nabla \chi_0\|^2_\infty, \|\nabla \chi_1\|^2_\infty)$. Note that one has used that $\chi_0 = 0$ on Γ_0, $\chi_1 = 0$ on Γ_1 and

$$\left(- \int_{\Gamma_0} + \int_{\Gamma_2} \right) \langle \chi_1 \tilde{u}_h^{(1)}, \chi_1 \tilde{u}_h^{(1)} \rangle \partial_n f \, d\sigma \geq 0,$$

which follows from $\partial_n f > 0$ on Γ_2 and from $\partial_n f < 0$ on Γ_0.

Now, since $\mathcal{L}_{\nabla f} + \mathcal{L}^*_{\nabla f}$ is a 0th order differential operator, and $\left| \tilde{u}_h^{(1)}(x) \right| \leq e^C |u_h^{(1)}(x)|$ a.e. on Ω_-, one obtains that for some constants C_2 (independent of C) and $C_3(C)$ depending on C,

$$\begin{aligned} C_3(C) h \geq \sum_{k\in\{0,1\}} \Big[&\left\| h d\chi_k \tilde{u}_h^{(1)} \right\|^2_{L^2(\dot{\Omega})} + \left\| h d^* \chi_k \tilde{u}_h^{(1)} \right\|^2_{L^2(\dot{\Omega})} + \langle (|\nabla f|^2 - |\nabla \varphi|^2) \chi_k \tilde{u}_h^{(1)}, \chi_k \tilde{u}_h^{(1)} \rangle_{L^2(\dot{\Omega})} \\ &- C_2 h \left\| \chi_k \tilde{u}_h^{(1)} \right\|^2_{L^2(\Omega_+)} \Big] + h \left(\int_{\Gamma_2} - \int_{\Gamma_1} \right) \langle \chi_0 \tilde{u}_h^{(1)}, \chi_0 \tilde{u}_h^{(1)} \rangle \partial_n f \, d\sigma. \end{aligned} \tag{B.153}$$

Let us first consider the case $k = 1$. Using $|\nabla \varphi| \leq |\nabla f|$ and (B.151)–(B.152), one gets:

$$\begin{aligned} &\langle (|\nabla f|^2 - |\nabla \varphi|^2) \chi_1 \tilde{u}_h^{(1)}, \chi_1 \tilde{u}_h^{(1)} \rangle_{L^2(\dot{\Omega})} - C_2 h \left\| \chi_1 \tilde{u}_h^{(1)} \right\|^2_{L^2(\Omega_+)} \\ &\geq \langle (|\nabla f|^2 - |\nabla \varphi|^2) \chi_1 \tilde{u}_h^{(1)}, \chi_1 \tilde{u}_h^{(1)} \rangle_{L^2(\Omega_+)} - C_2 h \left\| \chi_1 \tilde{u}_h^{(1)} \right\|^2_{L^2(\Omega_+)} \\ &\geq \left\langle \left(C h \frac{|\nabla f|^2}{f_+} - C_2 h \right) \chi_1 \tilde{u}_h^{(1)}, \chi_1 \tilde{u}_h^{(1)} \right\rangle_{L^2(\Omega_+)} \\ &\geq (KC - C_2) h \left\| \chi_1 \tilde{u}_h^{(1)} \right\|^2_{L^2(\Omega_+)}. \end{aligned} \tag{B.154}$$

Let us then consider the case $k=0$. In this case, one deduces from $\operatorname{supp}\chi_0 \subset V'_{\Gamma_1}$ where $|\nabla f|^2 = |\nabla f_+|^2 + |\nabla f_-|^2$, from $|\nabla\varphi|^2 = |\nabla f_+|^2$ on Ω_-, and from (B.150)–(B.152) the inequality:

$$\begin{aligned}
&\langle (|\nabla f|^2 - |\nabla\varphi|^2)\chi_0\tilde{u}_h^{(1)}, \chi_0\tilde{u}_h^{(1)}\rangle_{L^2(\dot\Omega)} - C_2 h \left\|\chi_0\tilde{u}_h^{(1)}\right\|^2_{L^2(\Omega_+)} \\
&= \left\||\nabla f_-|\chi_0\tilde{u}_h^{(1)}\right\|^2_{L^2(\dot\Omega)} + \langle (\underbrace{|\nabla f_+|^2 - |\nabla\varphi|^2}_{=0})\chi_0\tilde{u}_h^{(1)}, \chi_0\tilde{u}_h^{(1)}\rangle_{L^2(\Omega_-)} \\
&\quad + \langle (|\nabla f_+|^2 - |\nabla\varphi|^2 - C_2 h)\chi_0\tilde{u}_h^{(1)}, \chi_0\tilde{u}_h^{(1)}\rangle_{L^2(\Omega_+)} \\
&\geq \left\||\nabla f_-|\chi_0\tilde{u}_h^{(1)}\right\|^2_{L^2(\dot\Omega)} + (KC - C_2)h \left\|\chi_0\tilde{u}_h^{(1)}\right\|^2_{L^2(\Omega_+)} \\
&\geq (1 + 2C_4(C)h)\left\||\nabla f_-|\chi_0\tilde{u}_h^{(1)}\right\|^2_{L^2(\dot\Omega)} - (KC - C_2)h\left\|\chi_0\tilde{u}_h^{(1)}\right\|^2_{L^2(\Omega_-)}, \qquad \text{(B.155)}
\end{aligned}$$

where $C_4(C) := \frac{KC - C_2}{2\|\nabla f_-\|^2_{L^\infty(V'_{\Gamma_1})}}$ (see (B.131)) and C has been chosen large enough to ensure that $KC - C_2 > 0$.

In order to get a lower bound for the boundary term in (B.153), one uses the fact that the mixed Witten Laplacian $\Delta^{M,(1)}_{\hat f,\hat h}(\dot\Omega)$ associated with $\hat f = -\tilde\chi_0 f_-$ where $\tilde\chi_0 \in C^\infty(\overline{\Omega}, [0,1])$, $\tilde\chi_0 = 1$ on $\operatorname{supp}\chi_0$, $\operatorname{supp}\tilde\chi_0 \subset (V'_{\Gamma_1} + B(0,\alpha)) \cap \overline{\Omega}$ for $\alpha > 0$ such that f_- is smooth on $\operatorname{supp}\tilde\chi_0$ and $\hat h = \frac{h}{1 + C_4(C)h}$, is nonnegative. Starting from the inequality $(1 + C_4(C)h)\mathcal{Q}^{M,(1)}_{\hat f,\hat h}(\dot\Omega)(\chi_0\tilde{u}_h^{(1)}, \chi_0\tilde{u}_h^{(1)}) \geq 0$ and then applying Lemma B.56 to $\chi_0\tilde{u}_h^{(1)} \in D\left(\mathcal{Q}^{M,(1)}_{\hat f,\hat h}(\dot\Omega)\right)$ lead to (since $\chi_0 = 0$ on Γ_0):

$$\begin{aligned}
h\left(\int_{\Gamma_1} - \int_{\Gamma_2}\right)\langle \chi_0\tilde{u}_h^{(1)}, \chi_0\tilde{u}_h^{(1)}\rangle \partial_n f_-\, d\sigma &\geq -(1 + C_4(C)h)\left\||\nabla f_-|\chi_0\tilde{u}_h^{(1)}\right\|^2_{L^2(\dot\Omega)} \\
&- \frac{h^2}{1 + C_4(C)h}\left(\left\|d\chi_0\tilde{u}_h^{(1)}\right\|^2_{L^2(\dot\Omega)} + \left\|d^*\chi_0\tilde{u}_h^{(1)}\right\|^2_{L^2(\dot\Omega)}\right) - hC_5\|\chi_0\tilde{u}_h^{(1)}\|^2_{L^2(\dot\Omega)}, \qquad \text{(B.156)}
\end{aligned}$$

where C_5 is some positive constant independent of C (it only depends on f_-).

Injecting the estimates (B.154)–(B.156) in (B.153) and using $f = -f_- + f_+ + f(z)$ on V'_{Γ_1} with $\partial_n f_+ = 0$ on Γ_1, then leads to:

$$\begin{aligned}
C_3 h \geq &\sum_{k\in\{0,1\}} \frac{C_4 h^3}{1 + C_4 h}\left(\left\|d\chi_k\tilde{u}_h^{(1)}\right\|^2_{L^2(\dot\Omega)} + \left\|d^*\chi_k\tilde{u}_h^{(1)}\right\|^2_{L^2(\dot\Omega)}\right) + (KC - C_2)h\left\|\chi_1\tilde{u}_h^{(1)}\right\|^2_{L^2(\Omega_+)} \\
&+ C_4 h\left\||\nabla f_-|\chi_0\tilde{u}_h^{(1)}\right\|^2_{L^2(\dot\Omega)} - (KC - C_2)h\left\|\chi_0\tilde{u}_h^{(1)}\right\|^2_{L^2(\Omega_-)} \\
&- hC_5\|\chi_0\tilde{u}_h^{(1)}\|^2_{L^2(\dot\Omega)} + h\int_{\Gamma_2}\langle \chi_0 u|\chi_0 u\rangle_{T^*_\sigma\dot\Omega}\partial_n f_+\, d\sigma.
\end{aligned}$$

In the last computation one has used that $1 \geq \frac{C_4 h}{1 + C_4 h}$, $1 - \frac{1}{1 + C_4 h} = \frac{C_4 h}{1 + C_4 h}$. It follows moreover from (B.135) that $\partial_n f_+ > 0$ on $\operatorname{supp}\chi_0 \cap \Gamma_2$. Then, since $|\tilde{u}_h^{(1)}(x)| \leq e^C |u_h^{(1)}(x)|$

a.e. on Ω_-, there exists $C_6(C, C_2, K)$ such that

$$C_6 h \geq \sum_{k\in\{0,1\}} \frac{C_4 h^3}{1+C_4}\left(\left\|d\chi_k \tilde{u}_h^{(1)}\right\|^2_{L^2(\dot\Omega)} + \left\|d^*\chi_k \tilde{u}_h^{(1)}\right\|^2_{L^2(\dot\Omega)}\right) + 2C_4 \left\|\nabla f_-\right\|^2_{L^\infty(V'_{\Gamma_1})} h \left\|\chi_1 \tilde{u}_h^{(1)}\right\|^2_{L^2(\dot\Omega)}$$
$$+ C_4 h \left\||\nabla f_-|\chi_0 \tilde{u}_h^{(1)}\right\|^2_{L^2(\dot\Omega)} - hC_5 \|\chi_0 \tilde{u}_h^{(1)}\|^2_{L^2(\dot\Omega)}.$$

One has used that $1 + C_4 \geq 1 + C_4 h$, for $h \leq 1$ and $KC - C_2 = 2C_4 \left\|\nabla f_-\right\|^2_{L^\infty(V'_{\Gamma_1})}$. Additionally, since $|\nabla f_-| \geq c > 0$ on $\overline{V'_{\Gamma_1}}$ (see (B.131)), $\lim_{C\to\infty} C_4(C) = +\infty$ and C_5 is independent of C, one can then choose C such that $c^2 C_4 - C_5 > 0$. This implies the existence of a constant $C_7 > 0$ such that for $h_0 > 0$ small enough and for all $h \in (0, h_0]$,

$$\|\tilde{u}_h^{(1)}\|_{L^2(\dot\Omega)} + \|d\tilde{u}_h^{(1)}\|_{L^2(\dot\Omega)} + \|d^*\tilde{u}_h^{(1)}\|_{L^2(\dot\Omega)} \ \leq \ \frac{C_7}{h}. \tag{B.157}$$

Since $\varphi - f_+ \geq -C_8 h \ln \frac{1}{h}$ for some constant C_8, there exists $N_0 > 0$ such that:

$$\|e^{\frac{f_+}{h}} u_h^{(1)}\|_{L^2(\dot\Omega)} + \|d(e^{\frac{f_+}{h}} u_h^{(1)})\|_{L^2(\dot\Omega)} + \|d^*(e^{\frac{f_+}{h}} u_h^{(1)})\|_{L^2(\dot\Omega)} = O(h^{-N_0}). \tag{B.158}$$

One has in particular, owing to the trace result (B.121) stated in Proposition B.55 and since $f_+ = f - f(z)$ on Γ_1,

$$\left\|e^{\frac{f-f(z)}{h}} u_h^{(1)}\right\|_{L^2(\Gamma_1)} = O(h^{-N_0}). \tag{B.159}$$

<u>Step 2:</u> Agmon estimate in $\dot\Omega$.

One follows the same approach as in step 1 but with the function

$$\varphi = \begin{cases} \Psi - Ch \ln \dfrac{\Psi}{h}, \text{ if } \Psi > Ch, \\ \Psi - Ch \ln C, \text{ if } \Psi \leq Ch, \end{cases}$$

where the constant $C > 1$ will be fixed later on, and with the associated level sets:

$$\Omega_- = \left\{x \in \dot\Omega \text{ s.t. } \Psi(x) \leq Ch\right\} \quad \text{and} \quad \Omega_+ = \dot\Omega \setminus \Omega_-.$$

Applying formula (B.148) then leads to (note that $|\tilde{u}_h^{(1)}| \leq e^C |u_h|$ on Ω_-, $\partial_n f < 0$ on Γ_0 and $\partial_n f > 0$ on Γ_2):

$$C_2(C) h \left(1 + \int_{\Gamma_1} \langle \tilde{u}_h^{(1)}, \tilde{u}_h^{(1)} \rangle_{T^*_\sigma\Omega}\, d\sigma\right) \geq \left\|hd\tilde{u}_h^{(1)}\right\|^2_{L^2(\dot\Omega)} + \left\|hd^*\tilde{u}_h^{(1)}\right\|^2_{L^2(\dot\Omega)} \tag{B.160}$$
$$+ \langle (|\nabla f|^2 - |\nabla\varphi|^2)\tilde{u}_h^{(1)}, \tilde{u}_h^{(1)}\rangle_{L^2(\dot\Omega)} - C_1 h \left\|\tilde{u}_h^{(1)}\right\|^2_{L^2(\Omega_+)},$$

where $\tilde{u}_h^{(1)} := e^{\frac{\varphi}{h}} u_h^{(1)}$, the constant C_1 is independent of C, whereas C_2 is a constant depending on C. Besides, due to the relations

$$\Psi = f - f(z) \text{ on } \Gamma_1 \text{ and } e^{\frac{\varphi}{h}} \ \leq \ e^{\frac{\Psi}{h}} \text{ on } \dot\Omega,$$

the trace estimate obtained in (B.159) implies

$$\int_{\Gamma_1} \langle \tilde{u}_h^{(1)}, \tilde{u}_h^{(1)} \rangle_{T^*_\sigma \Omega} \, d\sigma = O(h^{-2N_0}). \tag{B.161}$$

Injecting (B.161) in (B.160) then gives

$$\begin{aligned} &\left\| h d\tilde{u}_h^{(1)} \right\|^2_{L^2(\dot{\Omega})} + \left\| h d^* \tilde{u}_h^{(1)} \right\|^2_{L^2(\dot{\Omega})} \\ &+ \langle (|\nabla f|^2 - |\nabla \varphi|^2) \tilde{u}_h^{(1)}, \tilde{u}_h^{(1)} \rangle_{L^2(\dot{\Omega})} - C_1 h \left\| \tilde{u}_h^{(1)} \right\|^2_{L^2(\Omega_+)} = O(h^{1-2N_0}). \end{aligned} \tag{B.162}$$

Since moreover $|\nabla \Psi|^2 \leq |\nabla f|^2$ (see (B.78)) and f has no critival point in $\overline{\dot{\Omega}}$, one gets:

$$|\nabla f|^2 - |\nabla \varphi|^2 \geq |\nabla f|^2 - |\nabla \Psi|^2 \left(1 - \frac{Ch}{\Psi}\right) \geq Ch \frac{|\nabla f|^2}{\Psi} \geq C C_3 h \text{ on } \Omega_+$$

where $C_3 > 0$ is independent of C. Since $|\nabla f|^2 \geq |\nabla \Psi|^2 = |\nabla \varphi|^2$ a.e. on Ω_-, adding the term $(CC_3 - C_1) h \left\| \tilde{u}_h^{(1)} \right\|^2_{L^2(\Omega_-)}$ to (B.162) leads to

$$\left\| h d\tilde{u}_h^{(1)} \right\|^2_{L^2(\dot{\Omega})} + \left\| h d^* \tilde{u}_h^{(1)} \right\|^2_{L^2(\dot{\Omega})} + (CC_3 - C_1) h \left\| \tilde{u}_h^{(1)} \right\|^2_{L^2(\dot{\Omega})} = O(h^{1-2N_0})$$

Now, taking $C > \frac{C_1}{C_3}$ gives, since $\varphi - \Psi \geq -C_4 h \ln \frac{1}{h}$, there exists $N_1 > 0$ such that:

$$\|e^{\frac{\Psi}{h}} u_h^{(1)}\|_{L^2(\dot{\Omega})} + \|d(e^{\frac{\Psi}{h}} u_h^{(1)})\|_{L^2(\dot{\Omega})} + \|d^*(e^{\frac{\Psi}{h}} u_h^{(1)})\|_{L^2(\dot{\Omega})} = O(h^{-N_1}). \tag{B.163}$$

This concludes the proof of (B.147). ∎

B.4.4 Comparison of the eigenform $u_{h,i}^{(1)}$ and its WKB approximation

Throughout this section, one assumes **[H1]**, **[H2]** and **[H3]**. In all this section, we consider, for a fixed critical point z_i, an ensemble of sets $\mathcal{S}_{M,i}$ associated with z_i (see Definition B.12) and an L^2-normalized eigenform $u_{h,i}^{(1)}$ of $\Delta_{f,h}^{M,(1)}(\dot{\Omega}_i)$ associated with the eigenvalue 0, as introduced at the end of Section B.4.1.3. For the ease of notation, we drop the subscript i in all this section.

B.4.4.1 Construction of the WKB expansion of $u_h^{(1)}$

Let z be a local minimum of $f|_{\partial\Omega}$. Before going through a rigorous construction of a WKB expansion $u_{z,wkb}^{(1)}$ of $u_h^{(1)}$ in a neighborhood of z, let us explain formally how we proceed. Let us recall that the 1-form $u_h^{(1)}$ satisfies:

$$\begin{cases} \Delta_{f,h}^{(1)} u_h^{(1)} = 0 \text{ in } \dot{\Omega}, \\ \mathbf{t} u_h^{(1)} = 0 \text{ and } \mathbf{t} d_{f,h}^* u_h^{(1)} = 0 \text{ on } \Gamma_1, \end{cases} \tag{B.164}$$

plus additional boundary conditions on $\Gamma_0 \cup \Gamma_2$ that we do not recall since the objective is to approximate $u_h^{(1)}$ in a neighborhood of z in $\overline{\dot{\Omega}}$. The behavior of $u_h^{(1)}$ in a neighborhood

of z exhibited in Proposition B.61 suggests to take $u^{(1)}_{z,wkb}$ of the form $u^{(1)}_{z,wkb}(x,h) = a^{(1)}(x,h)\, e^{-\frac{d_a(x,z)}{h}}$ where $a^{(1)}$ is expanded in powers of h: $a^{(1)}(x,h) = \sum_{k\geq 0} a^{(1)}_k(x)h^k$ and to look for 1-forms $(a^{(1)}_k)_{k\geq 0}$ so that $u^{(1)}_{z,wkb}$ is a nontrivial 1-form satisfying (compare with (B.164)):

$$\begin{cases} \Delta^{(1)}_{f,h} u^{(1)}_{z,wkb} = O(h^\infty)\, e^{-\frac{d_a(\cdot,z)}{h}} \text{ in } \dot\Omega, \\ \mathbf{t} u^{(1)}_{z,wkb} = 0 \text{ and } \mathbf{t} d^*_{f,h} u^{(1)}_h = 0 \text{ on } \Gamma_1, \end{cases} \tag{B.165}$$

where the meaning of $O(h^\infty)$ is formally $h^s O(h^\infty) = o_h(1)$ for any $s \in \mathbb{R}$. The boundary conditions in (B.165) ensures that when cutting suitably a solution to (B.165) near Γ_1, the resulting 1-form belongs to the form domain of $\Delta^{M,(1)}_{f,h}(\dot\Omega)$ (this is needed if one wants to approximate $u^{(1)}_h$ on $\partial\dot\Omega$). Instead of directly trying to solve (B.165), the construction of $u^{(1)}_{z,wkb}$ can be simply done as follows (see [34, Section 4.2]). Using the complex property, one considers $u^{(1)}_{z,wkb} = d_{f,h} u^{(0)}_{z,wkb}$ where the function $u^{(0)}_{z,wkb} = a^{(0)}(\cdot,h)\, e^{-\frac{d_a(.,z)}{h}}$ where $a^{(0)}(x,h) = \sum_{k\geq 0} a^{(0)}_k(x)h^k$ for a non trivial family of functions $(a_k)_{k\geq 0}$ such that:

$$\begin{cases} \Delta^{(0)}_{f,h} u^{(0)}_{z,wkb} = O(h^\infty)\, e^{-\frac{d_a(\cdot,z)}{h}} \text{ in } \dot\Omega, \\ u^{(0)}_{z,wkb} = e^{-\frac{1}{h}f} \text{ on } \Gamma_1. \end{cases} \tag{B.166}$$

This implies the boundary condition: $a^{(0)} = 1$ on Γ_1. Then, if $u^{(0)}_{z,wkb} = a^{(0)}\, e^{-\frac{d_a(.,z)}{h}}$ is a solution of (B.166), we set:

$$u^{(1)}_{z,wkb} = d_{f,h} u^{(0)}_{z,wkb}.$$

One can easily check that the 1-form $u^{(1)}_{z,wkb}$ then satisfies (B.165) and the extra boundary condition $\mathbf{t} d^*_{f,h} u^{(1)}_{z,wkb} = O(h^\infty)\, e^{-\frac{f-f(z)}{h}}$ on Γ_1. Indeed, it holds:

$$d_{f,h} u^{(0)}_{z,wkb} = e^{-\frac{d_a(\cdot,z)}{h}} \left(d(f - d_a(\cdot,z))\, a^{(0)} + h\, da^{(0)} \right),$$

which implies $\mathbf{t} u^{(1)}_{z,wkb} = 0$ since $a^{(0)} = 1$ and

$$f - d_a(\cdot,z) = f(z) \text{ on } \Gamma_1. \tag{B.167}$$

In addition, one has

$$d^*_{f,h} d_{f,h} u^{(0)}_{z,wkb} = \Delta^{(0)}_{f,h} u^{(0)}_{z,wkb} = O(h^\infty)\, e^{-\frac{d_a(\cdot,z)}{h}}$$

which implies $\mathbf{t} d^*_{f,h} u^{(1)}_{z,wkb} = O(h^\infty)\, e^{-\frac{d_a(\cdot,z)}{h}}$ and

$$\Delta^{(1)}_{f,h} d_{f,h} u^{(0)}_{z,wkb} = d_{f,h} \Delta^{(0)}_{f,h} u^{(0)}_{z,wkb} = O(h^\infty)\, e^{-\frac{d_a(\cdot,z)}{h}}.$$

Thus, the 1-form $u^{(1)}_{z,wkb}$ satisfies (B.165).

Expanding in powers of h the function $e^{\frac{d_a(x,z)}{h}}\, \Delta^{(0)}_{f,h}\Big(\big(\sum_{k\geq 0} a^{(0)}_k(x)h^k \big) e^{-\frac{d_a(x,z)}{h}} \Big)$, $u^{(0)}_{z,wkb}$ is a solution of (B.166) if it holds:

$$|\nabla d_a(x,z)| = |\nabla f(x)|, \text{ for } x \in \dot\Omega, \tag{B.168}$$

which is satisfied at least in a neighborhood of z (see Proposition B.52) and if $(a_k^{(0)})_{k\geq 0}$ satisfies the following transport equations, defined recursively by:

$$\begin{cases} (\Delta\Phi - \Delta f + 2\nabla\Phi\cdot\nabla)a_0^{(0)} = 0 & \text{in } \dot{\Omega} \\ (\Delta\Phi - \Delta f + 2\nabla\Phi\cdot\nabla)a_{k+1}^{(0)} = \Delta a_k^{(0)} & \text{in } \dot{\Omega},\ \forall k\geq 0, \end{cases} \tag{B.169}$$

with boundary conditions $\begin{cases} a_0^{(0)} = 1 & \text{on } \Gamma_1 \\ a_k^{(0)} = 0 & \text{on } \Gamma_1,\ \forall k\geq 1 \end{cases}$. The equation (B.168) together with the boundary condition (B.167) justify *a posteriori* the choice of the function $d_a(\cdot, z)$ in the exponential for the ansatz on $u_{z,wkb}^{(1)}$. Let us mention that $\partial_n f > 0$ on Γ_1 implies that there exists a non trivial solution $u_{z,wkb}^{(0)}$ to (B.166) in a neighborhood of Γ_1 since in that case the transport equations (B.169) are non degenerate. Let us now justify rigorously the construction of the WKB expansion $u_{z,wkb}^{(1)}$ of $u_h^{(1)}$, which is, in view of (B.168) and (B.169), possible near Γ_1.

A preliminary construction.

Let Φ be the solution of the eikonal equation (B.102) on a neighborhood $V_{\partial\Omega}$ of the boundary $\partial\Omega$. Let us introduce the formal transport operator

$$T := \Delta\Phi - \Delta f + 2\nabla\Phi\cdot\nabla.$$

Let us consider the solutions to the following transport equations, defined recursively by

$$\begin{cases} Ta_0 = 0 & \text{in } V_{\partial\Omega} \\ Ta_{k+1} = \Delta a_k & \text{in } V_{\partial\Omega}, \quad \forall k\geq 0, \end{cases} \tag{B.170}$$

with boundary conditions

$$\begin{cases} a_0 = 1 & \text{on } \partial\Omega \\ a_k = 0 & \text{on } \partial\Omega, \quad \forall k\geq 1. \end{cases} \tag{B.171}$$

For a fixed k, the transport equation can be solved locally around each $z\in\partial\Omega$ thanks to the condition $\partial_n\Phi = -\partial_n f < 0$ on $\partial\Omega$ and thus on a neighborhood of $\partial\Omega$ (independent of k) using a compactness argument. Therefore, up to choosing a smaller neighborhood $V_{\partial\Omega}$ of $\partial\Omega$ in $\overline{\Omega}$, there exists a unique sequence of $C^\infty(V_{\partial\Omega})$ functions $(a_k)_{k\geq 0}$ solution to (B.170)-(B.171).

There exists a function $a = a(x,h)$ (called a resummation of the formal symbol $\sum_{k=0}^{+\infty} a_k h^k$) C^∞ and uniformly bounded together with all its derivatives such that

$$a(x,h) = 1 \text{ on } \partial\Omega \quad \text{and} \quad a(x,h) \sim \sum_{k=0}^{+\infty} a_k(x)h^k.$$

This means that $a - \sum_{k=0}^{+\infty} a_k h^k$ is $O(h^\infty)$ in the following sense: for all compact K in $V_{\partial\Omega}$, for all $\alpha\in\mathbb{N}^d$, for all $N\in\mathbb{N}$,

$$\left\| \partial_x^\alpha \left(a - \sum_{k=0}^{N} a_k(x)h^k \right) \right\|_{L^\infty(K)} \leq C_{K,\alpha,N} h^{N+1}. \tag{B.172}$$

Such a construction is standard and can be found in [19] or in [34], where it is done using a Borel summation. Moreover a is unique up to a term of order $O(h^\infty)$. Let us now define on $V_{\partial\Omega}$:

$$u^{(0)}_{wkb}(x,h) := a(x,h)\, e^{-\frac{\Phi}{h}}.$$

By construction of the sequence $(a_k)_{k\geq 0}$, the function $u^{(0)}_{wkb}$ solves

$$\begin{cases} \Delta^{(0)}_{f,h} u^{(0)}_{wkb} = O(h^\infty)\, e^{-\frac{\Phi}{h}} \text{ in } V_{\partial\Omega}, \\ \qquad u^{(0)}_{wkb} = e^{-\frac{\Phi}{h}} = e^{-\frac{f}{h}} \text{ on } \partial\Omega, \end{cases}$$

where $O(h^\infty)$ is defined in (B.172). Indeed, using (B.44), $|\nabla f|^2 = |\nabla\Phi|^2$ on $V_{\partial\Omega}$, and the equations (B.170) satisfied by $(a_k)_{k\geq 0}$,

$$\begin{aligned} e^{\frac{\Phi}{h}} \Delta^{(0)}_{f,h} u^{(0)}_{wkb} &= -h^2 \Delta a(x,h) + h[a(x,h)\Delta\Phi + 2\nabla\Phi\cdot\nabla a(x,h)] - a(x,h)|\nabla\Phi|^2 \\ &\quad + a(x,h)|\nabla f|^2 - h a(x,h)\Delta f \\ &\sim hTa_0 + h^2 \sum_{k=0}^{+\infty} h^k (Ta_{k+1} - \Delta a_k) \\ &= O(h^\infty). \end{aligned}$$

In addition, it holds $u^{(0)}_{wkb} = e^{-\frac{\Phi}{h}}$ on $\partial\Omega$ since $a(x,h) = 1$ on $\partial\Omega$. Let us now define on $V_{\partial\Omega}$:

$$u^{(1)}_{wkb} := d_{f,h} u^{(0)}_{wkb}.$$

The 1-form $u^{(1)}_{wkb}$ satisfies:

$$\begin{cases} \Delta^{(1)}_{f,h} u^{(1)}_{wkb} = O(h^\infty) e^{-\frac{\Phi}{h}} \text{ in } V_{\partial\Omega}, \\ \qquad \mathbf{t} u^{(1)}_{wkb} = 0 \text{ on } \partial\Omega, \\ \mathbf{t} d^*_{f,h} u^{(1)}_{wkb} = O(h^\infty) e^{-\frac{\Phi}{h}} \text{ on } \partial\Omega, \end{cases} \tag{B.173}$$

where $O(h^\infty)$ is defined in (B.172). Indeed, one has $\mathbf{t} u^{(1)}_{wkb} = \mathbf{t} d_{f,h} u^{(0)}_{wkb} = d_{f,h} \mathbf{t} u^{(0)}_{wkb} = d_{f,h}\mathbf{t}\left(a(x,h)e^{-\frac{\Phi}{h}}\right) = d_{f,h}\mathbf{t} e^{-\frac{f}{h}} = d_{f,h} e^{-\frac{f}{h}} = 0$ since $a(x,h) = 1$ and $\Phi = f$ on $\partial\Omega$. Moreover $\mathbf{t} d^*_{f,h} u^{(1)}_{wkb} = \mathbf{t} d^*_{f,h} d_{f,h} u^{(0)}_{wkb} = \mathbf{t}\Delta^{(0)}_{f,h} u^{(0)}_{wkb} = O(h^\infty) e^{-\frac{\Phi}{h}}$. Finally, $\Delta^{(1)}_{f,h} u^{(1)}_{wkb} = \Delta^{(1)}_{f,h} d_{f,h} u^{(0)}_{wkb} = d_{f,h}\Delta^{(0)}_{f,h} u^{(0)}_{wkb} = (hd + df\wedge) O(h^\infty) e^{-\frac{\Phi}{h}} = O(h^\infty) e^{-\frac{\Phi}{h}}$.

<u>WKB expansion of $u^{(1)}_h$.</u>

Let z be a local minimum of $f|_{\partial\Omega}$. Let us now define the WKB expansion of $u^{(1)}_h$ on $V_{\partial\Omega}$ by:

$$u^{(1)}_{z,wkb} := e^{\frac{f(z)}{h}} u^{(1)}_{wkb} = e^{\frac{f(z)}{h}} d_{f,h} u^{(0)}_{wkb} = d_{f,h}\left(a(\cdot,h) e^{-\frac{\Phi - f(z)}{h}}\right). \tag{B.174}$$

One recalls (see Proposition B.52) that for any smooth open domain Γ such that $\overline{\Gamma} \subset \Gamma_1$ and $z \in \Gamma$, there exists a neighborhood of Γ in $\overline{\Omega}$, denoted by $V_\Gamma \subset V_{\partial\Omega} \cap (\Gamma_1 \cup \dot{\Omega})$, such that for all $x \in V_\Gamma$,

$$\Psi(x) = d_a(x,z) = \Phi(x) - f(z).$$

Lemma B.63. *Let us assume that the hypotheses **[H1]** and **[H3]** hold. Let us consider z a local minimum of $f|_{\partial\Omega}$ as introduced in hypothesis **[H2]**. The 1-form $u^{(1)}_{z,wkb}$ satisfies*

$$\begin{cases} \Delta^{(1)}_{f,h} u^{(1)}_{z,wkb} = O(h^\infty) e^{-\frac{\Phi - f(z)}{h}} \text{ in } V_{\partial\Omega}, \\ \mathbf{t} u^{(1)}_{z,wkb} = 0 \text{ on } \partial\Omega, \\ \mathbf{t} d^*_{f,h} u^{(1)}_{z,wkb} = O(h^\infty) e^{-\frac{\Phi - f(z)}{h}} \text{ on } \partial\Omega, \end{cases} \tag{B.175}$$

where $O(h^\infty)$ is defined in (B.172)*. For any $\chi \in C^\infty_c(V_\Gamma)$ such that $\chi = 1$ on a neighborhood of z, it holds: in the limit $h \to 0$,*

$$\int_\Omega |\chi(x) u^{(1)}_{z,wkb}(x)|^2 dx = C^2_{z,wkb}\ h^{\frac{d+1}{2}}\ (1 + O(h)), \tag{B.176}$$

where

$$C_{z,wkb} := \pi^{\frac{d-1}{4}} \frac{\sqrt{2\partial_n f(z)}}{(\det \operatorname{Hess} f|_{\partial\Omega}(z))^{\frac{1}{4}}}. \tag{B.177}$$

Furthermore, there exists $C > 0$ such that for h small enough,

$$\|\chi u^{(1)}_{z,wkb}\|_{H^1(\Omega)} \leq C h^{-1}, \tag{B.178}$$

and $\mathcal{Q}^{M,(1)}_{f,h}(\dot\Omega)(\chi u^{(1)}_{z,wkb}) = O(h^\infty)$.

Proof. Equation (B.175) is easily obtained from (B.173). Let us now prove (B.176) and (B.177). Notice that one can write (using (B.42))

$$\begin{aligned} u^{(1)}_{z,wkb} &= d_{f,h}\left[e^{-\frac{\Phi - f(z)}{h}} \sum_{k=0}^{+\infty} a_k h^k \right] \\ &= e^{-\frac{f}{h}} (hd) e^{\frac{f}{h}} \left[e^{-\frac{\Phi - f(z)}{h}} \sum_{k=0}^{+\infty} a_k h^k \right] \\ &= e^{-\frac{\Phi - f(z)}{h}} e^{-\frac{f - \Phi}{h}} (hd) e^{\frac{f-\Phi}{h}} \left[\sum_{k=0}^{+\infty} a_k h^k \right] \\ &= e^{-\frac{\Phi - f(z)}{h}} \left(d(f - \Phi) \wedge a_0 \right) \\ &\quad + e^{-\frac{\Phi - f(z)}{h}} \left[hd \sum_{k=0}^{+\infty} a_k h^k + d(f - \Phi) \wedge \sum_{k=1}^{+\infty} a_k h^k \right]. \end{aligned} \tag{B.179}$$

Recall that the function χ is supported in V_Γ and the function $x \mapsto \Phi(x) - f(z)$ has a unique minimum on V_Γ which is z since $\Phi(x) - f(z) = d_a(x, z) \geq 0$ on V_Γ. Therefore, in the limit $h \to 0$:

$$\sqrt{\int_\Omega \left| \chi(x) u^{(1)}_{z,wkb}(x) \right|^2 dx} = \sqrt{\int_\Omega \left| e^{-\frac{\Phi - f(z)}{h}} \chi d(f - \Phi) \wedge a_0 \right|^2} (1 + O(h)).$$

Additionaly, since $\chi(z) = 1$ and $|d(f - \Phi)(z)|^2 = |\nabla(f - \Phi)(z)|^2 = |\nabla_T(f - \Phi)(z)|^2 + (2\partial_n f(z))^2 = (2\partial_n f(z))^2$, one gets using Laplace's method

$$\int_\Omega \left| e^{-\frac{\Phi - f(z)}{h}} \chi d(f - \Phi) \wedge a_0 \right|^2 = (\pi h)^{\frac{d+1}{2}} \frac{2\partial_n f(z)}{\pi \sqrt{\det \operatorname{Hess} f|_{\partial\Omega}(z)}}\ (1 + O(h)). \tag{B.180}$$

Let us give more details on how to obtain (B.180). Recall that on supp(χ), $\Phi - f(z) = f_+ + f_-$, $f - \Phi = f - \Psi - f(z) = -2f_-$ and, on supp$(\chi) \cap \partial\Omega$, $\partial_n f = -\partial_n f_- = |\nabla f_-|$. Thus, using the coordinate set introduced in Definition B.9 and the co-area formula $dx = \frac{d\sigma_{\Sigma_\eta}}{|\nabla f_-|} d\eta$ (see for example [1])

$$\int_\Omega \left| e^{-\frac{\Phi(x)-f(z)}{h}} \chi(x) d(f-\Phi)(x) \wedge a_0(x) \right|^2 dx = 4 \int_{-\alpha}^0 e^{-2\frac{\eta}{h}} \int_{\Sigma_\eta} e^{-2\frac{f_+}{h}} \chi^2 a_0^2 |\nabla f_-| d\sigma_{\Sigma_\eta}\, d\eta$$
$$= 4 \int_{-\alpha}^0 e^{-2\frac{\eta}{h}} \int_{\partial\Omega} e^{-2\frac{f_+(x',0)}{h}} \chi^2(x',\eta) a_0^2(x',\eta) |\nabla f_-|(x',\eta) j(x',\eta) d\sigma_{\partial\Omega}(x')\, d\eta$$

where $\Sigma_\eta = \{x,\ f_-(x) = -\eta\}$, σ_{Σ_η} is the Lebesgue measure on Σ_η. In the last equality, $j(x',\eta)$ is the Jacobian of the parametrization of Σ_η by $x' \in \partial\Omega$. Using the Laplace formula, for any $\eta \in [-\eta_0, 0]$ with $\eta_0 > 0$ sufficiently small so that $\chi^2(z,\eta) \neq 0$ for all $\eta \in [-\eta_0, 0]$, one has

$$\int_{\partial\Omega} e^{-2\frac{f_+(x',0)}{h}} \chi^2(x',\eta) a_0^2(x',\eta) |\nabla f_-|(x',\eta) j(x',\eta) d\sigma_{\partial\Omega}(x')$$
$$= (\pi h)^{\frac{d-1}{2}} (\det \mathrm{Hess}\, f_+(z))^{-1/2} \chi^2(z,\eta) |\nabla f_-|(z,\eta) j(z,\eta) a_0^2(z,\eta)(1 + O(h)) \qquad \text{(B.181)}$$

where $O(h)$ is a function of η and h with L^∞ norm in $\eta \in [0, \eta_0]$ bounded from above by a constant times h (thanks to the regularity of the involved terms), for sufficiently small h. Thus, using again Laplace's method:

$$\int_\Omega \left| e^{-\frac{\Phi - f(z)}{h}} \chi d(f-\Phi) \wedge a_0 \right|^2$$
$$= 4 \int_{-\alpha}^0 e^{-2\frac{\eta}{h}} (\pi h)^{\frac{d-1}{2}} (\det \mathrm{Hess}\, f_+(z))^{-1/2} \chi^2(z,\eta) a_0^2(z,\eta) |\nabla f_-|(z,\eta) j(z,\eta)\, d\eta (1 + O(h))$$
$$= 2h(\pi h)^{\frac{d-1}{2}} (\det \mathrm{Hess}\, f_+(z))^{-1/2} \chi^2(z,0) a_0^2(z,0) |\nabla f_-|(z,0) j(z,0)(1 + O(h))$$

Since $\chi(z,0) = 1$, $a_0(z,0) = 1$, Hess $f_+(z) =$ Hess $f|_{\partial\Omega}(z)$ and $j(z,0) = 1$, this concludes the proof of (B.180), and thus of (B.176)-(B.177).

Now, writing

$$u^{(1)}_{z,wkb} = e^{-\frac{\Phi - f(z)}{h}} \left[d(f-\Phi) \wedge a(\cdot, h) + h\, da(\cdot, h) \right],$$

and noticing that $\Phi - f(z) \geq 0$ on suppχ, one has $\|\chi u^{(1)}_{z,wkb}\|_{H^1(\Omega)} \leq Ch^{-1}$.

It remains to prove the last statement. Using the fact that supp$[\Delta^{(1)}_{f,h}, \chi] \subset$ supp χ, $\Phi - f(z) = \Psi \geq c' > 0$ on supp$\nabla\chi$ and (B.175), one gets

$$\Delta^{(1)}_{f,h}(\chi u^{(1)}_{z,wkb}) = \chi \Delta^{(1)}_{f,h}\left(u^{(1)}_{z,wkb}\right) + [\Delta^{(1)}_{f,h}, \chi]\left(u^{(1)}_{z,wkb}\right)$$
$$= O(h^\infty) + O(e^{-\frac{c}{h}}) = O\left(h^\infty\right).$$

Therefore, from the Cauchy-Schwartz inequality, one has $\langle \chi u^{(1)}_{z,wkb}, \Delta^{(1)}_{f,h}(\chi u^{(1)}_{z,wkb}) \rangle_{L^2(\dot\Omega)} = O(h^\infty)$. The fact that $\mathcal{Q}^{M,(1)}_{f,h}(\dot\Omega)(\chi u^{(1)}_{z,wkb}) = O(h^\infty)$ then follows from an integration by parts and the boundary conditions in (B.175). ∎

B.4.4.2 A first estimate of the accuracy of the WKB approximation

Recall that $z \in \{z_1, \dots, z_n\}$ is a local minimum of $f|_{\partial\Omega}$ and that $u_h^{(1)}$ is a L^2-normalized eigenform of $\Delta_{f,h}^{M,(1)}(\dot{\Omega})$ associated with the eigenvalue 0. The objective of this section is to prove that $u_h^{(1)}$ is accurately approximated by the function $u_{z,wkb}^{(1)}$ defined in the previous section. The computations below are inspired by those made in [34, Chapter 4] where the authors were adapting [30, 35] to manifolds with boundary. The novelty is that we compare the two 1-forms on a neighborhood of B_z, instead of a neighborhood of z.

Take two smooth open sets $\Gamma_{St} \subset \Gamma'_{St} \subset \Gamma_1$ which are strongly stable (see Definition B.11 and Proposition B.57) and such that, for some positive ε, $(\Gamma_{St}+B(0,\varepsilon))\cap\partial\dot{\Omega} \subset \Gamma'_{St}$ and $(\Gamma'_{St} + B(0,\varepsilon)) \cap \partial\dot{\Omega} \subset \Gamma_1$, see Figure (B.15). The fact that Γ_{St} and Γ'_{St} are strongly stable and thus that $V_{\Gamma_{St}}$ and $V'_{\Gamma_{St}}$ are stable under the dynamics (B.183) -see below- will actually be needed only to get refined estimates in Section B.4.4.3. Let us now consider the system of coordinate (x', x_d) (see Definition B.9) which is well defined on V_{Γ_1} by assumption (see item 2 in Proposition B.58). Let us introduce the Lipschitz sets $V_{\Gamma_{St}}$ and $V_{\Gamma'_{St}}$

$$V_{\Gamma_{St}} = \{(x', x_d) \in \Gamma_{St} \times (-a, 0)\} \text{ and } V_{\Gamma'_{St}} = \{(x', x_d) \in \Gamma'_{St} \times (-a', 0)\} \tag{B.182}$$

where $0 < a < a'$ are small enough so that $V_{\Gamma_{St}} \subset V_{\Gamma'_{St}} \subset V_{\Gamma_1}$. By construction, there exists $\varepsilon > 0$ such that $V_{\Gamma_{St}}+B(0,\varepsilon) \subset V_{\Gamma'_{St}}$ and $V_{\Gamma'_{St}}+B(0,\varepsilon) \subset V_{\Gamma_1}\cap(\dot{\Omega}\cup\Gamma_1)$ (see again Figure B.15 for a schematic representation of these sets). In addition $V_{\Gamma_{St}} \cap \Gamma_1 = \Gamma_{St}$ and $V_{\Gamma'_{St}} \cap \Gamma_1 = \Gamma'_{St}$. Moreover, a and a' can be chosen sufficiently small so that the sets $\overline{V_{\Gamma_{St}}}$ and $\overline{V_{\Gamma'_{St}}}$ are stable under the dynamics

$$x'(t) = \begin{cases} -\nabla\Phi(x(t)) & \text{on } \Omega \\ -\nabla_T\Phi(x(t)) & \text{on } \partial\Omega. \end{cases} \tag{B.183}$$

This stability is a consequence of two facts. First, for $x(t)$ solution to (B.183), $\frac{d}{dt}f_-(x(t))' = -|\nabla f_-(x(t))|^2$ (since $\nabla\Phi\cdot\nabla f_- = |\nabla f_-|^2$ on V_{Γ_1}, thanks to (B.132), and $\nabla_T\Phi\cdot\nabla f_- = 0$ in $\partial\Omega$) so that $\forall t \geq 0$, $x_d(x(0)) \leq x_d(x(t)) \leq 0$. Second, by construction, for sufficiently small a and a',

$$\forall x \in \partial V_{\Gamma_{St}} \text{ such that } x'(x) \in \partial\Gamma_{St},\ \nabla\Phi(x)\cdot n_x(V_{\Gamma_{St}}) > 0$$

(where $n(V_{\Gamma_{St}})$ is the unit ouward normal to $V_{\Gamma_{St}}$). Indeed for any $z \in \partial\Gamma_{St}$, $\lim_{\sigma\to z} n_\sigma(V_{\Gamma_{St}}) = n_z(\Gamma_{St})$ (where the limit is taken for $\sigma \in \partial V_{\Gamma_{St}}$ with $x'(\sigma) \in \partial\Gamma_{St}$), see (B.140) for a proof, and since Γ_{St} is chosen strongly stable, for $z \in \partial\Gamma_{St}$, $\nabla\Phi(z)\cdot n_z(V_{\Gamma_{St}}) = (\nabla f_+ + \nabla f_-)\cdot n_z(\Gamma_{St}) = \nabla f_+ \cdot n_z(\Gamma_{St}) = \nabla f|_{\partial\Omega}\cdot n_z(\Gamma_{St}) > 0$. The argument is of course the same for $V_{\Gamma'_{St}}$.

Let us now introduce two smooth cut-off functions $0 \leq \chi \leq \eta \in \mathcal{C}_c^\infty(\dot{\Omega}\cup\Gamma_1)$ satisfying

$$\chi = 1 \text{ in a neighborhood of } \overline{V_{\Gamma_{St}}}, \quad \operatorname{supp}\chi \subset V_{\Gamma'_{St}} \tag{B.184}$$

$$\text{and } \eta = 1 \text{ in a neighborhood of } \overline{V_{\Gamma'_{St}}}, \quad \operatorname{supp}\eta \subset V_{\Gamma_1} \cap (\dot{\Omega}\cup\Gamma_1). \tag{B.185}$$

Notice that by construction, $\eta = 0$ on Γ_2. In the following, we moreover assume that χ and η are tensor products in the system of coordinates (x', x_d) (this will actually be needed only to get refined estimates in Section B.4.4.3):

$$\chi(x', x_d) = \chi_1(x')\chi_d(x_d) \text{ and } \eta(x', x_d) = \eta_1(x')\eta_d(x_d). \tag{B.186}$$

Let $\kappa \in \{\chi, \eta\}$. Owing to Lemma B.54, the 1-form $\kappa u_h^{(1)}$ belongs to $\Lambda^1 H_T^1(\dot{\Omega})$. The first a priori estimate on $\kappa(u_h^{(1)} - c(h)u_{z,wkb}^{(1)})$ is the following:

Proposition B.64. *Let us assume that the hypotheses **[H1]**, **[H2]** and **[H3]** hold. For $\kappa \in \{\chi, \eta\}$, one has*

$$\left\| \kappa(u_h^{(1)} - c_z(h)u_{z,wkb}^{(1)}) \right\|_{H^1(\dot{\Omega})} = O(h^\infty) \tag{B.187}$$

where

$$c_z(h)^{-1} = \langle u_h^{(1)}, \chi u_{z,wkb}^{(1)} \rangle_{L^2(\dot{\Omega})}. \tag{B.188}$$

The 1-form $u_h^{(1)}$ can be chosen such that $c_z(h) > 0$. Additionally, when $h \to 0$

$$c_z(h) = C_{z,wkb}^{-1} h^{-\frac{d+1}{4}} (1 + O(h^\infty)), \tag{B.189}$$

where $C_{z,wkb}$ is defined by (B.177).

Notice that $|c_z(h)|^{-1}$ is equivalent (in the limit $h \to 0$) to $\|\kappa u_{z,wkb}^{(1)}\|_{L^2(\dot{\Omega})}$ (see (B.176)), and can thus be simply understood as a normalizing factor.

Proof. Let us first consider the case $\kappa = \chi$, the other case is considered at the end of the proof. One defines $k(h) := \langle u_h^{(1)}, \chi u_{z,wkb}^{(1)} \rangle_{L^2(\dot{\Omega})} \in \mathbb{R}$. If $k(h) < 0$, then one changes $u_h^{(1)}$ to $-u_h^{(1)}$ so that one can suppose without loss of generality that

$$k(h) \geq 0.$$

For h small enough, one has (from Proposition B.59, item (iii))

$$\pi_{[0,ch^{3/2})}(\Delta_{f,h}^{M,(1)}(\dot{\Omega}))(\chi u_{z,wkb}^{(1)}) = k(h)u_h^{(1)}.$$

Let us define

$$\alpha_h := \chi(u_{z,wkb}^{(1)} - k(h)u_h^{(1)}).$$

Thus, the following identity holds for h small enough

$$\alpha_h = k(h)\,(1 - \chi)\,u_h^{(1)} + \pi_{[h^{3/2},+\infty]}(\Delta_{f,h}^{M,(1)}(\dot{\Omega}))(\chi u_{z,wkb}^{(1)}).$$

Notice that, using Cauchy-Schwarz inequality and Lemma B.63, there exist $C > 0$ and $h_0 > 0$ such that for all $h \in (0, h_0)$

$$|k(h)| \leq Ch^{\frac{d+1}{4}}.$$

Therefore, using Lemma C.8, Proposition B.61 and Lemma B.63 we get

$$\begin{aligned}
\|\alpha_h\|^2_{L^2(\dot\Omega)} &\leq 2k(h)^2\|\,(1-\chi)\,u_h^{(1)}\|^2_{L^2(\dot\Omega)} + 2\left\|\pi_{[ch^{3/2},+\infty]}\left(\Delta^{M,(1)}_{f,h}(\dot\Omega)\right)(\chi u^{(1)}_{z,wkb})\right\|^2_{L^2(\dot\Omega)}\\
&\leq Ch^{\frac{d+1}{2}}\left\|(1-\chi)\,u_h^{(1)}e^{\frac{\Psi}{h}}e^{\frac{-\Psi}{h}}\right\|^2_{L^2(\dot\Omega)} + Ch^{-3/2}\mathcal{Q}^{M,(1)}_{f,h}(\dot\Omega)(\chi u^{(1)}_{z,wkb})\\
&\leq Ch^{\frac{d+1}{2}}h^{-N_0}e^{-\frac{c}{h}} + Ch^{-3/2}\mathcal{Q}^{M,(1)}_{f,h}(\dot\Omega)(\chi u^{(1)}_{z,wkb})\\
&= O(h^\infty),
\end{aligned}$$

with $c := \inf_{\mathrm{supp}(1-\chi)}\Psi > 0$ (since $\chi = 1$ near z) and the integer N_0 is given by Proposition B.61. Moreover, since $d_{f,h} = hd + df\wedge$ and $d^*_{f,h} = hd^* + \mathbf{i}_{\nabla f}$, one obtains using the triangular inequality, the Gaffney inequality (B.116) (since $\alpha_h \in H^1_T(\dot\Omega)$), the fact that $\mathcal{Q}^{M,(1)}_{f,h}(\dot\Omega)(\chi u_h^{(1)}) = O(e^{-\frac{c}{h}})$ (from the Agmon estimate (B.147)) and $\mathcal{Q}^{M,(1)}_{f,h}(\dot\Omega)(\chi u^{(1)}_{z,wkb}) = O(h^\infty)$,

$$\begin{aligned}
\|\alpha_h\|^2_{H^1(\dot\Omega)} &\leq C(\|d\alpha_h\|^2_{L^2(\dot\Omega)} + \|d^*\alpha_h\|^2_{L^2(\dot\Omega)} + \|\alpha_h\|^2_{L^2(\dot\Omega)})\\
&\leq Ch^{-2}\left(\mathcal{Q}^{M,(1)}_{f,h}(\dot\Omega)(\alpha_h) + \|\alpha_h\|^2_{L^2(\dot\Omega)}\right)\\
&= O(h^\infty).
\end{aligned}$$

Moreover since $\|\chi u_h^{(1)}\|_{L^2(\dot\Omega)} = 1 + O(e^{-\frac{c}{h}})$ (from the Agmon estimate (B.147)), by considering $\|\chi(u^{(1)}_{z,wkb} - k(h)u_h^{(1)})\|_{L^2(\dot\Omega)} = O(h^\infty)$, one gets:

$$\begin{aligned}
k(h)^2 &= \frac{\|\chi u^{(1)}_{z,wkb}\|^2_{L^2(\dot\Omega)} + O(h^\infty)}{2 - \|\chi u_h^{(1)}\|^2_{L^2(\dot\Omega)}}\\
&= \frac{C^2_{z,wkb}h^{\frac{d+1}{2}} + O(h^\infty)}{1 + O(e^{-\frac{c}{h}})},
\end{aligned}$$

with $C_{z,wkb}$ is given by (B.177) in Lemma B.63. Therefore, since $k(h) \geq 0$, $k(h) = C_{z,wkb}h^{\frac{d+1}{4}}(1 + O(h^\infty))$. This concludes the proof of (C.115) for $\kappa = \chi$, by choosing

$$c_z(h) := k(h)^{-1}.$$

Let us now deal with the case $\kappa = \eta$. There exists $c > 0$ such that, for h sufficiently small,

$$\begin{aligned}
\|\eta(u^{(1)}_{z,wkb} - k(h)u_h^{(1)})\|_{H^1(\dot\Omega)} &\leq \|\alpha_h\|_{H^1(\dot\Omega)} + \|(\eta-\chi)(u^{(1)}_{z,wkb} - k(h)u_h^{(1)})\|_{H^1(\dot\Omega)}\\
&\leq O(h^\infty) + \|(\eta-\chi)u^{(1)}_{z,wkb}\|_{H^1(\dot\Omega)} + |k(h)|\|(\eta-\chi)u_h^{(1)}\|_{H^1(\dot\Omega)}\\
&\leq O(h^\infty) + e^{-\frac{c}{h}}.
\end{aligned}$$

The last inequality is the consequence of two facts. First, $\|(\eta-\chi)u_h^{(1)}\|_{H^1(\dot\Omega)} = e^{-\frac{c}{h}}$ thanks to Proposition B.61 and (B.116) together with the fact that $\chi = \eta$ near z. Second, a direct computation shows that

$$\|(\eta-\chi)u^{(1)}_{z,wkb}\|_{H^1(\dot\Omega)} \leq Ch^{-1}e^{-\frac{\inf_{\mathrm{supp}(\eta-\chi)}\Psi}{h}} \leq e^{-\frac{c}{h}}.$$

This concludes the proof of Proposition B.64. ∎

The estimate we obtained in Proposition B.64 is sufficient to get the result of Theorem B.1. The more precise estimates on Section B.4.4.3 are only needed to prove Theorem B.2.

B.4.4.3 A more accurate comparison on the WKB approximation

The objective of this section is to combine the techniques used to obtain the Agmon estimates of Proposition B.61 and the first estimate of the accuracy of the WKB approximation of Proposition B.64 in order to obtain a more precise estimate of the latter.

Let us start with estimates which are simple consequences of Proposition B.61 and Proposition B.64. Notice that, for $\kappa \in \{\chi, \eta\}$, one obviously gets from Proposition B.61 the following relation in $\Lambda^1 H^1(\dot{\Omega})$:

$$\exists N_0 \in \mathbb{N},\ e^{\frac{\Psi}{h}} \kappa (u_h^{(1)} - c_z(h) u_{z,wkb}^{(1)}) \ = O(h^{-N_0}). \tag{B.190}$$

For the term involving $u_{z,wkb}^{(1)}$, this is due to $\Psi(x) = \Phi(x) - f(z)$ on $\operatorname{supp} \kappa$ and the estimate (B.189) on $c_z(h)$. Let us now set

$$w_h := \kappa (u_h^{(1)} - c_z(h) u_{z,wkb}^{(1)}). \tag{B.191}$$

The 1-form w_h is in $C_c^\infty(\dot{\Omega} \cup \Gamma_1)$ and satisfies in $\dot{\Omega}$:

$$\begin{aligned}
\Delta_{f,h}^{(1)} w_h &= \kappa \Delta_{f,h}^{(1)} (u_h^{(1)} - c_z(h) u_{z,wkb}^{(1)}) + [\Delta_{f,h}^{(1)}, \kappa](u_h^{(1)} - c_z(h) u_{z,wkb}^{(1)}) \\
&= -c_z(h) \kappa \Delta_{f,h}^{(1)} u_{z,wkb}^{(1)} + [\Delta_{f,h}^{(1)}, \kappa](u_h^{(1)} - c_z(h) u_{z,wkb}^{(1)}) \\
&= (r_1 + r_1') e^{-\frac{\Psi}{h}} \ ,
\end{aligned} \tag{B.192}$$

where, owing to (B.175) and (B.189):

$$r_1 := -e^{\frac{\Psi}{h}} c_z(h) \kappa \Delta_{f,h}^{(1)} u_{z,wkb}^{(1)} = O(h^\infty) \tag{B.193}$$

in $\Lambda^1 L^2(\Omega)$ and, from (B.190):

$$\begin{aligned}
&r_1' := e^{\frac{\Psi}{h}} \, [\Delta_{f,h}^{(1)}, \kappa](u_h^{(1)} - c_z(h) u_{z,wkb}^{(1)}) = O(h^{-N_0}) \text{ in } \Lambda^1 L^2(\Omega) \text{ and} \\
&\operatorname{supp} r_1' \subset \operatorname{supp} \nabla \kappa.
\end{aligned} \tag{B.194}$$

Additionally, one gets similarly on the boundary Γ_1:

$$\mathbf{t} w_h|_{\Gamma_1} = 0 \text{ and } \mathbf{t} d_{f,h}^* w_h|_{\Gamma_1} = (r_2 + r_2') e^{-\frac{\Psi}{h}} = (r_2 + r_2') e^{-\frac{f - f(z)}{h}},$$

where owing to (B.175) and (B.189):

$$r_2 := \mathbf{t} e^{\frac{\Psi}{h}} \kappa \, d_{f,h}^* (u_h^{(1)} - c_z(h) u_{z,wkb}^{(1)})|_{\Gamma_1} = -\mathbf{t} e^{\frac{\Psi}{h}} \, \kappa \, c_z(h) \, d_{f,h}^* u_{z,wkb}^{(1)}|_{\Gamma_1} = O(h^\infty) \tag{B.195}$$

in $L^2(\partial\Omega)$ and

$$\begin{aligned}
&r_2' := \mathbf{t} e^{\frac{\Psi}{h}} h \, \mathbf{i}_{\nabla \kappa} (u_h^{(1)} - c_z(h) u_{z,wkb}^{(1)})|_{\Gamma_1} = O(h^{-N_0}) \text{ in } L^2(\partial \dot{\Omega}) \text{ with} \\
&\operatorname{supp} r_2' \subset \Gamma_1 \cap \operatorname{supp} \nabla \kappa.
\end{aligned} \tag{B.196}$$

We are now in position to prove the following proposition.

Proposition B.65. *Let us assume that the hypotheses **[H1]**, **[H2]** and **[H3]** hold. One has the following estimate in the limit $h \to 0$:*

$$\left\| e^{\frac{\Psi}{h}} (u_h^{(1)} - c_z(h) u_{z,wkb}^{(1)}) \right\|_{H^1(V_{\Gamma_{St}})} = O(h^\infty). \tag{B.197}$$

where $c_z(h)$ is defined by (B.188) *and where, we recall, $\Psi(x) = d_a(x,z)$ and $V_{\Gamma_{St}}$ is defined by* (B.182)*.*

Proof. As for the proof of Proposition B.61, one first proves an estimate along the boundary Γ_1 before propagating it in $V_{\Gamma_{St}}$.

Step 1. Comparison in Γ_1.

Let us consider w_h defined by (B.191) and the cut-off function $\kappa = \eta$ defined in (B.185). Like in the first step of the proof of Proposition B.61, we are going to prove an estimate of the form (B.197) with Ψ replaced by f_+. More precisely, we want to show that

$$\left\| e^{\frac{f_+}{h}} w_h \right\|_{H^1(V_{\Gamma'_{St}})} = \left\| e^{\frac{f_+}{h}} (u_h^{(1)} - c_z(h) u_{z,wkb}^{(1)}) \right\|_{H^1(V_{\Gamma'_{St}})} = \mathcal{O}(h^\infty), \tag{B.198}$$

which implies in particular the following estimate along the boundary, since $f_+ = f - f(z)$ in Γ_1,

$$\left\| e^{\frac{f-f(z)}{h}} (u_h^{(1)} - c_z(h) u_{z,wkb}^{(1)}) \right\|_{H^{1/2}(\Gamma'_{St})} = \mathcal{O}(h^\infty). \tag{B.199}$$

In the following, we denote (see Figure B.15 for a schematic representation of the set V_η)

$$V_\eta = \operatorname{supp} \eta.$$

In the system of coordinates (x', x_d), $x \in V_\eta$ if and only if $x'(x) \in \operatorname{supp} \eta_1$ and $x_d(x) \in \operatorname{supp} \eta_d$. We recall that V_η is a compact set of $\dot{\Omega} \cup \Gamma_1$. As for the proof of Proposition B.61, we introduce the sets

$$\Omega_- = \{x \in V_\eta \text{ s.t. } f_+(x) \leq Ch\} \text{ and } \Omega_+ = V_\eta \setminus \Omega_-,$$

and define the Lipschitz function $\varphi : V_\eta \to \mathbb{R}$ by

$$\varphi = \begin{cases} f_+ - Ch \ln \dfrac{f_+}{h} \text{ if } f_+ > Ch, \\ f_+ - Ch \ln C \text{ if } f_+ \leq Ch, \end{cases}$$

for some constant $C > 1$ that will be fixed at the end of this step. Notice for further purposes that

$$\lim_{h \to 0} \|\varphi - f_+\|_{L^\infty(V_\eta)} = 0. \tag{B.200}$$

We recall that in the system of coordinates (x', x_d), φ is independent of x_d.

The reasoning below is based on [35], see also [30, p. 49–52] for a presentation in the case without boundary. According to (B.198), we want to get an error of the form $\mathcal{O}(h^N)$ with N arbitrary. We are not going to work with the above phase function φ as

we did in the proof of Proposition B.61, but with a phase function φ_N also depending on some arbitrary $N \in \mathbb{N}$. Let us define

$$\tilde{w}_h = e^{\frac{\varphi_N}{h}} w_h = e^{\frac{\varphi_N}{h}} \eta(u_h^{(1)} - c_z(h) u_{z,wkb}^{(1)}).$$

Combining the integration by parts formula (B.148) (with $u = w_h$ and $\varphi = \varphi_N$) with the Green formula (B.115) (with $u = w_h$ and $v = e^{2\frac{\varphi_N}{h}} w_h$) leads to the estimate

$$\begin{aligned}\left\| e^{\frac{\varphi_N}{h}} \Delta_{f,h}^{(1)} w_h \right\|_{L^2(V_\eta)} \|\tilde{w}_h\|_{L^2(V_\eta)} + h \left\| e^{\frac{\varphi_N}{h}} \mathbf{t} d_{f,h}^* w_h \right\|_{L^2(\Gamma_1)} \|\tilde{w}_h\|_{L^2(\Gamma_1)} \\ \geq \|hd\tilde{w}_h\|_{L^2(V_\eta)}^2 + \|hd^*\tilde{w}_h\|_{L^2(V_\eta)}^2 - h \int_{\Gamma_1} \langle \tilde{w}_h, \tilde{w}_h \rangle_{T_\sigma^*\Omega} \partial_n f \, d\sigma \\ + \langle (|\nabla f|^2 - |\nabla \varphi_N|^2 + h\mathcal{L}_{\nabla f} + h\mathcal{L}_{\nabla f}^*) \tilde{w}_h, \tilde{w}_h \rangle_{L^2(V_\eta)}. \qquad \text{(B.201)}\end{aligned}$$

Let us explain formally how the function φ_N is chosen. Roughly speaking, using similar arguments as in the proof of Proposition B.61, it is natural to choose $\varphi_N = \varphi + Nh \ln \frac{1}{h}$ and to try to prove that the left-hand side of (B.201) is bounded from above by $\mathcal{O}(h^{-N_1}) \|\tilde{w}_h\|_{H^1(V_\eta)}$ for some $N_1 \in \mathbb{N}$ independent of N. This would indeed lead to an estimate of the form $\|\tilde{w}_h\|_{H^1(V_\eta)} = \mathcal{O}(h^{-N_1})$ (for some maybe larger N_1) and finally to the desired estimate on w_h since $\|\tilde{w}_h\|_{H^1(V_\eta)} \simeq h^{-N} \|e^{\frac{f_+}{h}} w_h\|_{H^1(V_\eta)}$. To get this upper bound, a trace theorem and (B.192)–(B.196) yield the following estimate from (B.201):

$$\|e^{\frac{\varphi_N - \Psi}{h}}\|_{L^\infty(V_\eta)} O(h^\infty) + \|e^{\frac{\varphi_N - \Psi}{h}}\|_{L^\infty(\mathrm{supp}(\nabla\eta))} O(h^{-N_1}) \geq \|\tilde{w}_h\|_{H^1(V_\eta)} \simeq h^{-N} \|e^{\frac{f_+}{h}} w_h\|_{H^1(V_\eta)}$$

for some $N_1 \in \mathbb{N}$ independent of N. It can be checked that $\|e^{\frac{\varphi_N - \Psi}{h}}\|_{L^\infty(V_\eta)} = \|e^{\frac{\varphi_N - \Psi}{h}}\|_{L^\infty(\mathrm{supp}(\nabla\eta))} = O(h^{-N})$ so that the first term is well controlled, but the second one is of order $O(h^{-N-N_1})$. These relations suggest a choice of φ_N satisfying $\varphi_N \leq f_+ \leq \Psi$ on $\mathrm{supp}\, \nabla\eta$ so that $\|e^{\frac{\varphi_N - \Psi}{h}}\|_{L^\infty(\mathrm{supp}(\nabla\eta))} = O(1)$. This would yield the desired estimate $\|e^{\frac{f_+}{h}} w_h\|_{H^1(V_\eta)} = O(h^{N-N_1})$.

Let us now enter the rigorous proof. The above considerations (see also [30, p. 49–52]) lead to define, for any $N \in \mathbb{N}$,

$$\varphi_N = \min\left\{ \varphi + Nh \ln \frac{1}{h}, \psi \right\}, \qquad \text{(B.202)}$$

where the Lipschitz function $\psi : V_\eta \to \mathbb{R}$ is defined by the following relation, for some $\varepsilon \in (0,1)$ that will be specified below:

$$\psi(x', x_d) = \psi(x', 0) = \min\left\{ \varphi(y', 0) + (1-\varepsilon) d_a^{\partial\Omega}(x', y'),\ y' \in \mathrm{supp}\, \nabla\eta_1 \right\}. \qquad \text{(B.203)}$$

Here, $d_a^{\partial\Omega}(x', y')$ denotes the Agmon distance associated with $f|_{\partial\Omega}$ between x' and y' along the boundary (see Definition B.7), i.e. the distance induced by the metric $|\nabla(f|_{\partial\Omega})|^2 \, ds^2$, where ds^2 denotes the restriction of the Euclidean metric to the boundary $\partial\Omega$.

<u>Step 1-a:</u> Preliminary estimates on φ_N.

Let us first show that there exists $\varepsilon \in (0,1)$ such that for any $h \in (0, h_0(N,\varepsilon))$ with $h_0 = h_0(N,\varepsilon)$ small enough,

$$\varphi_N = \varphi + Nh \ln \frac{1}{h} < \psi \text{ in } \; V_\eta \cap \left\{ x' \in \overline{\Gamma'_{St}} \right\}. \tag{B.204}$$

The proof of (B.204) is as follows. From (B.79) applied to $d_a^{\partial\Omega}$,

$$\forall (x',y') \in \overline{\Gamma'_{St}} \times \operatorname{supp} \nabla \eta_1 \ , \quad f_+(x',0) < f_+(y',0) + d_a^{\partial\Omega}(x',y'). \tag{B.205}$$

The inequality above is strict since if $f_+(x',0) = f_+(y',0) + d_a^{\partial\Omega}(x',y')$ for some $(x',y') \in \overline{\Gamma'_{St}} \times \operatorname{supp} \nabla\eta_1$, then there exists a generalized integral curve (in the sense of Definition B.8) of $-\nabla(f|_{\partial\Omega}) = -\nabla f_+$ joining $x' \in \overline{\Gamma'_{St}}$ to $y \in \operatorname{supp} \nabla\eta_1$ (this is a consequence of Corollary B.48 applied to the Agmon distance $d_a^{\partial\Omega}$ on $\partial\Omega$ rather than the Agmon distance d_a in $\overline{\Omega}$). But since Γ'_{St} is strongly stable, any integral curve of $-\nabla f_+$ remains in $\overline{\Gamma'_{St}}$, and thus cannot reach y' which is not in $\overline{\Gamma'_{St}}$ (see (B.185)).

From the strict inequality (B.205), there exists $\varepsilon_0 > 0$ such that for all $\varepsilon \in [0, \varepsilon_0)$,

$$\forall (x',y') \in \overline{\Gamma'_{St}} \times \operatorname{supp} \nabla \eta_1 \ , \quad f_+(x',0) \le f_+(y',0) + (1-\varepsilon) d_a^{\partial\Omega}(x',y'),$$

and thus, considering the limit $h \to 0$ (see (B.200)) and the infimum over $y' \in \operatorname{supp} \nabla\eta_1$ of the right-hand side, there exists $\varepsilon > 0$ used to define ψ (see (B.203)) and such that, for sufficiently small h,

$$\forall x' \in \overline{\Gamma'_{St}} \ , \quad f_+(x',0) < \psi(x',0).$$

Moreover, since $\lim_{h\to 0} \|\varphi + Nh \ln \frac{1}{h} - f_+\|_{L^\infty(V_\eta)} = 0$ (thanks to (B.200)), one obtains for h small enough, $\forall x' \in \overline{\Gamma'_{St}}$, $\varphi(x',0) + Nh \ln \frac{1}{h} < \psi(x',0)$, and by definition of φ_N, $\varphi_N(x',0) = \varphi(x',0) + Nh \ln \frac{1}{h}$ which leads to (B.204) for $x = (x',0)$, with $x' \in \overline{\Gamma'_{St}}$. The fact that φ_N and ψ does not depend on x_d in the system of coordinates (x', x_d) concludes the proof of (B.204).

Let us now prove that

$$\exists M < \frac{1}{1-\varepsilon}, \forall x \in V_\eta, |\nabla \psi(x)| \le M(1-\varepsilon) \left|\nabla f_+(x)\right|. \tag{B.206}$$

The triangular inequality applied to $d_a^{\partial\Omega}$ leads to the relation (since $\psi(x', x_d)$ does not depend on x_d)

$$\forall x, y \in V_\eta, \ |\psi(x', x_d) - \psi(y', y_d)| \le (1-\varepsilon) d_a^{\partial\Omega}(x',y'). \tag{B.207}$$

where we denote (x', x_d) (resp. (y', y_d)) the coordinates of x (resp. y) in the system of coordinates (B.129). Let us first show that (B.207) implies that

$$\text{for a.e. } x' \in V_\eta \cap \partial\Omega, \ \left|\nabla(\psi|_{\partial\Omega})(x')\right| \le (1-\varepsilon) \left|\nabla(f|_{\partial\Omega})(x')\right| = (1-\varepsilon) \left|\nabla(f_+|_{\partial\Omega})(x')\right|. \tag{B.208}$$

Indeed, let us consider a local parametrization in $\mathbb{R}^{d-1}$ of a neighborhood in $\partial\Omega$ of a point $x' \in \partial\Omega$. In this local chart, let us consider $y_\alpha = x' + \alpha \frac{\nabla(\psi|_{\partial\Omega})}{|\nabla(\psi|_{\partial\Omega})|}(x')$. One has, in the limit $\alpha \to 0$,

$$\psi(y'_\alpha, 0) - \psi(x',0) = \alpha |\nabla(\psi|_{\partial\Omega})(x')| + o(\alpha)$$

and likewise using the inequality (B.78) applied to $d_a^{\partial\Omega}$ (see also [19, p. 53])

$$d_a^{\partial\Omega}(x,' y'_\alpha) - d_a^{\partial\Omega}(x',x') \leq \alpha|\nabla(f|_{\partial\Omega})(x')| + o(\alpha).$$

By considering the limit $\alpha \to 0$, one thus deduces (B.208) from (B.207).

Now, one can check that, uniformly in $x' \in V_\eta \cap \partial\Omega$,

$$\lim_{x_d\to 0} |\nabla\psi(x',x_d)| = |\nabla(\psi|_{\partial\Omega})(x')| \text{ and } \lim_{x_d\to 0} |\nabla f_+(x',x_d)| = |\nabla(f_+|_{\partial\Omega})(x')|. \quad \text{(B.209)}$$

Indeed, using the fact that ψ does not depend on x_d, one first has almost everywhere (see (B.130)) $|\nabla\psi(x',x_d)| = |\nabla(\psi|_{\Sigma_{x_d}})(x')|$ where $\forall a > 0$, $\Sigma_a = \{x \in V_\eta,\, x_d(x) = a\}$ is endowed with the Riemannian structure induced by the Riemannian structure in Ω. Now, let us consider the smooth diffeomorphism $\Gamma_{x_d} : \Sigma_{x_d} \to \partial\Omega$ such that for all $x = (x',x_d) \in \Sigma_{x_d}$, $\Gamma_{x_d}(x) = (x',0) \in \partial\Omega$. The result (B.209) on ψ is then a consequence of the fact that $\psi|_{\partial\Omega} \circ \Gamma_{x_d} = \psi|_{\Sigma_{x_d}}$ and $\lim_{x_d\to 0} \|\Gamma_{x_d} - \mathrm{Id}\|_{W^{1,\infty}(\Sigma_{x_d})} = 0$ so that the Jacobian associated to the change of metric from Σ_{x_d} to $\partial\Omega$ converges to Id, uniformly on Σ_{x_d}. The same reasoning show that (B.209) also holds for f_+ since f_+ does not depend on x_d.

By combining (B.208) and (B.209), one obtains (B.206) for some $M > 1$. Moreover, M can be chosen as close to 1 as needed, up to modifying η (and thus $V_{\Gamma_{St}} \subset V_{\Gamma'_{St}} \subset V_\eta$) such that for all $x \in V_\eta$, $\|\Gamma_{x_d} - \mathrm{Id}\|_{W^{1,\infty}(\Sigma_{x_d})}$ is as close to 0 as needed.

Let us finally mention the following inequalities, valid for $h \in (0,h_0)$ with $h_0 = h_0(N,\varepsilon) > 0$ small enough:

$$\varphi_N \leq f_+ + Nh\ln\frac{1}{h} \leq \Psi + Nh\ln\frac{1}{h} \quad \text{in } V_\eta \quad \text{(B.210)}$$

$$\varphi_N = \psi \leq \varphi \leq f_+ \leq \Psi \quad \text{in } V_\eta \cap \{x' \in \operatorname{supp}\nabla\eta_1\} \quad \text{(B.211)}$$

and since $\Psi = f_+ + f_- > f_+$ on $\{x_d \in \operatorname{supp}\eta'_d\}$, one has

$$\varphi_N \leq f_+ + Nh\ln\frac{1}{h} \leq \Psi \quad \text{in } V_\eta \cap \{x_d \in \operatorname{supp}\eta'_d\}. \quad \text{(B.212)}$$

Step 1-b: Proof of (B.198).

We are now ready to prove (B.198). Controlling the left-hand side of (B.201) using the relations (B.192)–(B.196) gives

$$\begin{aligned}\left\|(r_1+r'_1)e^{\frac{\varphi_N-\Psi}{h}}\right\|_{L^2(V_\eta)} \|\tilde{w}_h\|_{L^2(V_\eta)} + \left\|(r_2+r'_2)e^{\frac{\varphi_N-\Psi}{h}}\right\|_{L^2(\Gamma_1)} \|\tilde{w}_h\|_{L^2(\Gamma_1)} \\ \geq \|hd\tilde{w}_h\|^2_{L^2(V_\eta)} + \|hd^*\tilde{w}_h\|^2_{L^2(V_\eta)} - h\int_{\Gamma_1} \langle\tilde{w}_h,\tilde{w}_h\rangle_{T^*_\sigma\Omega}\partial_n f\, d\sigma \\ + \langle(|\nabla f|^2 - |\nabla\varphi_N|^2 + h\mathcal{L}_{\nabla f} + h\mathcal{L}^*_{\nabla f})\tilde{w}_h,\tilde{w}_h\rangle_{L^2(V_\eta)}\,,\end{aligned}$$

where, since $\varphi_N - \Psi \leq Nh\ln\frac{1}{h}$ (by (B.210)) and $r_i = \mathcal{O}(h^\infty)$ for $i \in \{1,2\}$ (by (B.193) and (B.195)),

$$\left\|r_1 e^{\frac{\varphi_N-\Psi}{h}}\right\|_{L^2(V_\eta)} + \left\|r_2 e^{\frac{\varphi_N-\Psi}{h}}\right\|_{L^2(\Gamma_1)} = \mathcal{O}(h^\infty),$$

and, since $\varphi_N \leq \Psi$ on $\operatorname{supp}\nabla\eta$ (by (B.211)–(B.212)) and $\operatorname{supp} r'_i \subset \operatorname{supp}\nabla\eta$ for $i \in \{1,2\}$ (by (B.194) and (B.196)),

$$\left\|r'_1 e^{\frac{\varphi_N-\Psi}{h}}\right\|_{L^2(V_\eta)} + \left\|r'_2 e^{\frac{\varphi_N-\Psi}{h}}\right\|_{L^2(\Gamma_1)} = \mathcal{O}(h^{-N_0}).$$

This leads to the existence of $C_1 = C_1(N) > 0$ such that for h small enough:

$$C_1 h^{-N_0} \|\tilde{w}_h\|_{H^1(V_\eta)} \geq \|hd\tilde{w}_h\|^2_{L^2(V_\eta)} + \|hd^*\tilde{w}_h\|^2_{L^2(V_\eta)} - h\int_{\Gamma_1} \langle \tilde{w}_h, \tilde{w}_h\rangle_{T^*_\sigma\Omega} \partial_n f \, d\sigma$$
$$+ \langle (|\nabla f|^2 - |\nabla \varphi_N|^2 + h\mathcal{L}_{\nabla f} + h\mathcal{L}^*_{\nabla f})\tilde{w}_h, \tilde{w}_h\rangle_{L^2(V_\eta)}.$$

Since $\varphi_N \leq \varphi + Nh\ln\frac{1}{h}$, $\varphi \leq Ch$ on Ω_- and $\|w_h\|_{H^1(V_\eta)} = \mathcal{O}(h^\infty)$ (see (C.115))

$$\|\tilde{w}_h\|_{L^2(\Omega_-)} \leq e^C h^{-N} \|w_h\|_{L^2(\Omega_-)} \leq C_2(C, N). \tag{B.213}$$

Thus, since $\mathcal{L}_{\nabla f} + \mathcal{L}^*_{\nabla f}$ is a 0th order differential operator, we get the existence of $C_3 > 0$ independent of (C, N) and of $C_4 = C_4(C, N)$ such that:

$$C_4(h^{-N_0} \|\tilde{w}_h\|_{H^1(V_\eta)} + 1) \geq \|hd\tilde{w}_h\|^2_{L^2(V_\eta)} + \|hd^*\tilde{w}_h\|^2_{L^2(V_\eta)} - h\int_{\Gamma_1} \langle \tilde{w}_h, \tilde{w}_h\rangle_{T^*_\sigma\Omega} \partial_n f \, d\sigma$$
$$+ \langle |\nabla f_-|^2 \tilde{w}_h, \tilde{w}_h\rangle_{L^2(V_\eta)} + \langle (|\nabla f_+|^2 - |\nabla\varphi_N|^2 - C_3 h)\tilde{w}_h, \tilde{w}_h\rangle_{L^2(\Omega_+)}.$$

Moreover, by definition of φ_N, a.e. in Ω_+, $\nabla\varphi_N = \nabla\psi 1_{\{\varphi_N = \psi\}} + \nabla f_+(1 - \frac{Ch}{f_+})1_{\{\varphi_N < \psi\}}$. Now,

- On $\{\varphi_N = \psi\}$, since by (B.204) $\{\varphi_N = \psi\}$ avoids a neighborhood of $\{(z, x_d), x_d \in \operatorname{supp}\eta_d\} = \{x \in V_\eta, |\nabla f_+(x)| = 0\}$ (see (B.133)), we get
$$|\nabla f_+|^2 - |\nabla\varphi_N|^2 \geq \left(1 - M^2(1-\varepsilon)^2\right)|\nabla f_+|^2 \geq c_\varepsilon > 0,$$
where (B.206) have been used;
- On $\{\varphi_N < \psi\} \cap \Omega_+$, we get like in the proof of Proposition B.61 (see (B.150) and (B.152)),
$$|\nabla f_+|^2 - |\nabla\varphi_N|^2 \geq KCh.$$

Choosing $C > \max(1, \frac{C_3}{K})$, we obtain that for h small enough:

$$C_4(h^{-N_0} \|\tilde{w}_h\|_{H^1(V_\eta)} + 1) \geq \|hd\tilde{w}_h\|^2_{L^2(V_\eta)} + \|hd^*\tilde{w}_h\|^2_{L^2(V_\eta)} - h\int_{\Gamma_1} \langle \tilde{w}_h, \tilde{w}_h\rangle_{T^*_\sigma\Omega} \partial_n f \, d\sigma$$
$$+ \langle |\nabla f_-|^2 \tilde{w}_h, \tilde{w}_h\rangle_{L^2(V_\eta)} + (KC - C_3)h\left(\|\tilde{w}_h\|^2_{L^2(V_\eta)} - \|\tilde{w}_h\|^2_{L^2(\Omega_-)}\right) \tag{B.214}$$

We can now control from below the r.h.s. of the above estimate exactly as we did at the end of the first step of Proposition B.61: defining $C_5(C) := \frac{KC - C_3}{2\||\nabla f_-|^2\|_{L^\infty(V_\eta)}}$ (see (B.131)), one gets the inequality

$$(KC - C_3)h\|\tilde{w}_h\|^2_{L^2(V_\eta)} + \langle |\nabla f_-|^2\tilde{w}_h, \tilde{w}_h\rangle_{L^2(V_\eta)} \;\geq\; (1 + 2C_5 h)\langle |\nabla f_-|^2 \tilde{w}_h, \tilde{w}_h\rangle_{L^2(V_\eta)} \tag{B.215}$$

and from Lemma B.56 applied with $u = \tilde{w}_h$, $f = -\tilde{\eta} f_-$ where $\tilde{\eta} \in C^\infty(\overline{\Omega}, [0,1])$, $\tilde{\eta} = 1$ on $\operatorname{supp}\eta$, $\operatorname{supp}\tilde{\eta} \subset (\operatorname{supp}\eta + B(0,\alpha)) \cap \overline{\Omega}$ for $\alpha > 0$ such that f_- is smooth on $\operatorname{supp}\tilde{\eta}$ and $\frac{h}{1+C_5 h}$ instead of h, one gets the following lower bound:

$$\begin{aligned} -h\int_{\Gamma_1} \langle \tilde{w}_h, \tilde{w}_h\rangle \partial_n f \, d\sigma &= h\int_{\Gamma_1} \langle \tilde{w}_h, \tilde{w}_h\rangle \partial_n f_- \, d\sigma \\ &\geq -(1 + C_5 h)\||\nabla f_-|\tilde{w}_h\|^2_{L^2(V_\eta)} \\ &\quad - \frac{h^2}{1 + C_5 h}\left(\|d\tilde{w}_h\|^2_{L^2(V_\eta)} + \|d^*\tilde{w}_h\|^2_{L^2(V_\eta)}\right) - C_6 h\|\tilde{w}_h\|^2_{L^2(V_\eta)}, \end{aligned} \tag{B.216}$$

where C_6 is some positive constant independent of C (it only depends on f_-). Injecting the estimates (B.215) and (B.216) in (B.214) then leads to:

$$C_4(h^{-N_0}\|\tilde{w}_h\|_{H^1(V_\eta)}+1) \geq \frac{C_5h^3}{1+C_5h}\left(\|d\tilde{w}_h\|^2_{L^2(V_\eta)}+\|d^*\tilde{w}_h\|^2_{L^2(V_\eta)}\right)$$
$$+C_5h\,\||\nabla f_-|\tilde{w}_h\|^2_{L^2(V_\eta)}-(KC-C_3)h\,\|\tilde{w}_h\|^2_{L^2(\Omega_-)}-C_6h\|\tilde{w}_h\|^2_{L^2(V_\eta)}.$$

Then, since $|\nabla f_-|\geq c>0$ on $\overline{V_\eta}$ (see (B.131)), $\lim_{C\to\infty}C_5(C)=+\infty$. Therefore, since C_6 is independent of C, one can choose C such that $c^2C_5-C_6>0$, which implies, remembering also $\|\tilde{w}_h\|_{L^2(\Omega_-)}\leq C_2(C,N)$ (see (B.213)), the existence of a constant $C_7>0$ and a constant $h_0>0$ such that, for every $h\in(0,h_0)$,

$$\|\tilde{w}_h\|^2_{L^2(V_\eta)}+\|d\tilde{w}_h\|^2_{L^2(V_\eta)}+\|d^*\tilde{w}_h\|^2_{L^2(V_\eta)}\leq\frac{C_7}{h^3}(h^{-N_0}\|\tilde{w}_h\|_{H^1(V_\eta)}+1).$$

According to Gaffney's inequality (B.116), this finally leads to the existence of a positive constant C_8 such that

$$\|\tilde{w}_h\|_{H^1(V_\eta)}\ \leq\ C_8h^{-N_0-3}.$$

Moreover, according to (B.204), we have $\varphi_N=\varphi+Nh\ln\frac{1}{h}$ in $V_\eta\cap\left\{x'\in\overline{\Gamma'_{St}}\right\}$ and then $\varphi_N-Nh\ln\frac{1}{h}-f_+\geq -C_9h\ln\frac{1}{h}$ (with a constant C_9 independent of N) in $V_{\Gamma'_{St}}\subset V_\eta\cap\left\{x'\in\overline{\Gamma'_{St}}\right\}$. Therefore, there exists N_1 independent of N such that for h small enough,

$$\left\|e^{\frac{f_+}{h}}w_h\right\|_{H^1(V_{\Gamma'_{St}})}\leq C_Nh^{N-N_1},$$

from which (B.198) and (B.199) follow since N is arbitrary.

Step 2: Comparison in $V_{\Gamma_{St}}$.

We work now with the cut-off function χ defined in (B.184). Recall that $\eta\chi=\chi$. Similarly as in the previous step, let us define the sets

$$\Omega_-=\left\{x\in V_{\Gamma'_{St}}\text{ s.t. }\Psi(x)\leq Ch\right\}\text{ and }\Omega_+=V_{\Gamma'_{St}}\setminus\Omega_-,$$

and the function

$$\varphi_N=\min\left\{\varphi+Nh\ln\frac{1}{h},\psi\right\},$$

where φ and ψ are respectively defined by

$$\varphi=\begin{cases}\Psi-Ch\ln\dfrac{\Psi}{h}\text{ if }\Psi>Ch\\ \Psi-Ch\ln C\text{ if }\Psi\leq Ch,\end{cases}$$

and

$$\psi(x)=\min\left\{\varphi(y)+(1-\varepsilon)d_a\left(x,y\right),\ y\in\operatorname{supp}\nabla\chi\right\}.$$

The constant $C>1$ will be chosen at the end of the proof. Following the proof of (B.204), there exists $\varepsilon\in(0,1)$ such that for any $h\in(0,h_0)$ with $h_0=h_0(N,\varepsilon)$ small enough,

$$\varphi_N=\varphi+Nh\ln\frac{1}{h}<\psi\text{ in }\ V_{\Gamma_{St}}. \tag{B.217}$$

Indeed, using the fact that $\Psi(x) = d_a(x,z)$ and a triangular inequality,

$$\forall\,(x,y) \in \overline{V_{\Gamma_{St}}} \times \operatorname{supp}\nabla\chi, \quad \Psi(x) < \Psi(y) + d_a\,(x,y)\,.$$

The inequality is strict since if $\Psi(x) = \Psi(y) + d_a\,(x,y)$ for some $(x,y) \in \overline{V_{\Gamma_{St}}} \times \operatorname{supp}\nabla\chi$, then $\Phi(x) - \Phi(y) = d_a(x,y)$ and from Corollary B.53, up to modifying η such that $V_\eta \subset V_\alpha$ (see Corollary B.53 for the definition of V_α) there exists a generalized integral curve (in the sense of Definition B.8) of $\begin{cases} -\nabla\Phi \text{ on } V_\alpha \cap \Omega \\ -\nabla_T\Phi \text{ on } \partial\Omega \end{cases}$ joining $x \in \overline{V_{\Gamma_{St}}}$ to $y \notin \overline{V_{\Gamma_{St}}}$. This contradicts the fact that $\overline{V_{\Gamma_{St}}}$ is stable for (B.183). The end of the proof of (B.217) then follows exactly the same lines as the proof of (B.204).

Moreover, owing to the properties of d_a, one has analogously to (B.208) the following estimate valid a.e. in $V_{\Gamma'_{St}}$:

$$|\nabla\psi| \leq (1-\varepsilon)\,|\nabla f| = (1-\varepsilon)\,|\nabla\Psi|\,. \tag{B.218}$$

Let us finally mention the following inequalities, valid for $h \in (0,h_0)$ with $h_0 = h_0(N,\varepsilon) > 0$ small enough:

$$\varphi_N \leq \Psi + Nh\ln\frac{1}{h} \quad \text{in } V_{\Gamma'_{St}} \tag{B.219}$$

$$\text{and } \varphi_N = \psi \leq \varphi \leq \Psi \quad \text{on } \operatorname{supp}\nabla\chi. \tag{B.220}$$

We are now in position to prove (B.197). Let us define

$$\tilde{w_h} = e^{\frac{\varphi_N}{h}} w_h = e^{\frac{\varphi_N}{h}} \chi(u_h^{(1)} - c_z(h) u_{z,wkb}^{(1)}).$$

Using the relations (B.192)–(B.196) and the integration by parts formulae (B.148) and (B.115), there exists $C_1 > 0$ (only depending on f) such that

$$\begin{aligned}
&\left\|(r_1 + r_1')e^{\frac{\varphi_N - \Psi}{h}}\right\|_{L^2(V_{\Gamma'_{St}})} \|\tilde{w_h}\|_{L^2(V_{\Gamma'_{St}})} + \left\|(r_2 + r_2')e^{\frac{\varphi_N - \Psi}{h}}\right\|_{L^2(\Gamma_1)} \|\tilde{w_h}\|_{L^2(\Gamma_1)} \\
&+ C_1 h \int_{\Gamma_1} \langle \tilde{w_h}, \tilde{w_h}\rangle_{T^*_\sigma\Omega}\, d\sigma \geq \|hd\tilde{w_h}\|^2_{L^2(V_{\Gamma'_{St}})} + \|hd^*\tilde{w_h}\|^2_{L^2(V_{\Gamma'_{St}})} \\
&\qquad + \langle (|\nabla f|^2 - |\nabla\varphi_N|^2 - C_1 h)\tilde{w_h}, \tilde{w_h}\rangle_{L^2(\Omega_+)} - C_1 h\,\|\tilde{w_h}\|^2_{L^2(\Omega_-)}\,,
\end{aligned} \tag{B.221}$$

where we have used the fact that almost everywhere on Ω_-, $|\nabla\varphi_N|$ is either equal to $|\nabla\varphi| = |\nabla\Psi| = |\nabla f|$ or to $|\nabla\psi| \leq (1-\varepsilon)|\nabla f|$. Moreover, since $\varphi_N - \Psi \leq Nh\ln\frac{1}{h}$ (see (B.219)), one has from (B.193) and (B.195)

$$\left\|r_1 e^{\frac{\varphi_N - \Psi}{h}}\right\|_{L^2(V_{\Gamma'_{St}})} + \left\|r_2 e^{\frac{\varphi_N - \Psi}{h}}\right\|_{L^2(\Gamma_1)} = \mathcal{O}(h^\infty)$$

and, since $\varphi_N \leq \Psi$ on $\operatorname{supp}\nabla\chi$ (see (B.220)), one gets from (B.194) and (B.196)

$$\left\|r_1' e^{\frac{\varphi_N - \Psi}{h}}\right\|_{L^2(V_{\Gamma'_{St}})} + \left\|r_2' e^{\frac{\varphi_N - \Psi}{h}}\right\|_{L^2(\Gamma_1)} = \mathcal{O}(h^{-N_0}).$$

Additionally, since $\Psi = f - f(z)$ on Γ_1 and $\varphi_N - \Psi \leq Nh\ln\frac{1}{h}$ (see (B.219)), we deduce from the relation (B.199) obtained in the first step the following estimate:

$$\|\tilde{w_h}\|_{L^2(\Gamma_1)} = \left\|e^{\frac{\varphi_N}{h}}\chi(u_h^{(1)} - c_z(h)u_{z,wkb}^{(1)})\right\|_{L^2(\Gamma'_{St})} = \mathcal{O}(h^\infty).$$

Consequently, using in addition the relation

$$\|\tilde{w}_h\|_{L^2(\Omega_-)} \leq e^C h^{-N} \|w_h\|_{L^2(\Omega_-)} \leq C_2(C,N),$$

(since $\varphi_N \leq \varphi + Nh\ln\frac{1}{h}$, $\varphi \leq Ch$ on Ω_- and $\|w_h\|_{L^2(V_{\Gamma'_{St}})} = O(h^\infty)$ from (C.115)), we deduce from (B.221) the existence of some positive constant $C_3 = C_3(C, C_1, N)$ such that

$$C_3\left(h^{-N_0}\|\tilde{w}_h\|_{L^2(V_{\Gamma'_{St}})} + 1\right) \geq \|hd\tilde{w}_h\|^2_{L^2(V_{\Gamma'_{St}})} + \|hd^*\tilde{w}_h\|^2_{L^2(V_{\Gamma'_{St}})} + \langle(|\nabla f|^2 - |\nabla\varphi_N|^2 - C_1h)\tilde{w}_h, \tilde{w}_h\rangle_{L^2(\Omega_+)}. \quad \text{(B.222)}$$

Lastly, one has a.e. in Ω_+, $\nabla\varphi_N = \nabla\psi 1_{\{\varphi_N=\psi\}} + \nabla\Psi(1-\frac{Ch}{\Psi})1_{\{\varphi_N<\psi\}}$, and thus

- on $\{\varphi_N = \psi\}$, from (B.218),

$$|\nabla f|^2 - |\nabla\varphi_N|^2 \geq (2\varepsilon - \varepsilon^2)|\nabla f|^2 \geq c_\varepsilon > 0,$$

- on $\{\varphi_N < \psi\} \cap \Omega_+$, there exists $C_4 > 0$ independent of C such that,

$$|\nabla f|^2 - |\nabla\varphi_N|^2 \geq Ch\frac{|\nabla f|^2}{\Psi} \geq C_4Ch.$$

Taking $C > \frac{C_1}{C_4}$ and adding $(CC_4 - C_1)h\|\tilde{w}_h\|^2_{L^2(\Omega_-)}$ to (B.222) then leads to

$$C_5\left(h^{-N_0}\|\tilde{w}_h\|_{L^2(V_{\Gamma'_{St}})} + 1\right) \geq \|hd\tilde{w}_h\|^2_{L^2(V_{\Gamma'_{St}})} + \|hd^*\tilde{w}_h\|^2_{L^2(V_{\Gamma'_{St}})} + (CC_4 - C_1)h\|\tilde{w}_h\|^2_{L^2(V_{\Gamma'_{St}})},$$

for a constant C_5 depending on C and N. Using Gaffney's inequality (B.116), we consequently get the existence of $C_6 > 0$ such that

$$\|\tilde{w}_h\|_{H^1(V_{\Gamma'_{St}})} \leq C_6 h^{-N_0-3/2}.$$

Now, since $\varphi_N - Nh\ln\frac{1}{h} - \Psi \geq -C_7h\ln\frac{1}{h}$ in $V_{\Gamma_{St}}$ (with a constant C_7 independent of N, from the definition of φ and the fact that $\varphi_N - Nh\ln\frac{1}{h} = \varphi$ in $V_{\Gamma_{St}}$, see (B.217)), we also get the existence of N_2 independent of N such that for h small enough,

$$\left\|e^{\frac{\Psi}{h}}w_h\right\|_{H^1(V_{\Gamma_{St}})} \leq C_N h^{N-N_2},$$

for some constant $C_N > 0$, which concludes the proof of Proposition B.65. ∎

B.4.5 Proof of Theorem B.1

The aim of this section is to conclude the proof of Theorem B.1 by checking that the function $\tilde{u}$ and the family of 1-forms $(\tilde{\phi}_i)_{i=1,\dots,n}$ introduced in Section B.4.2 satisfy the estimates appearing in Proposition B.17 rewritten in the flat space (see Section B.2.2.2). In all this section, we assume in addition to the the hypotheses **[H1]**, **[H2]** and **[H3]**, that (B.20) and (B.21) hold.

From Sections B.4.2.1 and B.4.2.2, it only remains to prove (B.57), (B.58), (B.59) and (B.60). Let us start with a lemma about the normalisation term appearing in (B.146).

Lemma B.66. *Let us assume that the hypotheses **[H1]**, **[H2]** and **[H3]** hold. Let us define* $\Theta_i := \sqrt{\int_\Omega \left|\chi_i(x) u_{h,i}^{(1)}(x)\right|^2 dx}$. *There exist* $c > 0$ *and* $h_0 > 0$ *such that for all* $h \in (0, h_0)$,

$$\Theta_i^2 = 1 + O\left(e^{-\frac{c}{h}}\right).$$

Proof. On the one hand, one has the upper bound

$$\|\chi_i u_{h,i}^{(1)}\|_{L^2(\Omega)} = \|\chi_i u_{h,i}^{(1)}\|_{L^2(\dot\Omega_i)} \leq \|u_{h,i}^{(1)}\|_{L^2(\dot\Omega_i)} = 1.$$

On the other hand, the triangular inequality yields the lower bound

$$\|\chi_i u_{h,i}^{(1)}\|_{L^2(\dot\Omega_i)} \geq \|u_{h,i}^{(1)}\|_{L^2(\dot\Omega_i)} - \|(1-\chi_i) u_{h,i}^{(1)}\|_{L^2(\dot\Omega_i)} = 1 - \|(1-\chi_i) u_{h,i}^{(1)}\|_{L^2(\dot\Omega_i)}.$$

Thanks to Proposition B.61, there exist $N \in \mathbb{N}$ and $c > 0$ independent of h such that

$$\begin{aligned}
\|(1-\chi_i) u_{h,i}^{(1)}\|^2_{L^2(\dot\Omega_i)} &= \int_{\dot\Omega_i} \left|(1-\chi_i(x))\, u_{h,i}^{(1)}(x) e^{\frac{1}{h} d_a(x,z_i)} e^{-\frac{1}{h} d_a(x,z_i)}\right|^2 dx \\
&\leq \int_{\dot\Omega_i \setminus \mathcal{V}_i} \left|u_{h,i}^{(1)}(x) e^{\frac{1}{h} d_a(x,z_i)} e^{-\frac{1}{h} d_a(x,z_i)}\right|^2 dx \\
&\leq C\, h^{-N} e^{-\inf_{\dot\Omega_i \setminus \mathcal{V}_i} \frac{2}{h} d_a(.,z_i)} \leq C\, e^{-\frac{c}{h}},
\end{aligned}$$

where, we recall $\mathcal{V}_i = \{x \in \Omega,\, \chi_i = 1\}$. This concludes the proof of Lemma B.66. ∎

We are now in position to check the estimates stated in Section B.2.2.2.

<u>Step 1.</u> Study of the term $\left\|\left(1 - \pi_{[0,h^{\frac{3}{2}})}\left(\Delta_{f,h}^{D,(1)}(\Omega)\right)\right)\tilde\phi_i\right\|_{H^1(\Omega)}$.

We recall that from (B.116), $\tilde\phi_i$ belongs to $\Lambda^1 H_T^1(\Omega)$ and then we get from Lemma C.8 that there exist $c > 0$ and $h_0 > 0$ such that for all $h \in (0, h_0)$,

$$\begin{aligned}
\left\|\left(1 - \pi_{[0,h^{\frac{3}{2}})}\left(\Delta_{f,h}^{D,(1)}(\Omega)\right)\right)\tilde\phi_i\right\|^2_{L^2(\Omega)} &\leq c h^{-3/2}\left(\left\|d_{f,h}\tilde\phi_i\right\|^2_{L^2(\Omega)} + \left\|d^*_{f,h}\tilde\phi_i\right\|^2_{L^2(\Omega)}\right) \\
&= c h^{-3/2}\left(\left\|d_{f,h}\tilde\phi_i\right\|^2_{L^2(\dot\Omega_i)} + \left\|d^*_{f,h}\tilde\phi_i\right\|^2_{L^2(\dot\Omega_i)}\right).
\end{aligned}$$

Moreover, from Proposition B.59 (items (ii) et (iii))

$$d_{f,h}\tilde\phi_i = \Theta_i^{-1}\left(\chi_i\, d_{f,h} u_{h,i}^{(1)} + h\, d\chi_i \wedge u_{h,i}^{(1)}\right) = \Theta_i^{-1} h\, d\chi_i \wedge u_{h,i}^{(1)}, \tag{B.223}$$

and

$$d^*_{f,h}\tilde\phi_i = \Theta_i^{-1}\left(\chi_i\, d^*_{f,h} u_{h,i}^{(1)} - h\, u_{h,i}^{(1)} \cdot \nabla\chi_i\right) = -\Theta_i^{-1} h\, u_{h,i}^{(1)} \cdot \nabla\chi_i.$$

As a consequence, using Lemma B.66 and Proposition B.61, one gets for some $N \in \mathbb{N}$ and for some $c > 0$ which may change from one occurrence to another,

$$\begin{aligned}
\left\|\left(1 - \pi_{[0,h^{\frac{3}{2}})}\left(\Delta_{f,h}^{D,(1)}(\Omega)\right)\right)\tilde\phi_i\right\|^2_{L^2(\Omega)} &\leq c h^{-3/2}\left(\left\|h d\chi_i \wedge u_{h,i}^{(1)}\right\|^2_{L^2(\dot\Omega_i)} + \left\|h u_{h,i}^{(1)} \cdot \nabla\chi_i\right\|^2_{L^2(\dot\Omega_i)}\right) \\
&\leq c\, h^{1/2} \int_{\mathrm{supp}\nabla\chi_i} \left|u_{h,i}^{(1)}(x) e^{\frac{1}{h} d_a(x,z_i)} e^{-\frac{1}{h} d_a(x,z_i)}\right|^2 dx \\
&\leq c\, h^{1/2-N} e^{-\inf_{\mathrm{supp}\nabla\chi_i} \frac{2}{h} d_a(\cdot,z_i)}.
\end{aligned} \tag{B.224}$$

The function χ_i can be chosen such that the set $\left\{x \in \dot{\Omega}_i,\, \nabla\chi_i(x) \neq 0\right\}$ is as close as one wants to $\Gamma_{2,i}$ and to Γ_0 (see Figure B.14). Therefore by continuity of the Agmon distance, using (B.136)–(B.137), for any $\delta > 0$, one can choose χ_i satisfying the three conditions stated in Definition B.14 and such that

$$\inf_{z\in \mathrm{supp}\nabla\chi_i} d_a(z, z_i) \geq \min\left(d_a(x_0, z_i),\, \inf_{z\in B_{z_i}^c} d_a(z, z_i)\right) - \delta. \tag{B.225}$$

From (B.20), there exists $r > 0$ such that

$$\inf_{z\in B_{z_i}^c} d_a(z, z_i) \geq \max\left[f(z_n) - f(z_i), f(z_i) - f(z_1)\right] + r.$$

In addition, using (B.21), there exists $r' > 0$ such that

$$\begin{aligned} d_a(z_i, x_0) &\geq f(z_i) - f(x_0) \geq f(z_1) - f(x_0) \geq f(z_n) - f(z_1) + r' \\ &\geq \max[f(z_n) - f(z_i), f(z_i) - f(z_1)] + r'. \end{aligned}$$

Therefore, choosing χ_i such that $\delta < \min(r, r')$, there exists $\varepsilon' > 0$ such that

$$\inf_{z\in \mathrm{supp}\nabla\chi_i} d_a(z, z_i) \geq \max\left[f(z_n) - f(z_i), f(z_i) - f(z_1)\right] + \varepsilon'. \tag{B.226}$$

Using the estimate (B.226) in (B.224), there exist $\varepsilon_1 > 0$, $c > 0$, $N \in \mathbb{N}$ and $h_0 > 0$, such that for every $h \in (0, h_0)$

$$\begin{aligned} \left\|\left(1 - \pi_{[0,h^{\frac{3}{2}})}\left(\Delta_{f,h}^{D,(1)}(\Omega)\right)\right)\tilde{\phi}_i\right\|_{L^2(\Omega)}^2 &\leq ch^{-N} e^{-\frac{2}{h}(\max[f(z_n)-f(z_i), f(z_i)-f(z_1)]+\varepsilon')} \\ &\leq e^{-\frac{2}{h}(\max[f(z_n)-f(z_i), f(z_i)-f(z_1)]+\varepsilon_1)}. \end{aligned} \tag{B.227}$$

This last inequality leads to the desired estimate in the $L^2(\Omega)$-norm. In order to get the same upper bound in the $H^1(\Omega)$-norm, notice now that one has

$$\begin{aligned} &\left(1 - \pi_{[0,h^{\frac{3}{2}})}\left(\Delta_{f,h}^{D,(2)}(\Omega)\right)\right) d_{f,h}\tilde{\phi}_i = d_{f,h}\left(1 - \pi_{[0,h^{\frac{3}{2}})}\left(\Delta_{f,h}^{(D,1)}(\Omega)\right)\right)\tilde{\phi}_i \\ &= hd\left(1 - \pi_{[0,h^{\frac{3}{2}})}\left(\Delta_{f,h}^{D,(1)}(\Omega)\right)\right)\tilde{\phi}_i + df \wedge \left(1 - \pi_{[0,h^{\frac{3}{2}})}\left(\Delta_{f,h}^{D,(1)}(\Omega)\right)\right)\tilde{\phi}_i. \end{aligned}$$

Therefore it holds

$$\begin{aligned} hd\left(1 - \pi_{[0,h^{\frac{3}{2}})}\left(\Delta_{f,h}^{D,(1)}(\Omega)\right)\right)\tilde{\phi}_i = &\left(1 - \pi_{[0,h^{\frac{3}{2}})}\left(\Delta_{f,h}^{D,(2)}(\Omega)\right)\right) d_{f,h}\,\tilde{\phi}_i \\ &- df \wedge \left(1 - \pi_{[0,h^{\frac{3}{2}})}\left(\Delta_{f,h}^{D,(1)}(\Omega)\right)\right)\tilde{\phi}_i. \end{aligned}$$

Let us introduce $K_i := \max[f(z_n) - f(z_i), f(z_i) - f(z_1)]$. From (B.227), there exist $C > 0$ and $h_0 > 0$, such that for all $h \in (0, h_0)$

$$\left\|df \wedge \left(1 - \pi_{[0,h^{\frac{3}{2}})}\left(\Delta_{f,h}^{D,(1)}(\Omega)\right)\right)\tilde{\phi}_i\right\|_{L^2(\Omega)}^2 \leq Ce^{-\frac{2}{h}(K_i+\varepsilon_1)}.$$

Moreover, using (B.223) and (B.224) there exist $\varepsilon > 0$, $C > 0$ and $h_0 > 0$, such that for all $h \in (0, h_0)$,

$$\left\| \left(1 - \pi_{[0,h^{\frac{3}{2}})}(\Delta_{f,h}^{D,(2)}(\Omega))\right) d_{f,h}\tilde{\phi}_i \right\|_{L^2(\Omega)}^2 \leq \left\| d_{f,h}\tilde{\phi}_i \right\|_{L^2(\Omega)}^2 = \Theta_i^{-2} \left\| h d\chi_i \wedge u_{h,i}^{(1)} \right\|_{L^2(\dot{\Omega}_i)}^2$$
$$\leq C e^{-\frac{2}{h}(K_i+\varepsilon)}.$$

Thus one gets: there exist $\varepsilon > 0$, $C > 0$ and $h_0 > 0$, such that for all $h \in (0, h_0)$,

$$h^2 \left\| d \left(1 - \pi_{[0,h^{\frac{3}{2}})} \left(\Delta_{f,h}^{D,(1)}(\Omega)\right)\right) \tilde{\phi}_i \right\|_{L^2(\Omega)}^2 \leq C e^{-\frac{2}{h}(K_i+\varepsilon)}.$$

Similarly, there exist $\varepsilon > 0$, $C > 0$ and $h_0 > 0$, such that for all $h \in (0, h_0)$

$$h^2 \left\| d^* \left(1 - \pi_{[0,h^{\frac{3}{2}})} \left(\Delta_{f,h}^{D,(1)}(\Omega)\right)\right) \tilde{\phi}_i \right\|_{L^2(\Omega)}^2 \leq C e^{-\frac{2}{h}(K_i+\varepsilon)}.$$

As a consequence, using (B.116), there exist $\varepsilon > 0$, $C > 0$ and $h_0 > 0$, such that for all $h \in (0, h_0)$

$$\left\| \left(1 - \pi_{[0,h^{\frac{3}{2}})} \left(\Delta_{f,h}^{D,(1)}(\Omega)\right)\right) \tilde{\phi}_i \right\|_{H^1(\Omega)}^2 \leq C e^{-\frac{2}{h}(K_i+\varepsilon)}.$$

This concludes the proof of (B.57).

<u>Step 2</u>. Study of the terms $\displaystyle\int_\Omega \tilde{\phi}_i \cdot \tilde{\phi}_j$ for $(i,j) \in \{1, \dots, n\}^2$.

Let $(i,j) \in \{1, \dots, n\}^2$. Let us assume without loss of generality that $i < j$, so that $f(z_i) \leq f(z_j)$. From Proposition B.49, one has the inequality $d_a(z_i, z_j) > f(z_j) - f(z_i)$.

Now, according to Proposition B.61 and Lemma B.66 and to the triangular inequality for d_a, there exist $\varepsilon > 0$, $N \in \mathbb{N}$ and $h_0 > 0$ such that for all $h \in (0, h_0)$,

$$\begin{aligned}
\left| \int_\Omega \tilde{\phi}_i(x) \cdot \tilde{\phi}_j(x)\, dx \right| &\leq e^{-\frac{d_a(z_j,z_i)}{h}} \int_{\mathrm{supp}\chi_i \cap \mathrm{supp}\chi_j} e^{\frac{d_a(x,z_i)}{h}} |\tilde{\phi}_i(x)| e^{\frac{d_a(x,z_j)}{h}} |\tilde{\phi}_j(x)|\, dx \\
&\leq \Theta_i^{-1}\Theta_j^{-1} \left\| e^{\frac{d_a(.,z_i)}{h}} \chi_i u_{h,i}^{(1)} \right\|_{L^2(\dot{\Omega}_i)} \left\| e^{\frac{d_a(.,z_j)}{h}} \chi_j u_{h,j}^{(1)} \right\|_{L^2(\dot{\Omega}_j)} e^{-\frac{d_a(z_i,z_j)}{h}} \qquad \text{(B.228)} \\
&\leq C h^{-N} e^{-\frac{1}{h}(f(z_j)-f(z_i)+\varepsilon)}.
\end{aligned}$$

This concludes the proof of (B.58).

<u>Step 3.</u> Study of the terms $\displaystyle\int_{\Sigma_i} \tilde{\phi}_j \cdot n\, e^{-\frac{f}{h}}$ for $(i,j) \in \{1, \dots, n\}^2$.

By construction, for all $(i,j) \in \{1, \dots, n\}^2$ such that $i \neq j$, one has

$$\int_{\Sigma_i} \tilde{\phi}_j \cdot n\, e^{-\frac{1}{h}f} = 0.$$

Now, let us compute the term $\int_{\Sigma_i} \tilde{\phi}_i \cdot n\, e^{-\frac{1}{h}f}$. Let $u_{z_i,wkb}^{(1)}$ be the WKB expansion defined by (B.174). Following the beginning of Section B.4.4.2, let us consider

1. a neighborhood $V_{\Gamma_{St,i}}$ of Σ_i in $\overline{\Omega}$, which is stable under the dynamics (B.183) and such that, for some $\varepsilon > 0$, $V_{\Gamma_{St,i}} + B(0,\varepsilon) \subset V_{\Gamma_{1,i}} \cap (\Gamma_{1,i} \cup \dot{\Omega}_i)$

2. and a cut-off function $\chi_{wkb,i} \in C_c^\infty(\dot{\Omega}_i \cup \Gamma_{1,i})$ with $\chi_{wkb,i} \equiv 1$ on a neighborhood of $\overline{V_{\Gamma_{St,i}}}$ and such that $\operatorname{supp} \chi_{wkb,i} \subset V_{\Gamma_{1,i}} \cap (\dot{\Omega}_i \cup \Gamma_{1,i})$.

Using Proposition B.64, there exists $c_{z_i}(h) \in \mathbb{R}_+^*$ such that

$$\left\| \chi_{wkb,i} \left(u_{h,i}^{(1)} - c_{z_i}(h) u_{z_i,wkb}^{(1)} \right) \right\|_{H^1(\dot{\Omega}_i)} = O(h^\infty).$$

Let us now introduce

$$\tilde{\phi}_{z_i,wkb} := c_{z_i}(h) \chi_{wkb,i}\ u_{z_i,wkb}^{(1)} \tag{B.229}$$

so that

$$\int_{\Sigma_i} \tilde{\phi}_i \cdot n\ e^{-\frac{1}{h}f} = \int_{\Sigma_i} \tilde{\phi}_{z_i,wkb} \cdot n\ e^{-\frac{1}{h}f} + \int_{\Sigma_i} \left(\tilde{\phi}_i - \tilde{\phi}_{z_i,wkb} \right) \cdot n\, e^{-\frac{1}{h}f}.$$

Let us first deal with the term $\int_{\Sigma_i} \tilde{\phi}_{z_i,wkb} \cdot n\, e^{-\frac{1}{h}f}$. Using Laplace's method (the computation is similar to (B.181)), one gets when $h \to 0$ (since $\Phi = f$ and $\partial_n \Phi = -\partial_n f$ on $\partial\Omega$)

$$\begin{aligned}
\int_{\Sigma_i} \chi_{wkb,i}\ u_{z_i,wkb}^{(1)} \cdot n\, e^{-\frac{1}{h}f} &= \int_{\Sigma_i} e^{-\frac{\Phi - f(z_i)}{h}}\ a_0\, \partial_n (f - \Phi)\, e^{-\frac{1}{h}f}\ (1 + O(h)) \\
&= 2 e^{\frac{f(z_i)}{h}} \int_{\Sigma_i} e^{-\frac{2f}{h}}\ a_0\, \partial_n f\ (1 + O(h)) \\
&= \frac{2\, \partial_n f(z_i)\, \pi^{\frac{d-1}{2}}}{\sqrt{\det \operatorname{Hess} f|_{\partial\Omega}(z_i)}} h^{\frac{d-1}{2}}\ e^{-\frac{1}{h}f(z_i)} (1 + O(h)).
\end{aligned}$$

Then one obtains when $h \to 0$

$$\int_{\Sigma_i} \tilde{\phi}_{z_i,wkb} \cdot n\, e^{-\frac{1}{h}f} = c_{z_i}(h) \frac{2\, \partial_n f(z_i)\, \pi^{\frac{d-1}{2}}}{\sqrt{\det \operatorname{Hess} f|_{\partial\Omega}(z_i)}} h^{\frac{d-1}{2}}\ e^{-\frac{1}{h}f(z_i)} (1 + O(h)).$$

We recall from Proposition B.64 that in the limit $h \to 0$:

$$c_{z_i}(h) = C_{z_i,wkb}^{-1} h^{-\frac{d+1}{4}} (1 + O(h^\infty)),$$

where the constant $C_{z_i,wkb}$ is defined by (B.177). Therefore, in the limit $h \to 0$

$$\int_{\Sigma_i} \tilde{\phi}_{z_i,wkb} \cdot n\, e^{-\frac{1}{h}f} = \frac{\pi^{\frac{d-1}{4}} \sqrt{2 \partial_n f(z_i)}}{(\det \operatorname{Hess} f|_{\partial\Omega}(z_i))^{1/4}}\ h^{\frac{d-3}{4}}\ e^{-\frac{1}{h}f(z_i)} (1 + O(h)).$$

Let us now deal with the term $\int_{\Sigma_i} \left(\tilde{\phi}_i - \tilde{\phi}_{z_i,wkb} \right) \cdot n\ e^{-\frac{1}{h}f}$. One obtains using Lemmata B.63 and B.66, that there exist $C > 0$, $h_0 > 0$ and $\eta > 0$ such that for all

$h \in (0, h_0)$

$$\begin{aligned}
\left|\int_{\Sigma_i} \left(\tilde{\phi}_i - \tilde{\phi}_{z_i,wkb}\right) \cdot n \; e^{-\frac{1}{h}f}\right| &= \left|\int_{\Sigma_i} \left(\frac{u^{(1)}_{h,i}}{\Theta_i} - c_{z_i}(h) u^{(1)}_{z_i,wkb}\right) \cdot n \; e^{-\frac{1}{h}f}\right| \\
&= \frac{1}{\Theta_i}\left|\int_{\Sigma_i} \left(u^{(1)}_{h,i} - \Theta_i \; c_{z_i}(h) u^{(1)}_{z_i,wkb}\right) \cdot n \; e^{-\frac{1}{h}f}\right| \\
&\leq \frac{e^{-\frac{1}{h}f(z_i)}}{\Theta_i} \int_{\Sigma_i} \left|\left(u^{(1)}_{h,i} - c_{z_i}(h) u^{(1)}_{z_i,wkb}\right) \cdot n\right| \\
&\quad + e^{-\frac{1}{h}f(z_i)} \frac{|\Theta_i - 1|}{\Theta_i} |c_{z_i}(h)| \int_{\Sigma_i} \left|u^{(1)}_{z_i,wkb} \cdot n\right| \\
&\leq C e^{-\frac{1}{h}f(z_i)} \left\|\chi_{wkb,i} \left(u^{(1)}_{h,i} - c_{z_i}(h) u^{(1)}_{z_i,wkb}\right)\right\|_{H^1(\dot{\Omega}_i)} \\
&\quad + C e^{-\frac{1}{h}f(z_i)} \, e^{-\frac{\eta}{h}} h^{-\frac{d+1}{4}} \left\|\chi_{wkb,i} u^{(1)}_{z_i,wkb}\right\|_{H^1(\dot{\Omega}_i)}.
\end{aligned}$$

Therefore, one obtains using Proposition B.64 and (B.178)

$$e^{\frac{1}{h}f(z_i)} \left|\int_{\Sigma_i} \left(\tilde{\phi}_i - \tilde{\phi}_{z_i,wkb}\right) \cdot n \; e^{-\frac{1}{h}f}\right| = O(h^\infty) + C e^{-\frac{\eta}{h}} h^{-\frac{d+5}{4}} = O(h^\infty).$$

In conclusion, we have when $h \to 0$

$$\int_{\Sigma_i} \tilde{\phi}_i \cdot n \; e^{-\frac{1}{h}f} = \int_{\Sigma_i} \tilde{\phi}_{z_i,wkb} \cdot n \, e^{-\frac{1}{h}f} \; (1 + O(h^\infty)),$$

which gives the expected estimate

$$\int_{\Sigma_i} \tilde{\phi}_j \cdot n \, e^{-\frac{1}{h}f} = \begin{cases} B_i h^m \; e^{-\frac{1}{h}f(z_i)} \; (1 + O(h)) & \text{if } i = j, \\ 0 & \text{if } i \neq j, \end{cases} \tag{B.230}$$

where

$$m = \frac{d-3}{4} \quad \text{and} \quad B_i = \frac{\pi^{\frac{d-1}{4}} \sqrt{2\partial_n f(z_i)}}{(\det \operatorname{Hess} f|_{\partial\Omega}(z_i))^{1/4}}. \tag{B.231}$$

This concludes the proof of (B.60).

<u>Step 4.</u> Study of the term $\int_\Omega \nabla \tilde{u} \cdot \tilde{\phi}_i \, e^{-\frac{1}{h}f}$.

First one has the equality by Definition B.13,

$$\int_\Omega \nabla \tilde{u} \cdot \tilde{\phi}_i \, e^{-\frac{1}{h}f} = \frac{\int_\Omega \nabla \chi \cdot \tilde{\phi}_i \, e^{-\frac{1}{h}f}}{\sqrt{\int_\Omega \chi^2 e^{-\frac{2}{h}f}}},$$

where $\nabla \chi \cdot \tilde{\phi}_i = \mathbf{i}_{\nabla\chi} \tilde{\phi}_i = \tilde{\phi}_i(\nabla \chi)$. The denominator of the right-hand side being easily computed thanks to Laplace's method:

$$\sqrt{\int_\Omega \chi^2 e^{-\frac{2}{h}f}} = \frac{(\pi h)^{\frac{d}{4}}}{(\det \operatorname{Hess} f(x_0))^{1/4}} e^{-\frac{f(x_0)}{h}} (1 + O(h)).$$

Using an integration by parts and the fact that $d^*(u_{h,i}^{(1)}\ e^{-f/h}) = 0$ in $L^2(\dot{\Omega}_i)$ (see Proposition B.59 items (ii) and (iii)) which is valid for all h small enough, one obtains

$$\begin{aligned}\int_\Omega \nabla\chi\cdot\tilde{\phi}_i\, e^{-\frac{f}{h}} &= -\int_\Omega \nabla(1-\chi)\cdot\chi_i \frac{u_{h,i}^{(1)}}{\Theta_i}\, e^{-\frac{f}{h}}\\ &= \int_\Omega (1-\chi)\ \nabla\chi_i\cdot\frac{u_{h,i}^{(1)}}{\Theta_i}\, e^{-\frac{f}{h}} - \int_{\partial\Omega}(1-\chi)\ \tilde{\phi}_i\cdot n\, e^{-\frac{f}{h}}.\end{aligned}$$

Using the fact that $\chi = 0$ on $\partial\Omega$, one then obtains:

$$\begin{aligned}\int_{\partial\Omega}(1-\chi)\ \tilde{\phi}_i\cdot n\, e^{-\frac{f}{h}} &= \int_{\partial\Omega\cap\mathrm{supp}\chi_i}\tilde{\phi}_i\cdot n\, e^{-\frac{f}{h}}\\ &= \int_{\Sigma_i}\tilde{\phi}_i\cdot n\, e^{-\frac{f}{h}} + \int_{(\partial\Omega\cap\mathrm{supp}\chi_i)\setminus\Sigma_i}\tilde{\phi}_i\cdot n\, e^{-\frac{f}{h}}.\end{aligned}$$

Using (B.230), in the limit $h\to 0$:

$$\begin{aligned}\int_\Omega \nabla\chi\cdot\tilde{\phi}_i\, e^{-\frac{f}{h}} &= -B_i h^m\ e^{-\frac{1}{h}f(z_i)}\ (1+O(h))\\ &\quad - \int_{(\partial\Omega\cap\mathrm{supp}\chi_i)\setminus\Sigma_i}\tilde{\phi}_i\cdot n\, e^{-\frac{f}{h}} + \int_\Omega(1-\chi)\ \nabla\chi_i\cdot\frac{u_{h,i}^{(1)}}{\Theta_i}\, e^{-\frac{f}{h}}.\end{aligned}\tag{B.232}$$

Let us now prove that the two last terms in (B.232) are negligible compared to the first one.

On the compact set $(\partial\Omega\cap\mathrm{supp}\chi_i)\setminus\Sigma_i$ one has $f(z) > f(z_i)$ since $z_i\in\Sigma_i$ is the only global minimum of f on B_{z_i} and $\mathrm{supp}\,\chi_i\cap\partial\Omega\subset\Gamma_{1,i}\subset B_{z_i}$. Then, using Proposition B.61 and (B.116), there exist $\varepsilon>0$, $h_0>0$, $C>0$ and $N\in\mathbb{N}$ such that for all $h\in(0,h_0)$

$$\begin{aligned}\left|\int_{(\partial\Omega\cap\mathrm{supp}\chi_i)\setminus\Sigma_i}\tilde{\phi}_i\cdot n\, e^{-\frac{f}{h}}\right| &\le e^{-\frac{f(z_i)+\varepsilon}{h}}\left|\int_{(\partial\Omega\cap\mathrm{supp}\chi_i)\setminus\Sigma_i}\tilde{\phi}_i\cdot n\right|\\ &\le Ce^{-\frac{f(z_i)+\varepsilon}{h}}\left|\int_{(\partial\Omega\cap\mathrm{supp}\chi_i)\setminus\Sigma_i}\tilde{\phi}_i\cdot n\ e^{\frac{d_a(.,z_i)}{h}}\right|\\ &\le C\frac{e^{-\frac{f(z_i)+\varepsilon}{h}}}{\Theta_i}\ \left\|\chi_i u_{h,i}^{(1)}\ e^{\frac{d_a(.,z_i)}{h}}\right\|_{H^1(\dot{\Omega}_i)}\\ &\le Ce^{-\frac{f(z_i)+\varepsilon}{h}}h^{-N} \le Ce^{-\frac{f(z_i)+\varepsilon/2}{h}}.\end{aligned}\tag{B.233}$$

Let us now deal with the last term of (B.232). The support of $(1-\chi)\nabla\chi_i$ is included in the support of $\nabla\chi_i$ and does not contain x_0 since $\chi\equiv 1$ around x_0. The function χ_i can be chosen such that the set $\{x\in\dot{\Omega}_i,\ |\nabla\chi_i|\neq 0 \text{ and } \chi\neq 1\}$ is as close as one wants from $\Gamma_{2,i}$ (see Figure B.14). Therefore, by continuity of the Agmon distance, using (B.136), for any $\delta>0$, one can choose χ_i satisfying the three conditions stated in Definition B.14 and such that

$$\inf_{\mathrm{supp}(1-\chi)\nabla\chi_i}(d_a(\cdot,z_i)+f) \ge \inf_{B_{z_i}^c}(d_a(\cdot,z_i)+f) - \delta.$$

Thus, using the Cauchy-Schwarz inequality and Proposition B.61, there exists $N \in \mathbb{N}$ such that

$$\int_{\mathrm{supp}(1-\chi)\nabla\chi_i} \left|(1-\chi)\,\nabla\chi_i \cdot u_{h,i}^{(1)}\; e^{-\frac{f}{h}}\right| \leq C \left\| u_{h,i}^{(1)} e^{\frac{d_a(\cdot,z_i)}{h}} \right\|_{L^2(\dot{\Omega}_i)} e^{-\frac{1}{h}\inf_{\mathrm{supp}(1-\chi)\nabla\chi_i}(d_a(\cdot,z_i)+f)}$$
$$\leq Ch^{-N} e^{-\frac{1}{h}\inf_{B_{z_i}^c}(d_a(\cdot,z_i)+f-\delta)}. \tag{B.234}$$

Besides, from assumption (B.20)

$$\inf_{z\in B_{z_i}^c} [d_a(z,z_i)+f(z)] > f(z_i).$$

Indeed, the inequality (B.20) implies that there exists $r>0$ such that for all $z \in B_{z_i}^c$, $d_a(z,z_i) \geq f(z_i) - f(z_1) + r$ and therefore for all $z \in B_{z_i}^c$ one obtains

$$d_a(z,z_i) + f(z) \geq f(z_i) + (f(z) - f(z_1)) + r \geq f(z_i) + r.$$

Therefore, taking χ_i such that $\delta < r/2$, one has, when $h \to 0$

$$\int_{\mathrm{supp}(1-\chi)\nabla\chi_i} \left|(1-\chi)\,\nabla\chi_i \cdot u_{h,i}^{(1)}\; e^{-\frac{f}{h}}\right| = O\left(e^{-\frac{f(z_i)+c}{h}}\right)$$

for some constant $c>0$.

In conclusion, in the limit $h \to 0$,

$$\int_\Omega \nabla\tilde{u}\cdot\tilde{\phi}_i\, e^{-\frac{1}{h}f}dx = C_i h^p e^{-\frac{1}{h}(f(z_i)-f(x_0))}\;(1+O(h)),$$

with

$$C_i = -B_i\frac{(\det \mathrm{Hess} f(x_0))^{1/4}}{\pi^{\frac{d}{4}}} = -\frac{\pi^{-\frac{1}{4}}\sqrt{2\partial_n f(z_i)}(\det \mathrm{Hess} f(x_0))^{1/4}}{(\det \mathrm{Hess} f|_{\partial\Omega}(z_i))^{1/4}} \text{ and } p = m - \frac{d}{4} = -\frac{3}{4}, \tag{B.235}$$

where B_i and m have both been defined in (B.231). This concludes the proof of (B.59), and thus the proof of Theorem B.1.

B.5 Consequences and generalizations of Theorem B.1

B.5.1 Proofs of Proposition B.6, Proposition B.7, Corollary B.8 and Corollary B.10

B.5.1.1 Proof of Proposition B.6

Assume that **[H1]**, **[H2]** and **[H3]** hold. From Lemma B.18 and since the function $\tilde{u}$ is non negative in Ω, there exists $h_0>0$ such that for all $h \in (0,h_0)$

$$u_h = \frac{\pi_h^{(0)}\tilde{u}}{\left\|\pi_h^{(0)}\tilde{u}\right\|_{L_w^2}},$$

where u_h is the eigenfunction associated with the smallest eigenvalue of $-L_{f,h}^{(D),(0)}(\Omega)$ (see Proposition B.14) which satisfies (B.11) and $\tilde{u}$ is introduced in Definition B.13. Then, there exists $h_0 > 0$ such that for all $h \in (0, h_0)$,

$$\int_\Omega u_h \; e^{-\frac{2}{h}f} = \int_\Omega \frac{\pi_h^{(0)}\tilde{u}}{\left\|\pi_h^{(0)}\tilde{u}\right\|_{L^2_w}} e^{-\frac{2}{h}f} = \frac{1}{\left\|\pi_h^{(0)}\tilde{u}\right\|_{L^2_w}} \int_\Omega \left[\tilde{u} + \left(\pi_h^{(0)} - 1\right)\tilde{u}\right] e^{-\frac{2}{h}f}.$$

From the definition of χ (see Definition B.13) and using Laplace's method, one obtains (in the limit $h \to 0$)

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

and likewise

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

In addition, using Lemma B.18, one has $\left\|\pi_h^{(0)}\tilde{u}\right\|_{L^2_w} = 1 + O\left(e^{-\frac{c}{h}}\right)$. Therefore, it holds when $h \to 0$,

$$\frac{1}{\left\|\pi_h^{(0)}\tilde{u}\right\|_{L^2_w}} \int_\Omega \tilde{u} \; e^{-\frac{2}{h}f} = \frac{h^{\frac{d}{4}}\pi^{\frac{d}{4}}}{(\det \text{ Hess} f(x_0))^{1/4}} e^{-\frac{1}{h}f(x_0)}(1 + O(h)).$$

Moreover, from Lemma B.18, there exist $c > 0$, $h_0 > 0$ and $C > 0$ such that for $h \in (0, h_0)$

$$\frac{1}{\left\|\pi_h^{(0)}\tilde{u}\right\|_{L^2_w}} \left|\int_\Omega \left(\pi_h^{(0)} - 1\right)\tilde{u} \; e^{-\frac{2}{h}f}\right| \leq C \left\|(1 - \pi_h^{(0)})\tilde{u}\right\|_{L^2_w} \sqrt{\int_\Omega e^{-\frac{2}{h}f}} \leq C e^{-\frac{c}{h}} \; e^{-\frac{1}{h}f(x_0)}$$

Thus, one has when $h \to 0$,

$$\int_\Omega u_h \; e^{-\frac{2}{h}f} = \frac{\pi^{\frac{d}{4}}}{(\det \text{ Hess} f(x_0))^{1/4}} \; h^{\frac{d}{4}} \; e^{-\frac{1}{h}f(x_0)}(1 + O(h)).$$

This proves Proposition B.6.

B.5.1.2 Proof of Proposition B.7

The aim of this section is to prove (B.23). To this end, we first state in Proposition B.67 some estimates that the quasi-modes constructed in Section B.4.2 satisfy under hypotheses **[H1]**, **[H2]** and **[H3]**. Let us emphasize that these estimates are weaker than those obtained in Section B.4.5 where in addition to **[H1]**-**[H2]**-**[H3]**, also the hypotheses (B.20) and (B.21) were assumed. Then, we prove that the estimates of Proposition B.67 imply (B.23).

Proposition B.67. *Let us assume that the hypotheses **[H1]**, **[H2]** and **[H3]** hold. Then there exist $n+1$ quasi-modes $((\tilde{\psi}_i)_{i=1,\dots,n}, \tilde{u})$ which satisfy the following estimates:*

1. *$\forall i \in \{1,\dots,n\}$, $\tilde{\psi}_i \in \Lambda^1 H^1_{w,T}(\Omega)$ and $\tilde{u} \in \Lambda^0 H^1_{w,T}(\Omega)$. The function $\tilde{u}$ is non negative in Ω. Moreover $\forall i \in \{1,\dots,n\}$, $\left\|\tilde{\psi}_i\right\|_{L^2_w} = \|\tilde{u}\|_{L^2_w} = 1$.*

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

$$\left\|\left(1-\pi_h^{(1)}\right)\tilde{\psi}_i\right\|^2_{H^1_w} = O\left(e^{-\frac{\varepsilon_1}{h}}\right).$$

(b) For any $\delta > 0$, $\|\nabla\tilde{u}\|^2_{L^2_w} = O\left(e^{-\frac{2}{h}(f(z_1)-f(x_0)-\delta)}\right)$.

3. *There exists $\varepsilon_0 > 0$ such that $\forall (i,j) \in \{1,\dots,n\}^2$, $i<j$, in the limit $h \to 0$: $\left\langle \tilde{\psi}_i, \tilde{\psi}_j\right\rangle_{L^2_w} = O\left(e^{-\frac{\varepsilon_0}{h}}\right)$.*

4. *There exist $\varepsilon_0 > 0$, such that for all $i \in \{1,\dots,n\}$, in the limit $h \to 0$:*

$$\left\langle \nabla\tilde{u}, \tilde{\psi}_i\right\rangle_{L^2_w} = C_i\, h^p e^{-\frac{1}{h}(f(z_i)-f(x_0))}\left(1+O(h)\right) + O\left(e^{-\frac{1}{h}(f(z_1)-f(x_0)+\varepsilon_0)}\right),$$

where the constants p and $(C_i)_{i=1,\dots,n}$ are given by (B.235).

Proof. Thanks to the hypotheses **[H1]**, **[H2]** and **[H3]**, one can introduce the $n+1$ quasi-modes $((\tilde{\phi}_i)_{i=1,\dots,n}, \tilde{u})$ built in Section B.4.2. Recall that $\tilde{\psi}_i = e^{\frac{1}{h}f}\tilde{\phi}_i$ for $i \in \{1,\dots,n\}$.

Then, one easily obtains that $((\tilde{\psi}_i)_{i=1,\dots,n}, \tilde{u})$ satisfy the estimates stated in Proposition B.67, following exactly the computations made on $((\tilde{\phi}_i)_{i=1,\dots,n}, \tilde{u})$ in Section B.4.5: 2(a) follows from (B.224), 2(b) is a consequence of Lemma B.60, 3 follows from (B.228) and 4 is a consequence of (B.232)-(B.233)-(B.234) (in (B.234), one uses that for $\delta > 0$ small enough, there exists $c > 0$ such that $\inf_{B_{z_i^c}}(d_a(.,z_i) + f - \delta) \geq f(z_1) + c$. ∎

Let us now prove that the estimates stated in Proposition B.67 imply (B.23), which will conclude the proof of Proposition B.7.

Proof. From (B.51) together with the assumption $\|u_h\|_{L^2_w} = 1$, it holds

$$\lambda_h = -\langle L^{D,(0)}_{f,h}(\Omega)\, u_h, u_h\rangle_{L^2_w} = \frac{h}{2}\|\nabla u_h\|^2_{L^2_w} \tag{B.236}$$

where u_h is the eigenfunction associated with the smallest eigenvalue of $-L^{D,(0)}_{f,h}(\Omega)$ (see Proposition B.14). Recall that $\nabla u_h \in \operatorname{Ran}\pi_h^{(1)}$ (see (B.53)).

In addition, let us recall that from items 1, 2(a) and 3 in Proposition B.67 and using the proof of Lemma B.19, there exists h_0 such that for all $h \in (0,h_0)$,

$$\operatorname{span}\left(\pi_h^{(1)}\tilde{\psi}_i,\ i=1,\dots,n\right) = \operatorname{Ran}\pi_h^{(1)}.$$

Let us denote by $(\psi_i)_{i=1,\dots,n}$ the orthornormal basis of $\operatorname{Ran}\pi_h^{(1)}$ resulting from the Gram-Schmidt orthonormalisation procedure applied to the set $(\pi_h^{(1)}\tilde{\psi}_i)_{i=1,\dots,n}$ (see Lemma B.20) so that

$$\|\nabla u_h\|^2_{L^2_w} = \sum_{j=1}^n \left|\langle \nabla u_h, \psi_j\rangle_{L^2_w}\right|^2. \tag{B.237}$$

We now want to estimate the terms $\langle \nabla u_h, \psi_j \rangle_{L^2_w}$.

Using 2(b) in Proposition B.67 and using the proof of Lemma B.18, one has that for h small enough $\pi_h^{(0)}\tilde{u} \neq 0$ and therefore, since moreover $\tilde{u}$ is non negative in Ω, $u_h = \frac{\pi_h^{(0)}\tilde{u}}{\left\|\pi_h^{(0)}\tilde{u}\right\|_{L^2_w}}$. Thus one has (see (B.68)), for $j \in \{1, \dots, n\}$,

$$\begin{aligned}\langle \nabla u_h, \psi_j \rangle_{L^2_w} &= \frac{Z_j^{-1}}{\left\|\pi_h^{(0)}\tilde{u}\right\|_{L^2_w}} \left[\left\langle \nabla \tilde{u}, \tilde{\psi}_j \right\rangle_{L^2_w} + \left\langle \nabla \tilde{u}, \left(\pi_h^{(1)} - 1\right) \tilde{\psi}_j \right\rangle_{L^2_w} \right] \\ &\quad + \frac{Z_j^{-1}}{\left\|\pi_h^{(0)}\tilde{u}\right\|_{L^2_w}} \left[\sum_{i=1}^{j-1} \kappa_{ji} \left(\left\langle \nabla \tilde{u}, \tilde{\psi}_i \right\rangle_{L^2_w} + \left\langle \nabla \tilde{u}, \left(\pi_h^{(1)} - 1\right) \tilde{\psi}_i \right\rangle_{L^2_w} \right) \right]\end{aligned}$$

where $(\kappa_{ji})_{1 \le i < j \le n}$ and $(Z_j)_{1 \le j \le n}$ are defined in Lemma B.20.

Now, using the items 1, 2(a) and 3 of Proposition B.67 and the proof of Lemma B.22, one obtains that there exist $\varepsilon_0 > 0$ and $h_0 > 0$ such that $\forall h \in (0, h_0)$, $\forall (i,j) \in \{1, \dots, n\}^2$, it holds

$$\kappa_{ji} = O\left(e^{-\frac{\varepsilon_0}{h}}\right) \text{ and } Z_i = 1 + O\left(e^{-\frac{\varepsilon_0}{h}}\right), \tag{B.238}$$

Injecting (B.238) and the estimates 2 and 4 of Proposition B.67 into (B.68) leads to the existence of $\varepsilon' > 0$ and $h_0 > 0$ such that $\forall h \in (0, h_0)$,

$$\langle \nabla u_h, \psi_j \rangle_{L^2_w} = C_i \; h^p e^{-\frac{1}{h}(f(z_j) - f(x_0))} \left(1 + O(h)\right) + O\left(e^{-\frac{1}{h}(f(z_1) - f(x_0) + \varepsilon')}\right), \tag{B.239}$$

where the constants p and $(C_i)_{i=1,\dots,n}$ are given by (B.235). Using (B.239) in (B.236) and (B.237), there exists $\varepsilon' > 0$ such that in the limit $h \to 0$

$$\lambda_h = \frac{h}{2} \sum_{j=1}^{n} C_i^2 \; h^{2p} e^{-\frac{2}{h}(f(z_i) - f(x_0))} \left(1 + O(h)\right) + O\left(e^{-\frac{2}{h}(f(z_1) - f(x_0) + \varepsilon')}\right).$$

Therefore, the estimate (B.23) holds and Proposition B.7 is proved. ∎

B.5.1.3 Proof of Corollary B.8

According to (B.14) one has for $i \in \{1, \dots, n\}$:

$$\mathbb{P}^{\nu_h}[X_{\tau_\Omega} \in \Sigma_i] = -\frac{h}{2\lambda_h} \frac{\int_{\Sigma_i} (\partial_n u_h)(z)\, e^{-\frac{2}{h} f(z)} \sigma(dz)}{\int_\Omega u_h(y) e^{-\frac{2}{h} f(y)} dy}.$$

Let us assume that **[H1]**, **[H2]** and **[H3]** together with the inequalities (B.20) and (B.21) hold. From Proposition B.6 and Proposition B.7, one obtains when $h \to 0$

$$\begin{aligned}\lambda_h \frac{2}{h} \int_\Omega u_h \; e^{-\frac{2}{h} f} dx &= 2\pi^{\frac{d-2}{4}} \left(\det \operatorname{Hess} f(x_0)\right)^{\frac{1}{4}} h^{\frac{d-6}{4}} \\ &\quad \times \sum_{k=1}^{n_0} \frac{\partial_n f(z_k)}{\sqrt{\det \operatorname{Hess} f|_{\partial\Omega}(z_k)}} \, e^{-\frac{1}{h}(2f(z_1) - f(x_0))} (1 + O(h)).\end{aligned}$$

Then, using in addition Theorem B.1 to estimate $\int_{\Sigma_i} (\partial_n u_h)\, e^{-\frac{2}{h} f} d\sigma$ $(i \in \{1, \dots, n\})$, one proves Corollary B.8.

B.5.1.4 Proof of Corollary B.10

Before starting the proof of Corollary B.10, let us notice that under the assumptions stated in Corollary B.8, for all $i \in \{1, ..., n\}$ and for any test function $F \in C^\infty(\partial\Omega)$ satisfying $\operatorname{supp} F \subset B_{z_i}$ and $z_i \in \operatorname{int}(\operatorname{supp} F)$, when $h \to 0$,

$$\mathbb{E}^{\nu_h}[F(X_{\tau_\Omega})] = \frac{\partial_n f(z_i)}{\sqrt{\det \operatorname{Hess} f_{|\partial\Omega}(z_i)}} \left(\sum_{k=1}^{n_0} \frac{\partial_n f(z_k)}{\sqrt{\det \operatorname{Hess} f_{|\partial\Omega}(z_k)}} \right)^{-1} e^{-\frac{2}{h}(f(z_i)-f(z_1))}(F(z_i)+O(h)). \tag{B.240}$$

The strategy for the proof of Corollary B.10 is to first extend (B.240) to a deterministic initial condition, and then to deduce the result of Corollary B.10.

Let us first notice that we can assume without loss of generality (up to increasing α if α is smaller than $f(x_0) + f(z_i) - f(z_1)$, see (B.26)) that

$$f(x_0) + f(z_i) - f(z_1) < \alpha < 2f(z_1) - f(z_i). \tag{B.241}$$

For such an α, let us define

$$K_\alpha := f^{-1}((-\infty, \alpha]) \cap \Omega.$$

We would like to show that (B.240) holds when $X_0 = x \in f^{-1}((-\infty, \alpha]) \cap \Omega$, for any test function $F \in C^\infty(\partial\Omega)$ satisfying $\operatorname{supp} F \subset B_{z_i}$ and $z_i \in \operatorname{int}(\operatorname{supp} F)$.

Let us introduce the principal eigenfunction $\tilde{u}_h$ of $-L_{f,h}^{D,(0)}(\Omega)$:

$$\begin{cases} -L_{f,h}^{(0)}\tilde{u}_h = \lambda_h \tilde{u}_h \text{ on } \Omega, \\ \tilde{u}_h = 0 \text{ on } \partial\Omega, \end{cases} \tag{B.242}$$

with $\tilde{u}_h > 0$ on Ω and normalized such that

$$\int_\Omega \tilde{u}_h^2 \, dx = 1. \tag{B.243}$$

Notice that u_h solution to (B.12) only differs from $\tilde{u}_h$ by a multiplicative constant so that, from Proposition C.3

$$\nu_h(dx) = Z_h(\Omega)^{-1}\tilde{u}_h(x)e^{-\frac{2}{h}f(x)}dx, \tag{B.244}$$

where, for any set $O \subset \Omega$,

$$Z_h(O) = \int_O \tilde{u}_h \, e^{-\frac{2}{h}f}.$$

For $F \in C^\infty(\partial\Omega)$, let us define $w_h(x) = \mathbb{E}^x[F(X_{\tau_\Omega})]$ for all $x \in \overline{\Omega}$. The function w_h is such that: $\forall h > 0$ and $x \in \Omega$,

$$|w_h(x)| \leq \|F\|_{L^\infty}.$$

Moreover, a standard Feynman-Kac formula shows that w_h satisfies

$$\begin{cases} L_{f,h}^{(0)} w_h = 0 \text{ on } \Omega, \\ w_h = F \text{ on } \partial\Omega, \end{cases} \tag{B.245}$$

where, we recall, the differential operator $L^{(0)}_{f,h}$ is defined by (B.10). Our objective is to compare $w_h(x)$ with $\mathbb{E}^{\nu_h}[F(X_{\tau_\Omega})]$.

By the Markov property, using (B.244), we have

$$\begin{aligned}\mathbb{E}^{\nu_h}[F(X_{\tau_\Omega})] &= \left(\int_\Omega \tilde{u}_h\, e^{-\frac{2}{h}f}\right)^{-1}\left(\int_\Omega w_h\, \tilde{u}_h\, e^{-\frac{2}{h}f}\right)\\ &= Z_h^{-1}(\Omega)\left(\int_{\Omega\setminus K_\alpha} w_h\, \tilde{u}_h\, e^{-\frac{2}{h}f}\right) + Z_h^{-1}(\Omega)\left(\int_{K_\alpha} w_h\, \tilde{u}_h\, e^{-\frac{2}{h}f}\right). \quad \text{(B.246)}\end{aligned}$$

In order to estimate the first term in (B.246), we need a leveling property for $\tilde{u}_h$, which is stated in [15, Theorem 2.4].

Lemma B.68. *Let us assume that **[H1]**, **[H2]** and **[H3]** hold and let us consider $\tilde{u}_h$ the principal eigenfunction of $L^{D,(0)}_{f,h}(\Omega)$ (see* (B.242)*) with normalization* (B.243)*. Then, for any compact set $K \subset \Omega$,*

$$\lim_{h\to 0}\left\|\tilde{u}_h - \left(\int_\Omega dx\right)^{-1/2}\right\|_{L^\infty(K)} = 0.$$

Notice that the reason why we consider a smooth test function F rather than 1_{Σ_i} is that we would like to apply the results in [15].

A direct consequence of Lemma B.68 is the following limit,

$$\lim_{h\to 0} h\ln\left(Z_h(\Omega)\right) = -2f(x_0). \quad \text{(B.247)}$$

Indeed, from the normalization of $\tilde{u}_h$, we get $Z_h(\Omega) \le e^{-\frac{2}{h}f(x_0)}$, and from Lemma B.68 we have, for h small enough and for $r > 0$ such that the open ball $B(x_0, 2r)$ is included in Ω,

$$Z_h(\Omega) \ge Z_h(B(x_0,r)) \ge \frac{1}{2}\left(\int_\Omega dx\right)^{-1/2}\int_{B(x_0,r)} e^{-\frac{2f}{h}}.$$

Since $\lim_{h\to 0} h\ln\left(\int_{B(x_0,r)} e^{-\frac{2f}{h}}\,dx\right) = -2f(x_0)$, we get (B.247).

Now, for the first term in (B.246), using (B.247), we have for any $\delta > 0$, for h small enough,

$$\begin{aligned}Z_h(\Omega)^{-1}\left|\int_{\Omega\setminus K_\alpha} w_h\, \tilde{u}_h\, e^{-\frac{2}{h}f}\right| &\le \|F\|_{L^\infty}\, e^{\frac{\delta}{h}}\, e^{-\frac{2}{h}\left(\inf_{\Omega\setminus K_\alpha} f - f(x_0)\right)}\\ &= \|F\|_{L^\infty}\, e^{\frac{\delta}{h}}\, e^{-\frac{2}{h}(\alpha - f(x_0))}\end{aligned}$$

and thus, thanks to (B.241), by choosing δ small enough, there exists $c > 0$ such that, for all h small enough,

$$Z_h(\Omega)^{-1}\left|\int_{\Omega\setminus K_\alpha} w_h\, \tilde{u}_h\, e^{-\frac{2}{h}f}\right| \le \|F\|_{L^\infty}\, e^{-\frac{2}{h}(f(z_i) - f(z_1) + c)}. \quad \text{(B.248)}$$

In order to estimate the second term in (B.246), we need a leveling property for w_h.

Lemma B.69. *Let us assume that **[H1]**, **[H2]** and **[H3]** hold, as well as* (B.241)*. Let us consider w_h solution to* (B.245)*. Then there exists $C > 0$ such that for any $\delta > 0$, for any h small enough, for all $x, y \in K_\alpha$,*

$$|w_h(x) - w_h(y)| \leq C\, e^{\frac{\delta}{h}}\, e^{-\frac{2}{h}(f(z_1)-\alpha)}.$$

Proof. From [21, Theorem 1], it is known that for any $\delta > 0$, for any h small enough and for all $x, y \in K_\alpha$,

$$|w_h(x) - w_h(y)| \leq C\, e^{\frac{\delta}{h}}\, e^{-\frac{2}{h}V_\Omega(K_\alpha)},$$

where $V_\Omega(K_\alpha)$ is defined by,

$$V_\Omega(K_\alpha) = \inf_{x\in K_\alpha} \inf_{T>0} \inf_{\gamma\in \mathrm{Abs}(T,x,\partial\Omega)} \frac{1}{4}\int_0^T |\dot\gamma + \nabla f(\gamma)|^2\, dt$$

where $\mathrm{Abs}(T, x, \partial\Omega)$ is the set of absolutely continuous functions $\gamma : [0, T] \to \overline{\Omega}$ satisfying $\gamma(0) = x$ and $\gamma(T) \in \partial\Omega$. For any $\gamma \in \mathrm{Abs}(T, x, \partial\Omega)$, we have

$$\int_0^T |\dot\gamma + \nabla f(\gamma)|^2 dt - \int_0^T |\dot\gamma - \nabla f(\gamma)|^2 dt = 4\int_0^T \dot\gamma \cdot \nabla f(\gamma) dt = 4\left(f(\gamma(T)) - f(x)\right),$$

and therefore, it holds

$$\int_0^T |\dot\gamma + \nabla f(\gamma)|^2 dt \geq 4\left(f(\gamma(T)) - f(x)\right) \geq 4\left(f(z_1) - f(x)\right).$$

Finally we obtain

$$V_\Omega(K_\alpha) \geq f(z_1) - \max_{x\in K_\alpha} f(x) = f(z_1) - \alpha.$$

This concludes the proof of Lemma B.69. ∎

We are now in position to estimate the second term in (B.246). Using Lemma B.69, we get, for any $\delta > 0$, in the limit $h \to 0$, uniformly in $y_0 \in K_\alpha$,

$$Z_h^{-1}(\Omega)\left(\int_{K_\alpha} w_h\, \tilde u_h\, e^{-\frac{2}{h}f} dx\right) = w_h(y_0)\frac{Z_h(K_\alpha)}{Z_h(\Omega)} + O\left(e^{\frac{\delta}{h}}\, e^{-\frac{2}{h}(f(z_1)-\alpha)}\right)\frac{Z_h(K_\alpha)}{Z_h(\Omega)}.$$

Therefore, by choosing $\delta > 0$ small enough, thanks to (B.241), there exists $c > 0$ such that, in the limit $h \to 0$,

$$Z_h^{-1}(\Omega)\left(\int_{K_\alpha} w_h\, \tilde u_h\, e^{-\frac{2}{h}f} dx\right) = w_h(y_0)\frac{Z_h(K_\alpha)}{Z_h(\Omega)} + O\left(e^{-\frac{2}{h}(f(z_i)-f(z_1)+c)}\right)\frac{Z_h(K_\alpha)}{Z_h(\Omega)}. \tag{B.249}$$

In addition we have $\frac{Z_h(K_\alpha)}{Z_h(\Omega)} = 1 + O\left(e^{-\frac{c}{h}}\right)$ for some $c > 0$ independent of h. Indeed $\frac{Z_h(K_\alpha)}{Z_h(\Omega)} = 1 - \frac{Z_h(\Omega\setminus K_\alpha)}{Z_h(\Omega)}$ and using (B.247), we get for any $\delta > 0$,

$$\frac{Z_h(\Omega\setminus K_\alpha)}{Z_h(\Omega)} \leq e^{\frac{\delta}{h}}\, e^{-\frac{2}{h}\left(\min_{\Omega\setminus K_\alpha} f - f(x_0)\right)} = O\left(e^{-\frac{c}{h}}\right), \tag{B.250}$$

for some $c > 0$ independent of h by choosing δ small enough. Gathering the results (B.248)–(B.249)–(B.250) in (B.246), there exists $c > 0$ independent of h such that, in the limit $h \to 0$, it holds: uniformly in $y_0 \in K_\alpha$,

$$\mathbb{E}^{\nu_h}[F(X_{\tau_\Omega})] = w_h(y_0)\left(1 + O\left(e^{-\frac{c}{h}}\right)\right) + O\left(e^{-\frac{2}{h}(f(z_i)-f(z_1)+c)}\right).$$

Let $i \in \{1, \dots, n\}$ and let us assume that $\operatorname{supp} F \subset B_{z_i}$ and $z_i \in \operatorname{int}(\operatorname{supp} F)$. Then, combining the last estimate with (B.240) implies that uniformly in $x \in f^{-1}((-\infty, \alpha]) \cap \Omega$, in the limit $h \to 0$:

$$\mathbb{E}^x[F(X_{\tau_\Omega})] = \frac{\partial_n f(z_i)}{\sqrt{\det \operatorname{Hess} f_{|\partial\Omega}(z_i)}} \left(\sum_{k=1}^{n_0} \frac{\partial_n f(z_k)}{\sqrt{\det \operatorname{Hess} f_{|\partial\Omega}(z_k)}}\right)^{-1} e^{-\frac{2}{h}(f(z_i)-f(z_1))}(F(z_i)+O(h)). \tag{B.251}$$

Let $\Sigma_i \subset \partial\Omega$ containing z_i and such that $\overline{\Sigma}_i \subset B_{z_i}$. Then, there exit $F, G \in C^\infty(\partial\Omega)$ such that $\operatorname{supp} F \subset B_{z_i}$, $z_i \in \operatorname{int}(\operatorname{supp} F)$, $\operatorname{supp} G \subset B_{z_i}$, $z_i \in \operatorname{int}(\operatorname{supp} G)$, $F \le 1_{\Sigma_i} \le G$ and $F(z_i) = G(z_i) = 1$. From the inequality

$$\mathbb{E}^x[F(X_{\tau_\Omega})] \le \mathbb{P}^x[X_{\tau_\Omega} \in \Sigma_i] \le \mathbb{E}^x[G(X_{\tau_\Omega})],$$

together with (B.251) applied to F and G, one gets in the limit $h \to 0$:

$$\mathbb{P}^x[X_{\tau_\Omega} \in \Sigma_i] = \frac{\partial_n f(z_i)}{\sqrt{\det \operatorname{Hess} f_{|\partial\Omega}(z_i)}} \left(\sum_{k=1}^{n_0} \frac{\partial_n f(z_k)}{\sqrt{\det \operatorname{Hess} f_{|\partial\Omega}(z_k)}}\right)^{-1} e^{-\frac{2}{h}(f(z_i)-f(z_1))}(1+O(h)).$$

This concludes the proof of Corollary B.10.

B.5.2 Proofs of Theorem B.2 and Corollary B.11

In this section, we prove Theorem B.2. The proof is similar to the one made for Theorem B.1: the estimates of Proposition B.17 and the construction of the quasi-mode associated with z_{j_0} are modified. The proof of Theorem B.2 is organized as follows. In Section B.5.2.1, we give the estimates required for the $n+1$ quasi-modes. Then, in Section B.5.2.2, we prove that these estimates imply Theorem B.2. In Section B.5.2.3, the construction of the quasi-modes is given and we check that they satisfy the estimates stated in Section B.5.2.1.

B.5.2.1 Statement of the assumptions required for the quasi-modes

For the ease of notation, for $p \in \{0, 1\}$, the orthogonal projector $\pi_{[0, \frac{\sqrt{h}}{2})}\left(-L_{f,h}^{D,(p)}(\Omega)\right)$ is still denoted by $\pi_h^{(p)}$, see (B.54).

The next proposition gives the assumption we need on the quasi-modes $(\tilde{\psi}_i)_{i=1,\dots,n}$ whose span approximates $\operatorname{Ran} \pi_h^{(1)}$, and $\tilde{u}$ whose span approximates $\operatorname{Ran} \pi_h^{(0)}$, in order to prove Theorem B.2. It is the equivalent of Proposition B.17 in the more general setting of Theorem B.2.

Proposition B.70. *Let us assume that the hypotheses **[H1]**, **[H2]** and **[H3]** hold. Let Σ_i denotes an open set included in $\partial\Omega$ containing z_i ($i \in \{1,\dots,n\}$) and such that $\overline{\Sigma}_i \subset B_{z_i}$. Let $k_0 \in \{1,\dots,n\}$ and f^* such that*

$$f(z_{k_0}) \leq f^* \leq f(z_{k_0+1}),$$

(with the convention $f(z_{k_0+1}) = +\infty$ if $k_0 = n$). Finally, let $\Sigma \subset \partial\Omega$ be a smooth open set such that $\overline{\Sigma} \subset B_{z_{j_0}}$, for some $j_0 \in \{1,\dots,k_0\}$ and $\inf_\Sigma f = f^*$.

Let us assume that there exist n quasi-modes $(\tilde{\psi}_i)_{i=1,\dots,n}$ and a family of quasi-modes $(\tilde{u} = \tilde{u}_\delta)_{\delta>0}$ satisfying the following conditions:

1. *$\forall i \in \{1,\dots,n\}$, $\tilde{\psi}_i \in \Lambda^1 H^1_{w,T}(\Omega)$ and $\tilde{u} \in \Lambda^0 H^1_{w,T}(\Omega)$. The function $\tilde{u}$ is non negative in Ω. Moreover, $\forall i \in \{1,\dots,n\}$, $\left\|\tilde{\psi}_i\right\|_{L^2_w} = \|\tilde{u}\|_{L^2_w} = 1$.*

2. *(a) There exists $\varepsilon_1 > 0$ such that for all $i \in \{1,\dots,k_0\}$, it holds in the limit $h \to 0$:*

$$\left\|\left(1-\pi_h^{(1)}\right)\tilde{\psi}_i\right\|^2_{H^1_w} = O\left(e^{-\frac{2}{h}(\max[f^*-f(z_i),f(z_i)-f(z_1)]+\varepsilon_1)}\right),$$

and for all $i \in \{k_0+1,\dots,n\}$, $\left\|\left(1-\pi_h^{(1)}\right)\tilde{\psi}_i\right\|^2_{H^1_w} = O\left(e^{-\frac{2}{h}(f^*-f(z_1)+\varepsilon_1)}\right)$.

(b) For any $\delta > 0$, $\|\nabla\tilde{u}\|^2_{L^2_w} = O\left(e^{-\frac{2}{h}(f(z_1)-f(x_0)-\delta)}\right)$.

3. *There exists $\varepsilon_0 > 0$, $\forall (i,j) \in \{1,\dots,n\}^2$, if $i < j \leq k_0$ in the limit $h \to 0$:*

$$\left\langle \tilde{\psi}_i, \tilde{\psi}_j \right\rangle_{L^2_w} = O\left(e^{-\frac{1}{h}(f(z_j)-f(z_i)+\varepsilon_0)}\right),$$

and if $k_0 < j$, $i < j$, in the limit $h \to 0$:

$$\left\langle \tilde{\psi}_i, \tilde{\psi}_j \right\rangle_{L^2_w} = O\left(e^{-\frac{1}{h}(f^*-f(z_1)+\varepsilon_0)}\right).$$

4. *(a) There exists $\varepsilon' > 0$ and there exist constants $(C_i)_{i=1,\dots,n}$ and p which do not depend on h such that for $i \in \{1,\dots,k_0\}$, in the limit $h \to 0$:*

$$\left\langle \nabla\tilde{u}, \tilde{\psi}_i \right\rangle_{L^2_w} = C_i\ h^p e^{-\frac{1}{h}(f(z_i)-f(x_0))}\,(1+O(h)),$$

and for $i \in \{k_0+1,\dots,n\}$, in the limit $h \to 0$:

$$\left\langle \nabla\tilde{u}, \tilde{\psi}_i \right\rangle_{L^2_w} = C_i\ h^p e^{-\frac{1}{h}(f(z_i)-f(x_0))}\,(1+O(h)) + O\left(e^{-\frac{1}{h}(f^*-f(x_0)+\varepsilon')}\right).$$

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

$$\int_{\Sigma_i} \tilde{\psi}_j \cdot n\, e^{-\frac{2}{h}f} d\sigma = \begin{cases} B_i\, h^m\, e^{-\frac{1}{h}f(z_i)}\ (1+O(h)) & \text{if } i = j \\ 0 & \text{if } i \neq j. \end{cases}$$

(c) *There exist C^* and p^* independent of h such that for all $i \in \{1, \dots, n\}$, in the limit $h \to 0$:*

$$\int_\Sigma \tilde{\psi}_i \cdot n\, e^{-\frac{2}{h}f} d\sigma = \delta_{j_0,i}\, C^* h^{q^*} e^{-\frac{1}{h}(2f^* - f(z_{j_0}))}(1 + O(h)).$$

Let u_h be the eigenfunction associated with the smallest eigenvalue of $-L_{f,h}^{(D),(0)}(\Omega)$ (see Proposition B.14) which satisfies (B.11)*. Then, one has:*

- *For all $i \in \{1, \dots, k_0\}$, in the limit $h \to 0$*

$$\int_{\Sigma_i} (\partial_n u_h)\, e^{-\frac{2}{h}f} d\sigma = C_i B_i h^{p+m}\, e^{-\frac{1}{h}(2f(z_i) - f(x_0))}\ (1 + O(h)).$$

  Moreover, if $f(z_{k_0}) < f(z_{k_0+1})$, there exists $\varepsilon > 0$ such that for all $i \in \{k_0 + 1, \dots, n\}$ in the limit $h \to 0$

$$\int_{\Sigma_i} (\partial_n u_h)\, e^{-\frac{2}{h}f} d\sigma = \left(\int_{\Sigma_{k_0}} (\partial_n u_h)\, e^{-\frac{2}{h}f} d\sigma \right) O\left(e^{-\frac{\varepsilon}{h}}\right).$$

- *In the limit $h \to 0$:*

$$\int_{\Sigma} (\partial_n u_h)\, e^{-\frac{2}{h}f} d\sigma = C^* C_{j_0} h^{q^*+p}\, e^{-\frac{1}{h}(2f^* - f(x_0))}\ (1 + O(h)).$$

The estimates (B.22), (B.31) and (B.34) in Theorem B.2 are a consequence of this proposition and of the construction of the appropriate quasi-modes $((\tilde{\psi}_i)_{i=1,\dots,n}, \tilde{u})$, see Section B.5.2.3, which will show that $(B_i)_{i=1,\dots,n}$, m, $(C_i)_{i=1,\dots,n}$, p are given by (B.231)-(B.235) and C^*, q^* are given by Lemma B.77. Moreover, the remainder estimates (B.24), (B.32) and (B.35) in Theorem B.2 are a consequence of the asymptotics (B.22), (B.31) and (B.34) together with Proposition B.6, Proposition B.7 and (B.14).

B.5.2.2 Proof of Proposition B.70

The proof of Proposition B.70 follows closely the same steps as the proof of Proposition B.17. We only highlight the main differences. In all this section, we assume that the hypotheses **[H1]**, **[H2]** and **[H3]** hold. Let $f^* \in \mathbb{R}$, $k_0 \in \{1, \dots, n\}$, $j_0 \in \{1, \dots, k_0\}$, $(\Sigma_i)_{i \in \{1,\dots,n\}}$ and Σ be as stated in Proposition B.70. In addition, let us assume the existence of $n+1$ quasi-modes $(\tilde{u}, (\tilde{\psi}_i)_{i=1,\dots,n})$ satisfying all the conditions of Proposition B.70. In the following, ε denotes a positive constant independent of h, smaller than $\min(\varepsilon_1, \varepsilon_0, \varepsilon')$, and whose precise value may vary (a finite number of times) from one occurence to the other.

Let us recall a result relating $\tilde{u}$ with u_h on the one hand, and span $\left(\tilde{\psi}_j, j = 1, \dots, n\right)$ with $\operatorname{Ran} \pi_h^{(1)}$ on the other hand. The following lemma is a direct consequence of Lemma B.18, Lemma B.19 and the assumptions 1, 2 and 3 of Proposition B.70.

Lemma B.71. *Let us assume that the assumptions of Proposition B.70 hold. Then, there exist $c > 0$ and $h_0 > 0$ such that for $h \in (0, h_0)$,*

$$\left\| \pi_h^{(0)} \tilde{u} \right\|_{L^2_w} = 1 + O\left(e^{-\frac{c}{h}}\right).$$

In addition, there exists $h_0 > 0$ such that for all $h \in (0, h_0)$,

$$\operatorname{span}\left(\pi_h^{(1)} \tilde{\psi}_i,\, i = 1, \ldots, n\right) = \operatorname{Ran} \pi_h^{(1)}.$$

A direct consequence of Lemma B.71 and the fact that $\tilde{u}$ is non negative in Ω is that it holds for h small enough:

$$u_h = \frac{\pi_h^{(0)} \tilde{u}}{\left\| \pi_h^{(0)} \tilde{u} \right\|_{L^2_w}}. \tag{B.252}$$

Let us denote by $(\psi_i)_{i=1,\ldots,n}$ the orthonormal basis of $\operatorname{Ran} \pi_h^{(1)}$ resulting from the Gram-Schmidt orthonormalization procedure on the set $(\pi_h^{(1)} \tilde{\psi}_i)_{i=1,\ldots,n}$ (see Lemma B.20). Then, since $\nabla u_h \in \operatorname{Ran}\left(\pi_h^{(1)}\right) = \operatorname{span}(\psi_j, j = 1, \ldots, n)$ (see (B.53)) and $\langle \psi_j, \psi_i \rangle_{L^2_w} = \delta_{i,j}$, one has for any $\Gamma \subset \partial\Omega$

$$\int_\Gamma (\partial_n u_h)\, e^{-\frac{2}{h} f} d\sigma = \sum_{j=1}^n \langle \nabla u_h, \psi_j \rangle_{L^2_w} \int_\Gamma \psi_j \cdot n\, e^{-\frac{2}{h} f} d\sigma. \tag{B.253}$$

Let $(\kappa_{ji})_{(i,j) \in \{1,\ldots,n\}^2,\, i<j}$ and $(Z_j)_{j \in \{1,\ldots,n\}}$ be the matrix and vector obtained through the Gram-Schimdt othonormalization procedure, see Lemma B.20.

Now, to prove Proposition B.70, the strategy consists in proving precise estimates when $h \to 0$, of the terms

$$\kappa_{ji},\ Z_j,\ \langle \nabla u_h, \psi_j \rangle_{L^2_w} \text{ and } \left(\int_\Gamma \psi_j \cdot n\, e^{-\frac{2}{h} f} d\sigma \right)_{\Gamma \in \{\Sigma, \Sigma_1, \ldots, \Sigma_n\}}$$

for $(i, j) \in \{1, \ldots, n\}^2$, $i < j$. Then, they will be used to obtain a precise estimate of (B.253) when $h \to 0$. This is the purpose of the next steps.

<u>Step 1.</u> Estimates on the terms $(\kappa_{ji})_{(i,j) \in \{1,\ldots,n\}^2,\, i<j}$ and of $(Z_i)_{i \in \{1,\ldots,n\}}$.

Lemma B.72. *Let us assume that the assumptions of Proposition B.70 hold. Then, there exist $\varepsilon > 0$ and $h_0 > 0$ such that for all $(i, j) \in \{1, \ldots, n\}^2$ with $i < j$ and all $h \in (0, h_0)$, if $j \leq k_0$:*

$$\left\langle \pi_h^{(1)} \tilde{\psi}_i, \pi_h^{(1)} \tilde{\psi}_j \right\rangle_{L^2_w} = O\left(e^{-\frac{1}{h}(f(z_j) - f(z_i) + \varepsilon)}\right),$$

and if $j > k_0$:

$$\left\langle \pi_h^{(1)} \tilde{\psi}_i, \pi_h^{(1)} \tilde{\psi}_j \right\rangle_{L^2_w} = O\left(e^{-\frac{1}{h}(f^* - f(z_1) + \varepsilon)}\right).$$

Proof. The proof follows the same lines as the proof of Lemma B.21. If $i < j$ and $j \leq k_0$, from assumption 2(a) in Proposition B.70 and since $f^* \geq f(z_1)$, one gets

$$\begin{aligned}\left\langle (1-\pi_h^{(1)})\tilde{\psi}_i, (1-\pi_h^{(1)})\tilde{\psi}_j \right\rangle_{L^2_w} &\leq \|(1-\pi_h^{(1)})\tilde{\psi}_i\|_{L^2_w} \|(1-\pi_h^{(1)})\tilde{\psi}_j\|_{L^2_w} \\ &\leq O\left(e^{-\frac{1}{h}(f^*-f(z_i)+f(z_j)-f(z_1)+\varepsilon)}\right) = O\left(e^{-\frac{1}{h}(f(z_j)-f(z_i)+\varepsilon)}\right).\end{aligned}$$

If $i < j$ and $k_0 < j$, from assumptions 1 and 2(a) in Proposition B.70, one gets

$$\left\langle (1-\pi_h^{(1)})\tilde{\psi}_i, (1-\pi_h^{(1)})\pi_h^{(1)}\tilde{\psi}_j \right\rangle_{L^2_w} \leq \|\tilde{\psi}_i\|_{L^2_w} \|(1-\pi_h^{(1)})\tilde{\psi}_j\|_{L^2_w} \leq O\left(e^{-\frac{1}{h}(f^*-f(z_1)+\varepsilon)}\right).$$

Lemma B.72 is then a consequence of (C.130) together with assumption 3 in Proposition B.70. ∎

Lemma B.73. *Let us assume that the assumptions of Proposition B.70 hold. Then, there exist $\varepsilon > 0$ and $h_0 > 0$ such that for all $(i,j) \in \{1,\dots,n\}^2$ with $i < j$ and all $h \in (0,h_0)$, if $j \leq k_0$:*

$$\kappa_{ji} = O\left(e^{-\frac{1}{h}(f(z_j)-f(z_i)+\varepsilon)}\right),$$

and if $j > k_0$:

$$\kappa_{ji} = O\left(e^{-\frac{1}{h}(f^*-f(z_1)+\varepsilon)}\right).$$

In addition, there exist $c > 0$ and $h_0 > 0$ such that for all $j \in \{1,\dots,n\}$ and $h \in (0,h_0)$,

$$Z_j = 1 + O\left(e^{-\frac{c}{h}}\right).$$

Proof. If $i < j$ and $j \leq k_0$, the estimates on κ_{ji} and Z_j are proved by induction as in the proof of Lemma B.22. Let us now deal with the case $i < j$ and $k_0 < j$. For $j = k_0 + 1$, it follows from (B.66) that for all $i < k_0 + 1$,

$$\kappa_{(k_0+1)i} = -\sum_{k=i}^{k_0}\sum_{l=1}^{k} \frac{1}{Z_k^2} \langle \pi_h^{(1)}\tilde{\psi}_{k_0+1}, \pi_h^{(1)}\tilde{\psi}_l\rangle_{L^2_w}\ \kappa_{kl}\kappa_{ki},$$

where we use the notation $\kappa_{ii} = 1$ for every $i \in \{1,\dots,n\}$. Since $1 \leq k \leq k_0$, one has $Z_k^{-1} = 1 + O\left(e^{-\frac{c}{h}}\right)$. In addition, since $1 \leq l \leq k \leq k_0$ and $1 \leq i \leq k \leq k_0$, one has $\kappa_{kl}\kappa_{ki} = O(1)$. From Lemma B.72, one has for $1 \leq l < k_0 + 1$, $\langle \pi_h^{(1)}\tilde{\psi}_{k_0+1}, \pi_h^{(1)}\tilde{\psi}_l\rangle_{L^2_w} = O\left(e^{-\frac{1}{h}(f^*-f(z_1)+\varepsilon)}\right)$. Therefore, one obtains for all $i < k_0 + 1$,

$$\kappa_{(k_0+1)i} = O\left(e^{-\frac{1}{h}(f^*-f(z_1)+\varepsilon)}\right).$$

The fact that $Z_{k_0+1} = 1 + O\left(e^{-\frac{c}{h}}\right)$, comes from the fact that the terms $(\kappa_{(k_0+1)i})_{i\in\{1,\dots,k_0\}}$ are exponentially small and the fact that $\left\|\pi_h^{(1)}\tilde{\psi}_{k_0+1}\right\|_{L^2_w} = 1 + O\left(e^{-\frac{c}{h}}\right)$. In order to prove by induction the estimates on κ_{ji} for $i < j$ and $j > k_0$, let us now assume that for some $k \in \{k_0+1,\dots,n\}$ and for all $j \in \{k_0+1,\dots,k\}$, $i \in \{1,\dots,j-1\}$,

$$\kappa_{ji} = O\left(e^{-\frac{1}{h}(f^*-f(z_1)+\varepsilon)}\right) \text{ and } Z_j = 1 + O\left(e^{-\frac{c}{h}}\right).$$

It follows from (B.66), for $q \in \{1, \dots, k\}$,

$$\kappa_{(k+1)q} = -\sum_{j=q}^{k} \sum_{l=1}^{j} \frac{1}{Z_j^2} \langle \pi_h^{(1)} \tilde{\psi}_{k+1}, \pi_h^{(1)} \tilde{\psi}_l \rangle_{L^2_w} \ \kappa_{jl} \kappa_{jq},$$

where we used the notation $\kappa_{ii} = 1$. Since $1 \leq j \leq k$, one has $Z_j^{-1} = 1 + O\left(e^{-\frac{c}{h}}\right)$. In addition, since $1 \leq l \leq j \leq k$ and $1 \leq q \leq j \leq k$, one has $\kappa_{jl}\kappa_{jq} = O(1)$. From Lemma B.72, one has for $1 \leq l < k+1$ and $k > k_0$, $\langle \pi_h^{(1)} \tilde{\psi}_{k+1}, \pi_h^{(1)} \tilde{\psi}_l \rangle_{L^2_w} = O\left(e^{-\frac{1}{h}(f^* - f(z_1) + \varepsilon)}\right)$. Therefore, one obtains for all $1 \leq q < k+1$,

$$\kappa_{(k+1)q} = O\left(e^{-\frac{1}{h}(f^* - f(z_1) + \varepsilon)}\right).$$

The fact that $Z_{k+1} = 1 + O\left(e^{-\frac{c}{h}}\right)$, comes from the fact that the $(\kappa_{(k+1)q})_{q \in \{1,\dots,k\}}$ are exponentially small and the fact that $\left\| \pi_h^{(1)} \tilde{\psi}_{k+1} \right\|_{L^2_w} = 1 + O\left(e^{-\frac{c}{h}}\right)$. This concludes the proof by induction. ∎

<u>Step 2.</u> Estimates on the interaction terms $(\langle \nabla u_h, \psi_j \rangle_{L^2_w})_{j \in \{1,\dots,n\}}$.

Lemma B.74. *Let us assume that the assumptions of Proposition B.70 hold. Then, for $j \in \{1, \dots, k_0\}$, in the limit $h \to 0$:*

$$\langle \nabla u_h, \psi_j \rangle_{L^2_w} = C_j \ h^p e^{-\frac{1}{h}(f(z_j) - f(x_0))} \left(1 + O(h)\right),$$

and for $j \in \{k_0 + 1, \dots, n\}$, there exists $\varepsilon' > 0$ such that in the limit $h \to 0$:

$$\langle \nabla u_h, \psi_j \rangle_{L^2_w} = C_j \ h^p e^{-\frac{1}{h}(f(z_j) - f(x_0))} \left(1 + O(h)\right) + O\left(e^{-\frac{1}{h}(f^* - f(x_0) + \varepsilon')}\right).$$

Proof. For $j \in \{1, \dots, k_0\}$, the proof of the estimate of $\langle \nabla u_h, \psi_j \rangle_{L^2_w}$ is exactly the same as for Lemma B.23. Let $j \in \{k_0 + 1, \dots, n\}$. Using (B.67)–(B.61)–(B.64)–(B.65), one has

$$\langle \nabla u_h, \psi_j \rangle_{L^2_w} = a_j + b_j + c_j,$$

where a_j, b_j and c_j are defined by

$$a_j = \frac{Z_j^{-1}}{\left\| \pi_h^{(0)} \tilde{u} \right\|_{L^2_w}} \left(\left\langle \nabla \tilde{u}, \tilde{\psi}_j \right\rangle_{L^2_w} + \left\langle \nabla \tilde{u}, \left(\pi_h^{(1)} - 1\right) \tilde{\psi}_j \right\rangle_{L^2_w} \right),$$

$$b_j = \frac{Z_j^{-1}}{\left\| \pi_h^{(0)} \tilde{u} \right\|_{L^2_w}} \sum_{i=1}^{k_0} \kappa_{ji} \ \left(\left\langle \nabla \tilde{u}, \tilde{\psi}_i \right\rangle_{L^2_w} + \left\langle \nabla \tilde{u}, \left(\pi_h^{(1)} - 1\right) \tilde{\psi}_i \right\rangle_{L^2_w} \right) \ ,$$

and

$$c_j = \frac{Z_j^{-1}}{\left\| \pi_h^{(0)} \tilde{u} \right\|_{L^2_w}} \sum_{i=k_0+1}^{j-1} \kappa_{ji} \ \left(\left\langle \nabla \tilde{u}, \tilde{\psi}_i \right\rangle_{L^2_w} + \left\langle \nabla \tilde{u}, \left(\pi_h^{(1)} - 1\right) \tilde{\psi}_i \right\rangle_{L^2_w} \right) \ ,$$

with the convention $\sum_{i=k_0+1}^{k_0} = 0$. From Lemmata B.71 and B.73, one has $\frac{Z_j^{-1}}{\left\|\pi_h^{(0)}\tilde{u}\right\|_{L^2_w}} = 1+O\left(e^{-\frac{c}{h}}\right)$. Using assumptions 2 and 4(a) in Proposition B.70 and Lemma B.73, there exists $\delta_0 > 0$ such that for all $\delta \in (0, \delta_0)$,

$$
\begin{aligned}
a_j &= C_j h^p e^{-\frac{1}{h}(f(z_j)-f(x_0))}(1+O(h)) + O\left(e^{-\frac{1}{h}(f^*-f(x_0)+\varepsilon)}\right) + O\left(e^{-\frac{1}{h}(f^*-f(x_0)-\delta+\varepsilon)}\right),\\
b_j &= \sum_{i=1}^{k_0} O\left(e^{-\frac{1}{h}(f^*-f(z_1)+\varepsilon+f(z_i)-f(x_0)-\delta)}\right) + O\left(e^{-\frac{1}{h}(f^*-f(z_1)+\varepsilon+f(z_1)-f(x_0)-\delta+f(z_i)-f(z_1)+\varepsilon)}\right)\\
&= O\left(e^{-\frac{1}{h}(f^*-f(x_0)-\delta+\varepsilon)}\right),\\
c_j &= \sum_{i=k_0+1}^{j-1} O\left(e^{-\frac{1}{h}(f^*-f(z_1)+\varepsilon)}\right)\left(O\left(e^{-\frac{1}{h}(f(z_i)-f(x_0)-\delta)}\right) + O\left(e^{-\frac{1}{h}(f^*-f(x_0)+\varepsilon)}\right)\right)\\
&\quad + O\left(e^{-\frac{1}{h}(f^*-f(z_1)+\varepsilon+f(z_1)-f(x_0)-\delta+f^*-f(z_1)+\varepsilon)}\right) = O\left(e^{-\frac{1}{h}(f^*-f(x_0)-\delta+\varepsilon)}\right).
\end{aligned}
$$

Therefore, choosing $\delta \in (0, \varepsilon)$, there exists $\varepsilon' > 0$ such that

$$
\langle \nabla u_h, \psi_j \rangle_{L^2_w} = C_j h^p e^{-\frac{1}{h}(f(z_j)-f(x_0))}(1+O(h)) + O\left(e^{-\frac{1}{h}(f^*-f(x_0)+\varepsilon')}\right).
$$

This concludes the proof of Lemma B.74. ∎

Step 3. Estimates on the boundary terms $\left(\int_\Gamma \psi_j \cdot n\, e^{-\frac{2}{h}f} d\sigma\right)_{j\in\{1,\dots,n\},\Gamma\in\{\Sigma,\Sigma_1,\dots,\Sigma_n\}}$.

Lemma B.75. *Let us assume that the assumptions of Proposition B.70 hold. Then, there exists $\varepsilon > 0$ such that in the limit $h \to 0$ one has:*

- *If $k \in \{1, \dots, k_0\}$ and $j \in \{1, \dots, k_0\}$,*

$$
\begin{aligned}
\int_{\Sigma_k} \psi_j \cdot n\, e^{-\frac{2}{h}f} d\sigma &= \delta_{j,k} B_k h^m e^{-\frac{1}{h}f(z_k)}(1+O(h)) + O\left(e^{-\frac{1}{h}(2f(z_k)-f(z_j)+\varepsilon)}\right)\\
&\quad + 1_{j>k} O\left(e^{-\frac{1}{h}(f(z_k)+\varepsilon)}\right).
\end{aligned}
$$

- *If $k \in \{1, \dots, k_0\}$ and $j \in \{k_0+1, \dots, n\}$,* $\int_{\Sigma_k} \psi_j \cdot n\, e^{-\frac{2}{h}f} d\sigma = O\left(e^{-\frac{1}{h}(f(z_k)+\varepsilon)}\right)$.

- *If $k \in \{k_0+1, \dots, n\}$ and $j \in \{1, \dots, k_0\}$,* $\int_{\Sigma_k} \psi_j \cdot n\, e^{-\frac{2}{h}f} d\sigma = O\left(e^{-\frac{1}{h}(2f(z_{k_0})-f(z_j)+\varepsilon)}\right)$

- *If $k \in \{k_0+1, \dots, n\}$ and $j \in \{k_0+1, \dots, n\}$,*

$$
\int_{\Sigma_k} \psi_j \cdot n\ e^{-\frac{2}{h}f} d\sigma = \delta_{j,k} O\left(h^m e^{-\frac{1}{h}f(z_k)}\right) + O\left(e^{-\frac{1}{h}(f(z_{k_0+1})+\varepsilon)}\right).
$$

Proof. For all $(j,k) \in \{1,\dots,n\}^2$, using (B.64)–(B.65) and Lemmata B.73 and B.71 together with assumption 4(b) in Proposition B.70, one has in the limit $h \to 0$:

$$\begin{aligned}\int_{\Sigma_k} \psi_j \cdot n\ e^{-\frac{2}{h}f} d\sigma &= Z_j^{-1}\left[\int_{\Sigma_k} \tilde{\psi}_j \cdot n\ e^{-\frac{2}{h}f} d\sigma + \int_{\Sigma_k} (\pi_h^{(1)} - 1)\tilde{\psi}_j \cdot n\ e^{-\frac{2}{h}f} d\sigma\right] \\ &\quad + Z_j^{-1} \sum_{i=1}^{j-1} \kappa_{ji}\ \left(\int_{\Sigma_k} \tilde{\psi}_i \cdot n\ e^{-\frac{2}{h}f} d\sigma + \int_{\Sigma_k} (\pi_h^{(1)} - 1)\tilde{\psi}_i \cdot n\ e^{-\frac{2}{h}f} d\sigma\right) \\ &= \delta_{j,k} B_k h^m e^{-\frac{1}{h}f(z_k)}(1 + O(h)) + \frac{1}{h}\left\|\left(1 - \pi_h^{(1)}\right)\tilde{\psi}_j\right\|_{H_w^1} O\left(e^{-\frac{1}{h}f(z_k)}\right) \\ &\quad + \sum_{i=1}^{j-1} \kappa_{ji}\delta_{i,k} O\left(h^m e^{-\frac{1}{h}f(z_k)}\right) + \frac{\kappa_{ji}}{h}\left\|\left(1 - \pi_h^{(1)}\right)\tilde{\psi}_i\right\|_{H_w^1} O\left(e^{-\frac{1}{h}f(z_k)}\right).\end{aligned} \tag{B.254}$$

Let us know deal separately with the two cases $k \in \{1,\dots,k_0\}$ and $k \in \{k_0+1,\dots,n\}$. In the following, we use assumption 2(a) in Proposition B.70 and Lemma B.73 to estimate (B.254).

Case 1: $k \in \{1,\dots,k_0\}$. If $j \in \{1,\dots,k_0\}$, from (B.254), one gets in the limit $h \to 0$:

$$\begin{aligned}\int_{\Sigma_k} \psi_j \cdot n\ e^{-\frac{2}{h}f} d\sigma &= \delta_{j,k} B_k h^m e^{-\frac{1}{h}f(z_k)}(1 + O(h)) + O\left(e^{-\frac{1}{h}(f^* - f(z_j) + f(z_k) + \varepsilon)}\right) \\ &\quad + \sum_{i=1}^{j-1} \delta_{i,k} O\left(e^{-\frac{1}{h}(f(z_k)+\varepsilon)}\right) + \sum_{i=1}^{j-1} O\left(e^{-\frac{1}{h}(f(z_j) - f(z_i) + f^* - f(z_i) + f(z_k) + \varepsilon)}\right).\end{aligned}$$

Since $f^* \geq f(z_k)$ for all $k \in \{1,\dots,k_0\}$ and since there exists $i < j$ such that $\delta_{i,k} = 1$ if and only if $j > k$, there exists $\varepsilon > 0$ such that for all $(k,j) \in \{1,\dots,k_0\}^2$ and for all h small enough,

$$\int_{\Sigma_k} \psi_j \cdot n\, e^{-\frac{2}{h}f} d\sigma = \delta_{j,k} B_k h^m e^{-\frac{1}{h}f(z_k)}(1 + O(h)) + O\left(e^{-\frac{1}{h}(2f(z_k) - f(z_j) + \varepsilon)}\right) + 1_{j>k} O\left(e^{-\frac{1}{h}(f(z_k)+\varepsilon)}\right).$$

If $j \in \{k_0+1,\dots,n\}$, from (B.254), one gets

$$\int_{\Sigma_k} \psi_j \cdot n\ e^{-\frac{2}{h}f} d\sigma = O\left(e^{-\frac{1}{h}(f^* - f(z_1) + f(z_k) + \varepsilon)}\right) + \sum_{i=1}^{j-1} O\left(e^{-\frac{1}{h}(f(z_k)+\varepsilon)}\right).$$

Case 2: $k \in \{k_0+1,\dots,n\}$. If $j \in \{1,\dots,k_0\}$, from (B.254) and since $f(z_k) \geq f^* \geq f(z_{k_0})$, one has

$$\begin{aligned}\int_{\Sigma_k} \psi_j \cdot n\ e^{-\frac{2}{h}f} d\sigma &= O\left(e^{-\frac{1}{h}(f^* - f(z_j) + \varepsilon + f(z_k))}\right) + \sum_{i=1}^{j-1} O\left(e^{-\frac{1}{h}(f^* + f(z_k) + f(z_j) - 2f(z_i) + \varepsilon)}\right) \\ &= O\left(e^{-\frac{1}{h}(2f(z_{k_0}) - f(z_j) + \varepsilon)}\right).\end{aligned}$$

If $j \in \{k_0+1,\dots,n\}$, from (B.254), one gets

$$\int_{\Sigma_k} \psi_j \cdot n\ e^{-\frac{2}{h}f} d\sigma = \delta_{j,k} O\left(h^m e^{-\frac{1}{h}f(z_k)}\right) + O\left(e^{-\frac{1}{h}(f(z_k)+\varepsilon)}\right),$$

which leads to the desired estimate since $f(z_k) \geq f(z_{k_0+1})$. This concludes the proof of Lemma B.75. ∎

Lemma B.76. *Let us assume that the assumptions of Proposition B.70 hold. Then, for $j \in \{1, \dots, k_0\}$ one has when $h \to 0$:*

$$\int_\Sigma \psi_j \cdot n\, e^{-\frac{2}{h}f} d\sigma = \delta_{j_0,j}\, C^* h^{q^*} e^{-\frac{1}{h}(2f^* - f(z_{j_0}))}\,(1 + O(h)) + O\left(e^{-\frac{1}{h}(2f^* - f(z_j) + \varepsilon)}\right)$$

and for $j \in \{k_0 + 1, \dots, n\}$ one has $\displaystyle\int_\Sigma \psi_j \cdot n\, e^{-\frac{2}{h}f} d\sigma = O\left(e^{-\frac{1}{h}(2f^* - f(z_1) + \varepsilon)}\right)$.

Proof. Let $j \in \{1, \dots, n\}$. Using (B.64)–(B.65) and Lemmata B.73 and B.71 together with assumption 4(c) in Proposition B.70, one has

$$\begin{aligned}
\int_\Sigma \psi_j \cdot n\; e^{-\frac{2}{h}f} d\sigma &= Z_j^{-1} \left[\int_\Sigma \tilde{\psi}_j \cdot n\; e^{-\frac{2}{h}f} d\sigma + \int_\Sigma (\pi_h^{(1)} - 1)\tilde{\psi}_j \cdot n\; e^{-\frac{2}{h}f} d\sigma \right] \\
&\quad + Z_j^{-1} \sum_{i=1}^{j-1} \kappa_{ji} \left(\int_\Sigma \tilde{\psi}_i \cdot n\; e^{-\frac{2}{h}f} d\sigma + \int_\Sigma (\pi_h^{(1)} - 1)\tilde{\psi}_i \cdot n\; e^{-\frac{2}{h}f} d\sigma \right) \\
&= \delta_{j_0,j}\, C^* h^{q^*} e^{-\frac{1}{h}(2f^* - f(z_{j_0}))}(1 + O(h)) + \frac{1}{h} \left\| \left(1 - \pi_h^{(1)}\right) \tilde{\psi}_j \right\|_{H_w^1} O\left(e^{-\frac{1}{h}f^*}\right) \\
&\quad + \sum_{i=1}^{j-1} \delta_{j_0,i} \kappa_{ji} O\left(h^{q^*} e^{-\frac{1}{h}(2f^* - f(z_{j_0}))}\right) + \frac{\kappa_{ji}}{h} \left\| \left(1 - \pi_h^{(1)}\right) \tilde{\psi}_i \right\|_{H_w^1} O\left(e^{-\frac{1}{h}f^*}\right).
\end{aligned} \tag{B.255}$$

Let us first deal with the case $j \in \{1, \dots, k_0\}$. Using assumption 2(a) in Proposition B.70 and Lemma B.73, one gets from (B.255)

$$\begin{aligned}
\int_\Sigma \psi_j \cdot n\; e^{-\frac{2}{h}f} d\sigma &= \delta_{j_0,j}\, C^* h^{q^*} e^{-\frac{1}{h}(2f^* - f(z_{j_0}))}\,(1 + O(h)) + O\left(e^{-\frac{1}{h}(f^* - f(z_j) + \varepsilon + f^*)}\right) \\
&\quad + \sum_{i=1}^{j-1} O\left(e^{-\frac{1}{h}(2f^* + f(z_j) - 2f(z_i) + \varepsilon)}\right) \\
&= \delta_{j_0,j}\, C^* h^{q^*} e^{-\frac{1}{h}(2f^* - f(z_{j_0}))}\,(1 + O(h)) + O\left(e^{-\frac{1}{h}(2f^* - f(z_j) + \varepsilon)}\right).
\end{aligned}$$

Let us now deal with the case $j \in \{k_0+1, \dots, n\}$. In that case, one obtains from (B.255), assumption 2(a) in Proposition B.70, Lemma B.73 together with the fact that $f^* \geq f(z_i)$ for all $i \in \{1, \dots, k_0\}$ and $f^* \geq f(z_{k_0}) \geq f(z_{j_0})$,

$$\begin{aligned}
\int_\Sigma \psi_j \cdot n\; e^{-\frac{2}{h}f} d\sigma &= O\left(e^{-\frac{1}{h}(f^* - f(z_1) + \varepsilon + f^*)}\right) + \sum_{i=1}^{j-1} \delta_{j_0,i}\, O\left(e^{-\frac{1}{h}(f^* - f(z_1) + 2f^* - f(z_{j_0}) + \varepsilon)}\right) \\
&\quad + \sum_{i=1}^{k_0} O\left(e^{-\frac{1}{h}(2f^* - f(z_1) + f^* - f(z_i) + \varepsilon)}\right) + \sum_{i=k_0+1}^{j-1} O\left(e^{-\frac{1}{h}(2f^* - 2f(z_1) + \varepsilon + f^*)}\right) \\
&= O\left(e^{-\frac{1}{h}(2f^* - f(z_1) + \varepsilon)}\right).
\end{aligned}$$

This concludes the proof of Lemma B.76. ∎

Step 4. Estimates on the boundary terms $\left(\int_\Gamma (\partial_n u_h)\, e^{-\frac{2}{h}f} d\sigma\right)_{\Gamma\in\{\Sigma,\Sigma_1,\dots,\Sigma_n\}}$.

We are now in position to conclude the proof of Proposition B.70.

Proof. Let us assume that the assumptions of Proposition B.70 hold. The proof is divided into two cases.

Case 1: $\Gamma = \Sigma_k$ in (B.253) for some $k \in \{1,\dots,n\}$. If $k \in \{1,\dots,k_0\}$, from Lemmata B.74 and B.75 and the fact that $f^* \geq f(z_{k_0}) \geq f(z_k)$, one obtains that there exists $\varepsilon > 0$ such that for all $j \in \{1,\dots,n\}$, in the limit $h \to 0$

$$\langle \nabla u_h, \psi_j\rangle_{L^2_w} \int_{\Sigma_k} \psi_j \cdot n\, e^{-\frac{2}{h}f} d\sigma = \delta_{jk} B_k C_k h^{m+p} e^{-\frac{1}{h}(2f(z_k)-f(x_0))}(1+O(h)) + O\left(e^{-\frac{1}{h}(2f(z_k)-f(x_0)+\varepsilon)}\right).$$

Therefore, from (B.253), one gets for all $k \in \{1,\dots,k_0\}$, in the limit $h \to 0$

$$\int_{\Sigma_k} (\partial_n u_h)\; e^{-\frac{2}{h}f} d\sigma = B_k C_k h^{m+p} e^{-\frac{1}{h}(2f(z_k)-f(x_0))}(1+O(h)).$$

If $k \in \{k_0+1,\dots,n\}$. From Lemmata B.74 and B.75, one has for $j \in \{1,\dots,k_0\}$:

$$\langle \nabla u_h, \psi_j\rangle_{L^2_w} \int_{\Sigma_k} \psi_j \cdot n\, e^{-\frac{2}{h}f} d\sigma = O\left(h^p e^{-\frac{1}{h}(2f(z_{k_0})-f(x_0)+\varepsilon)}\right).$$

and for $j \in \{k_0+1,\dots,n\}$ (since $f(z_j) \geq f(z_{k_0+1})$ and $f(z_{k_0}) \leq f^* \leq (z_{k_0+1})$):

$$\langle \nabla u_h, \psi_j\rangle_{L^2_w} \int_{\Sigma_k} \psi_j \cdot n\, e^{-\frac{2}{h}f} d\sigma = \delta_{jk} O\left(h^{p+m} e^{-\frac{1}{h}(2f(z_k)-f(x_0))}\right) + O\left(e^{-\frac{1}{h}(2f(z_{k_0})-f(x_0)+\varepsilon)}\right).$$

Therefore, if one assumes that $f(z_{k_0+1}) > f(z_{k_0})$, from (B.253), one gets for all $k \in \{k_0+1,\dots,n\}$ and for all h small enough

$$\int_{\Sigma_k} (\partial_n u_h)\; e^{-\frac{2}{h}f} d\sigma = O\left(e^{-\frac{1}{h}(2f(z_{k_0})-f(x_0)+\varepsilon)}\right).$$

Case 2: $\Gamma = \Sigma$ in (B.253). From (B.253) and using Lemma B.76 and Lemma B.74, one has

$$\begin{aligned}\int_\Sigma \partial_n u_h\; e^{-\frac{2}{h}f} d\sigma &= C_{j_0} C^* h^{q^*+p} e^{-\frac{1}{h}(2f^*-f(x_0))}(1+O(h)) + \sum_{j=1, j\neq j_0}^{k_0} O\left(h^p e^{-\frac{1}{h}(-f(x_0)+2f^*+\varepsilon)}\right) \\ &\quad + \sum_{j=k_0+1}^{n} O\left(h^p e^{-\frac{1}{h}(f(z_j)-f(x_0)+2f^*-f(z_1)+\varepsilon)}\right) + O\left(e^{-\frac{1}{h}(f^*-f(x_0)+2f^*-f(z_1)+\varepsilon)}\right) \\ &= C_{j_0} C^* h^{q^*} e^{-\frac{1}{h}(2f^*-f(x_0))}(1+O(h)),\end{aligned}$$

which is the desired result. Proposition B.70 is proved. ∎

B.5.2.3 Construction of the quasi-modes which satisfy the estimates of Proposition B.70

In this section, we first construct the quasi-modes $(\tilde{\psi}_i)_{i\in\{1,\dots,n\}}$ and the family of quasi-modes $(\tilde{u}=\tilde{u}_\delta)_{\delta>0}$. Then, we prove that they satisfy the estimates stated in Proposition B.70. In all this section, one assumes that the hypotheses **[H1]**, **[H2]** and **[H3]** hold. Let $(\Sigma_i)_{i\in\{1,\dots,n\}}$ and Σ be as in Proposition B.70.

Construction of the quasi-modes.

The $n+1$ quasi-modes $((\tilde{\psi}_i)_{i\in\{1,\dots,n\}},\tilde{u})$ are constructed as in Section B.4.2 except $\tilde{\psi}_{j_0}$ (where we recall that $j_0\in\{1,\dots,n\}$ is such that $\overline{\Sigma}\subset B_{z_{j_0}}$). Recall that for all $j\in\{1,\dots,n\}$, $\tilde{\psi}_j$ is defined as:

$$\tilde{\psi}_j = e^{\frac{1}{h}f}\tilde{\phi}_j \in \Lambda^1 H^1_{w,T}(\Omega). \tag{B.256}$$

for a well chosen $\tilde{\phi}_j\in\Lambda^1 H^1_T(\Omega)$.

Thanks to the hypotheses **[H1]**, **[H2]** and **[H3]**, one can introduce the n quasi-modes $((\tilde{\phi}_i)_{i\in\{1,\dots,n\}\setminus\{j_0\}},\tilde{u})$ built in Section B.4.2 (see Definitions B.13 and B.14).

The construction of $\tilde{\phi}_{j_0}$ requires to take into account the set Σ in addition to the set Σ_{j_0} when defining the cut off function χ_{j_0} in Definition B.14. Let us make this precise. Let $\mathcal{S}_{M,j_0}:=\{\dot{\Omega}_{j_0},\Gamma_0,\Gamma_{1,j_0},\Gamma_{2,j_0},V_{\Gamma_{1,j_0}}\}$ be an ensemble of sets associated with z_{j_0}, see Definition B.12. Thanks to Proposition B.57, the set Γ_{1,j_0} can be taken such that

$$\overline{\Sigma}_{j_0}\cup\overline{\Sigma}\subset\Gamma_{1,j_0}.$$

We recall that Section B.4.1 was dedicated to the construction of a domain $\dot{\Omega}_{j_0}\subset\Omega$ and a mixed Witten Laplacian $\Delta^{M,(1)}_{f,h}(\dot{\Omega}_{j_0})$ (see (B.122)) associated with this ensemble of sets $\mathcal{S}_{M,j_0}$. Proposition B.59 gives the spectral properties of the operator $\Delta^{M}_{f,h}(\dot{\Omega}_{j_0})$. In the following, we consider a normalized eigenform $u^{(1)}_{h,j_0}\in D\left(\Delta^{M,(1)}_{f,h}(\dot{\Omega}_{j_0})\right)$ associated with the first eigenvalue 0, i.e. such that

$$\Delta^{M,(1)}_{f,h}(\dot{\Omega}_{j_0})\,u^{(1)}_{h,j_0}=0 \text{ in } \dot{\Omega}_{j_0} \text{ and } \left\|u^{(1)}_{h,j_0}\right\|_{L^2(\dot{\Omega}_{j_0})}=1.$$

The quasi-mode $\tilde{\phi}_{j_0}$ is then defined as the following truncation of $u^{(1)}_{h,j_0}$.

Definition B.15. *Let us assume that the hypotheses **[H1]**, **[H2]** and **[H3]** hold. Let $\chi_{j_0}\in C^\infty\left(\overline{\Omega}\right)$ be such that:*

1. *$\chi_{j_0}\in C^\infty_c\left(\dot{\Omega}_{j_0}\cup\Gamma_{1,j_0}\right)$ (and thus $\chi_{j_0}=0$ on $\Gamma_{2,j_0}\cup\Gamma_0$ and $\chi_{j_0}=0$ on on a neighborhood of $\partial\Omega\setminus\Gamma_{1,j_0}$),*
2. *$\chi_{j_0}=1$ on a neighborhood of $\Sigma_{j_0}\cup\Sigma$ in $\overline{\dot{\Omega}_{j_0}}$,*
3. *$0\le\chi_{j_0}\le 1$.*

The quasi-mode $\tilde{\phi}_{j_0}$ is defined on Ω by:

$$\tilde{\phi}_{j_0}:=\frac{\chi_{j_0}u^{(1)}_{h,j_0}}{\sqrt{\int_\Omega\left|\chi_{j_0}(x)u^{(1)}_{h,j_0}(x)\right|^2dx}}. \tag{B.257}$$

The quasi-modes satisfy the estimates stated in proposition B.70.

Using in addition to **[H1]**-**[H2]**-**[H3]** the hypotheses (B.29) and (B.30), one easily obtains that $((\tilde{\psi}_i)_{i=1,\dots,n}, \tilde{u})$ satisfy the estimates 1, 2, 3, 4(a) and 4(b) stated in Proposition B.70, following exactly the computations made on $((\tilde{\phi}_i)_{i=1,\dots,n}, \tilde{u})$ in Section B.4.5: 2(a) follows from (B.224)-(B.225)-(B.29)-(B.30), 2(b) is proven in Lemma B.60, 3 follows from (B.228)-(B.29), 4(b) is proven in Step 3 in Section B.4.5 and 4(a) is a consequence of (B.232)-(B.233)-(B.234)-(B.29). In particular, one gets that the constants $(B_i)_{i=1,\dots,n}$, m, $(C_i)_{i=1,\dots,n}$ and p in Proposition B.70 are given by (B.231)-(B.235).

The following lemma deals with the assumption 4(c) in Proposition B.70 which requires to use Proposition B.65.

Lemma B.77. *Let us assume that the hypotheses **[H1]**, **[H2]** and **[H3]** hold. Let $j \in \{1, \dots, n\}$. Then, when $h \to 0$, one has*

$$\int_\Sigma \tilde{\psi}_j \cdot n\, e^{-\frac{2}{h}f} d\sigma = \delta_{j_0,j} \frac{B^* \sqrt{2}\,(\det \mathrm{Hess} f|_{\partial\Omega}(z_{j_0}))^{\frac{1}{4}}}{\pi^{\frac{d-1}{4}} \sqrt{\partial_n f(z_{j_0})}}\, h^{p^* - \frac{d+1}{4}} e^{-\frac{1}{h}(2f^* - f(z_{j_0}))}\,(1 + O(h))\,,$$

where B^* and p^* are defined by (B.33).

Proof. By construction, if $j \neq j_0$ then $\tilde{\psi}_j \equiv 0$ on $B_{z_{j_0}}$. Let us deal with the case $j = j_0$. Using (B.256), one has

$$\int_\Sigma \tilde{\psi}_{j_0} \cdot n\, e^{-\frac{2}{h}f} d\sigma = \int_\Sigma \tilde{\phi}_{j_0} \cdot n\; e^{-\frac{1}{h}f} d\sigma. \tag{B.258}$$

Let $u^{(1)}_{z_{j_0},wkb}$ be the WKB expansion defined by (B.174). Following the beginning of Section B.4.4.2, let us consider

1. a neighborhood $V_{\Gamma_{St,j_0}}$ of Σ in $\overline{\Omega}$, which is stable under the dynamics (B.183) and such that, for some $\varepsilon > 0$, $V_{\Gamma_{St,j_0}} + B(0,\varepsilon) \subset V_{\Gamma_{1,j_0}} \cap (\dot{\Omega}_{j_0} \cup \Gamma_{1,j_0})$
2. and a cut-off function $\chi_{wkb,j_0} \in C_c^\infty(\dot{\Omega}_{j_0} \cup \Gamma_{1,j_0})$ with $\chi_{wkb,j_0} \equiv 1$ on a neighborhood of $\overline{V_{\Gamma_{St,j_0}}}$ such that $\operatorname{supp} \chi_{wkb,j_0} \subset V_{\Gamma_{1,j_0}} \cap (\dot{\Omega}_{j_0} \cup \Gamma_{1,j_0})$.

Using Proposition B.65, there exists $c_{z_{j_0}}(h) \in \mathbb{R}_+^*$ such that

$$\left\| e^{\frac{1}{h} d_a(\cdot, z_{j_0})} \left(u^{(1)}_{h,j_0} - c_{z_{j_0}}(h) u^{(1)}_{z_{j_0},wkb} \right) \right\|_{H^1(V_{\Gamma_{St,j_0}})} = O(h^\infty).$$

Let us now introduce

$$\tilde{\phi}_{z_{j_0},wkb} := c_{z_{j_0}}(h) \chi_{wkb,j_0}\; u^{(1)}_{z_{j_0},wkb}$$

so that

$$\int_\Sigma \tilde{\phi}_{j_0} \cdot n\; e^{-\frac{1}{h}f} d\sigma = \int_\Sigma \tilde{\phi}_{z_{j_0},wkb} \cdot n\; e^{-\frac{1}{h}f} d\sigma + \int_\Sigma \left(\tilde{\phi}_{j_0} - \tilde{\phi}_{z_{j_0},wkb} \right) \cdot n\, e^{-\frac{1}{h}f} d\sigma. \tag{B.259}$$

Let us first deal with the term $\int_\Sigma \tilde{\phi}_{z_{j_0},wkb} \cdot n\, e^{-\frac{1}{h}f}$ in (B.259). Using (B.33), one has (since $\Phi = f$, $\partial_n \Phi = -\partial_n f$ and $a_0 = 1$ on $\partial\Omega$, see (B.179)) when $h \to 0$,

$$\begin{aligned}
\int_\Sigma \tilde{\phi}_{z_{j_0},wkb} \cdot n\, e^{-\frac{1}{h}f} d\sigma &= c_{z_{j_0}}(h) \int_\Sigma \chi_{wkb,j_0}\; u^{(1)}_{z_{j_0},wkb} \cdot n\; e^{-\frac{1}{h}f} \\
&= 2\, c_{z_{j_0}}(h) \int_\Sigma \partial_n f\; e^{-\frac{1}{h}(2f - f(z_{j_0}))}\; (1 + O(h)) \\
&= 2\, c_{z_{j_0}}(h)\, B^*\, h^{p^*}\; e^{-\frac{1}{h}(2f^* - f(z_{j_0}))}\, (1 + O(h))\,.
\end{aligned}$$

Then using (B.189), one obtains in the limit $h \to 0$:

$$\int_\Sigma \tilde{\phi}_{z_{j_0},wkb} \cdot n\, e^{-\frac{1}{h}f} d\sigma = \frac{B^* \sqrt{2}\, (\det \mathrm{Hess} f|_{\partial\Omega}(z_{j_0}))^{\frac{1}{4}}}{\pi^{\frac{d-1}{4}} \sqrt{\partial_n f(z_{j_0})}} h^{p^* - \frac{d+1}{4}} e^{-\frac{1}{h}(2f^* - f(z_{j_0}))} \left(1 + O(h)\right). \tag{B.260}$$

Let us now estimate the term $\int_\Sigma \left(\tilde{\phi}_{j_0} - \tilde{\phi}_{z_{j_0},wkb}\right) \cdot n\ e^{-\frac{1}{h}f}$ in (B.259). Since $d_a(\cdot, z_{j_0}) = f - f(z_{j_0}) = \Phi - f(z_{j_0})$ on Σ, one obtains using Lemma B.66: there exist $C > 0$, $h_0 > 0$ and $\eta > 0$ such that for all $h \in (0, h_0)$,

$$\begin{aligned}
\left| \int_\Sigma \left(\tilde{\phi}_{j_0} - \tilde{\phi}_{z_{j_0},wkb}\right) \cdot n\ e^{-\frac{1}{h}f} d\sigma \right| &= \left| \int_\Sigma \left(\frac{u^{(1)}_{h,j_0}}{\Theta_{j_0}} - c_{z_{j_0}}(h) u^{(1)}_{z_{j_0},wkb} \right) \cdot n\ e^{-\frac{1}{h}f} d\sigma \right| \\
&\leq \frac{e^{-\frac{1}{h}(2f^* - f(z_{j_0}))}}{\Theta_{j_0}} \int_\Sigma \left| \left(u^{(1)}_{h,j_0} - c_{z_{j_0}}(h) u^{(1)}_{z_{j_0},wkb} \right) e^{\frac{d_a(\cdot, z_{j_0})}{h}} d\sigma \right| \\
&\quad + e^{-\frac{1}{h}(2f^* - f(z_{j_0}))} \frac{|\Theta_{j_0} - 1|}{\Theta_{j_0}} |c_{z_{j_0}}(h)| \int_\Sigma \left| u^{(1)}_{z_{j_0},wkb} e^{\frac{\Phi - f(z_{j_0})}{h}} d\sigma \right| \\
&\leq C e^{-\frac{1}{h}(2f^* - f(z_{j_0}))} \left\| e^{\frac{d_a(\cdot, z_{j_0})}{h}} \left(u^{(1)}_{h,j_0} - c_{z_{j_0}}(h) u^{(1)}_{z_{j_0},wkb} \right) \right\|_{H^1(V_{\Gamma_{St,j_0}})} \\
&\quad + C e^{-\frac{1}{h}(2f^* - f(z_{j_0}))} |c_{z_{j_0}}(h)| e^{-\frac{\eta}{h}} \left\| \chi_{wkb,j_0}\, u^{(1)}_{z_{j_0},wkb} e^{\frac{\Phi - f(z_{j_0})}{h}} \right\|_{H^1(\dot{\Omega}_{j_0})}.
\end{aligned}$$

Since it holds $u^{(1)}_{z_{j_0},wkb} e^{\frac{\Phi - f(z_{j_0})}{h}} = d_{f - (\Phi - f(z_{j_0})),h} a(\cdot, h) = h da(\cdot, h) + \nabla(f - \Phi) \wedge a(\cdot, h)$ (see (B.174)), there exists $C > 0$ such that for all h small enough,

$$\left\| \chi_{wkb,j_0}\, u^{(1)}_{z_{j_0},wkb} e^{\frac{\Phi - f(z_{j_0})}{h}} \right\|_{H^1(\dot{\Omega}_{j_0})} \leq C.$$

Then, one obtains using Proposition B.65 and (B.189):

$$e^{\frac{1}{h}(2f^* - f(z_{j_0}))} \left| \int_\Sigma \left(\tilde{\phi}_{j_0} - \tilde{\phi}_{z_{j_0},wkb}\right) \cdot n\ e^{-\frac{1}{h}f} \right| = O(h^\infty) + C e^{-\frac{\eta}{h}} h^{-\frac{d+1}{4}} = O(h^\infty). \tag{B.261}$$

Injecting the estimates (B.260)–(B.261) in (B.259) and using (B.258) imply that in the limit $h \to 0$:

$$\int_\Sigma \tilde{\psi}_{j_0} \cdot n\, e^{-\frac{2}{h}f} d\sigma = \frac{B^* \sqrt{2}\, (\det \mathrm{Hess} f|_{\partial\Omega}(z_{j_0}))^{\frac{1}{4}}}{\pi^{\frac{d-1}{4}} \sqrt{\partial_n f(z_{j_0})}}\ h^{p^* - \frac{d+1}{4}}\ e^{-\frac{1}{h}(2f^* - f(z_{j_0}))} \left(1 + O(h)\right).$$

This proves Lemma B.77. ∎

In conclusion, the n quasi-modes $(\tilde{\psi}_i)_{i=1,\dots,n}$ and the family of quasi-modes $(\tilde{u} = \tilde{u}_\delta)_{\delta > 0}$ satisfy all the conditions of Proposition B.70. This concludes the proof of Theorem B.2.

B.5.2.4 Proof of Corollary B.11

Let us assume that the hypotheses **[H1]**-**[H2]**-**[H3]** hold and let us assume that $f|_{\partial\Omega}$ has only two local minima z_1 and z_2 such that $f(z_1) < f(z_2)$. Let $\Sigma \subset \partial\Omega$ be a smooth open set such that $\overline{\Sigma} \subset B_{z_1}$ and

$$f^* := \inf_{\Sigma} f.$$

In addition, let us assume that (B.37) and (B.38) hold and let us assume that $f^* = f(z_2)$. Then, the inequalities (B.37) and (B.38) are exactly (B.29) and (B.30) (in the case $n = 2$ with $j_0 = 1$ and $k_0 = 2$). Therefore, (B.35) holds. It remains to compute the prefactor in (B.35). To this end, we need the constants B^* and p^* in (B.33). Let us assume that there is only one minimizer z^* of f on Σ. This implies that $z^* \in \partial\Sigma$ since z_1 is the only critical point of $f|_{\partial\Omega}$ in B_{z_1}. Furthermore, we assume that z^* is a non degenerate minimum of $f_{|\partial\Sigma}$ with $\partial_{n(\partial\Sigma)} f(z^*) < 0$ where $n(\partial\Sigma)$ is the unit outward normal to $\partial\Sigma \subset \partial\Omega$. Then, using Laplace's method, in the limit $h \to 0$:

$$\int_{\Sigma} \partial_n f \, e^{-\frac{2}{h} f} d\sigma = -\frac{\partial_n f(z^*)(\pi h)^{\frac{d}{2}}}{2\pi \partial_{n(\partial\Sigma)} f(z^*) \sqrt{\det \text{Hess} f_{|\partial\Sigma}(z^*)}} e^{-\frac{2}{h} f^*} (1 + O(h)),$$

with by convention, $\det \text{Hess} f_{|\partial\Sigma}(z^*) = 1$ if $d = 2$. This specifies the constants B^* and p^* appearing in (B.33). This ends the proof of Corollary B.11.

Bibliography of Chapter B

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Chapter C

The exit from a metastable state: concentration of the exit point on the low energy saddle points

Abstract

We consider the first exit time and the first exit point distribution from a bounded domain Ω of the stochastic process $(X_t)_{t\geq 0}$ solution to the overdamped Langevin dynamics:

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

sarting from the quasi stationary distribution in Ω. In the small temperature regime ($h \to 0$), it is proven that the support of the distribution of the first exit point concentrates on the points realizing the minimum of f on $\partial\Omega$. The proof holds under rather general assumptions on f and relies on tools from semi-classical analysis. The case when X_0 is a deterministic initial condition in Ω is also discussed.

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C.1 Introduction and main results

C.1.1 Overdamped Langevin dynamics and purpose of this work

One of the major issues in molecular dynamics is to have access to the different conformations of large molecules (such as proteins). In a constant temperature environment, a prototypal dynamics used in practice to describe the motion of the atoms in a molecule is the overdamped Langevin dynamics in $\mathbb{R}^d$:

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

where $X_t \in \mathbb{R}^d$ is the position vector of the N atoms ($d = 3N$), $f : \mathbb{R}^d \to \mathbb{R}$ is the potential energy function (assumed to be C^∞ in the following), the parameter $h > 0$ is the temperature and $(B_t)_{t\geq 0}$ is a standard d-dimensional Brownian motion. The overdamped Langevin dynamics (C.1) contains two terms : the term $-\nabla f(X_t)$ sends the process towards local minima of f, while the noise term $\sqrt{h}\, dB_t$ drives X_t from one basin of attraction of the dynamics $\dot{x} = -\nabla f(x)$ to another one. If the temperature is small ($h \ll 1$), the process $(X_t)_{t\geq 0}$ remains during a very long period of time trapped around a neighborhood of a local minimum of f, called a metastable state, before going to another region. Consequently, the process $(X_t)_{t\geq 0}$ has long periods of "inactivity" where no transition occurs between the metastable states. In the configuration space, the move from a metastable state to another corresponds to a change of configuration of the molecule. To have access to the different conformations of the molecule, it is needed to simulate $(X_t)_{t\geq 0}$ over long period of times which are unreachable in practice. Kinetic Monte Carlo algorithms are used in practice to overcome this difficulty (see for instance [27], [3, 10, 28, 31, 32]). One of the major ingredients in these algorithms is the transition rates between the different conformations of the molecule. These rates are computed in practice using the so-called Eyring-Kramers formula which predicts both the average time spent by the process (C.1) in a state and the probability to go to another state (see for instance [13,31]). The problem can be formulated as follows: given a metastable state $\Omega \subset \mathbb{R}^d$, what is the behaviour of the exit event of the process (C.1) from Ω (i.e. the time spent in Ω and the exit point distribution on $\partial\Omega$) in the small temperature regime ($h \to 0$)? In this work, we are mainly interested in the behaviour of the exit point distribution on $\partial\Omega$ when $h \to 0$. Let us consider a domain $\Omega \subset \mathbb{R}^d$ and the associated exit event from Ω. More precisely, let us introduce

$$\tau_\Omega = \inf\{t \geq 0 | X_t \notin \Omega\} \tag{C.2}$$

the first exit time from Ω. Let $\mathcal{Y} \subset \partial\Omega$. The law of X_{τ_Ω} concentrates on $\mathcal{Y}$ if for every neighborhood $\mathcal{V}_\mathcal{Y}$ of $\mathcal{Y}$ in $\partial\Omega$

$$\lim_{h\to 0} \mathbb{P}\left[X_{\tau_\Omega} \in \mathcal{V}_\mathcal{Y}\right] = 1,$$

and if for all $x \in \mathcal{Y}$ and for all neighborhoods $\mathcal{V}_x$ of x in $\partial\Omega$

$$\lim_{h\to 0} \mathbb{P}\left[X_{\tau_\Omega} \in \mathcal{V}_x\right] > 0.$$

Intuitively, one expects that the law of X_{τ_Ω} concentrates on $\arg\min_{\partial\Omega} f$.
The concentration of the law of X_{τ_Ω} in the small temperature regime ($h \to 0$) has been

studied using formal computations in [23] in the case when $\partial\Omega$ is characteristic (i.e $\partial_n f(x) = 0$ for all $x \in \partial\Omega$) and in the case when $\partial\Omega$ is noncharacteristic (i.e $\partial_n f(x) > 0$ for all $x \in \partial\Omega$). Our work is motivated by [23], and aims at generalizing and proving rigorously the results in [23]. In particular, we exhibit a general geometric setting in which the law of X_{τ_Ω} concentrates on points belonging to $\arg\min_{\partial\Omega} f$, with relative probabilities to leave through each point in $\arg\min_{\partial\Omega} f$ explicitly given by first and second order derivatives of f around these points. When $\partial_n f > 0$ on $\partial\Omega$ and the function f has only one critical point in Ω which is a strict minimum of f in Ω, the concentration of the law of X_{τ_Ω} on $\arg\min_{\partial\Omega} f$ has been obtained in [19], [18] and [26]. In [11], the most probable places of exit from Ω of the process (C.1) in the limit $h \to 0$ have been obtained in some specific cases. The results in [11], [26] and [18] also cover the non reversible case (i.e. when the drift in (C.1) is not the gradient of some function f). We refer to [5] for a comprehensive review of the literature. Let us mention that some results on the concentration of the law of X_{τ_Ω} in the small temperature regime can be obtained from [22].

In this work, we improve on these previous results. For instance, we do not assume that $\partial_n f > 0$ on $\partial\Omega$, we have no restriction on the number of critical points of f in Ω and f is allowed to have critical points in Ω with larger energies than $\min_{\partial\Omega} f$.

The introduction is organized as follows. In Section C.1.2, we introduce the quasi stationary distribution associated with Ω and the process (C.1), and we explain why it is relevant to study the exit event from a metastable domain Ω assuming that the process (C.1) is initially distributed according the quasi stationary distribution. In Section C.1.3, we introduce assumptions on f which will be used throughout this paper and we define the set of generalized saddle points of f. Finally, Section C.1.4 is dedicated to the statement of the main results of this work.

C.1.2 The quasi stationary distribution

The quasi stationary distribution is the cornerstone of our analysis. Here and in the following, we assume that the domain $\Omega \subset \mathbb{R}^d$ is smooth, open and bounded. Let us give the definition of the quasi stationary distribution associated with the overdamped Langevin process (C.1) and Ω:

Definition C.1. *Let $\Omega \subset \mathbb{R}^d$ and consider the dynamics (C.1). A quasi stationary distribution is a probability measure ν_h supported in Ω such that for all measurable sets $A \subset \Omega$ and for all $t \geq 0$*

$$\nu_h(A) = \frac{\displaystyle\int_\Omega \mathbb{P}^x \left[X_t \in A, t < \tau_\Omega\right] \nu_h(dx)}{\displaystyle\int_\Omega \mathbb{P}^x \left[t < \tau_\Omega\right] \nu_h(dx)}.$$

Here and in the following, the superscript x indicates that the stochastic process starts from $x \in \mathbb{R}^d$: $X_0 = x$. In words, if X_0 is distributed according to ν_h, then $\forall t > 0$, X_t is still distributed according to ν_h conditionally on $X_s \in \Omega$ for all $s \in (0, t)$. We have the following results from [20]:

Proposition C.1. *Let $\Omega \subset \mathbb{R}^d$ be a bounded domain and consider the dynamics* (C.1)*. Then, there exists a probability measure ν_h with support in Ω such that, whatever the law of the initial condition X_0 with support in Ω,*

$$\lim_{t\to\infty} \|\mathrm{Law}(X_t|t < \tau_\Omega) - \nu_h\|_{TV} = 0. \tag{C.3}$$

Here, $\mathrm{Law}(X_t|t < \tau_\Omega)$ denotes the law of X_t conditional to the event $\{t < \tau_\Omega\}$. A corollary of this proposition is that the quasi stationary distribution ν_h exists and is unique. For a given initial distribution of the process (C.1), if the convergence in (C.3) is much quicker than the exit from Ω, the exit from the domain Ω is said to be metastable. When the exit from Ω is metastable, it is thus relevant to study the exit event from a metastable state Ω assuming that the process (C.1) is initially distributed according to the quasi stationary distribution ν_h.

Let us introduce the infinitesimal generator of the dynamics (C.1), which is the differential operator

$$L^{(0)}_{f,h} = -\nabla f \cdot \nabla + \frac{h}{2}\,\Delta \tag{C.4}$$

with Dirichlet boundary conditions on $\partial\Omega$. In the notation $L^{(0)}_{f,h}$, the superscript (0) indicates that we consider an operator on functions, namely 0-forms. The basic observation to define our functional framework is that the operator $L^{(0)}_{f,h}$ is self-adjoint on the weighted L^2 space

$$L^2_w(\Omega) = \left\{ u : \Omega \to \mathbb{R}, \int_\Omega u^2 e^{-\frac{2}{h}f} < \infty \right\}$$

(the weighted Sobolev spaces $H^k_w(\Omega)$ are defined similarly). Indeed, for any smooth test functions u and v with compact supports in Ω, one has

$$\int_\Omega (L^{(0)}_{f,h}u)v\, e^{-\frac{2}{h}f} = \int_\Omega (L^{(0)}_{f,h}v)u\, e^{-\frac{2}{h}f} = -\frac{h}{2}\int_\Omega \nabla u \cdot \nabla v\, e^{-\frac{2}{h}f}.$$

This gives a proper framework to introduce the Dirichlet realization $L^{D,(0)}_{f,h}$ on Ω of the operator $L^{(0)}_{f,h}$:

Proposition C.2. *The Friedrich's extension associated with the quadratic form*

$$\phi \in C^\infty_c(\Omega) \mapsto \frac{h}{2}\int_\Omega |\nabla\phi|^2\, e^{-\frac{2}{h}f},$$

is denoted $-L^{D,(0)}_{f,h}$. It is a non negative unbounded self adjoint operator on $L^2_w(\Omega)$ with domain

$$D\left(L^{D,(0)}_{f,h}\right) = H^1_{w,0}(\Omega) \cap H^2_w(\Omega)$$

where $H^1_{w,0}(\Omega) = \{u \in H^1_w(\Omega),\ u = 0 \text{ on } \partial\Omega\}$.

The compact injection $H^1_w(\Omega) \subset L^2_w(\Omega)$ implies that the operator $L^{D,(0)}_{f,h}$ has a compact resolvent and its spectrum is consequently purely discrete. Let us introduce $\lambda_h > 0$ the principal eigenvalue of $-L^{D,(0)}_{f,h}$:

$$\lambda_h = \inf \sigma\big(-L^{D,(0)}_{f,h}\big). \tag{C.5}$$

From standard results on elliptic operator (see for example [9,12]), λ_h is non degenerate and its associated eigenfunction u_h has a sign on Ω. Moreover, $u_h \in C^\infty(\overline{\Omega})$. Without loss of generality, one can then assume that:

$$u_h > 0 \text{ on } \Omega \quad \text{and} \quad \int_\Omega u_h^2 e^{-\frac{2}{h}f} = 1. \tag{C.6}$$

The eigenvalue-eigenfunction couple (λ_h, u_h) satisfies:

$$\begin{cases} -L_{f,h}^{(0)} u_h = \lambda_h u_h \text{ on } \Omega, \\ \qquad u_h = 0 \text{ on } \partial\Omega. \end{cases} \tag{C.7}$$

The link between the quasi stationary distribution ν_h and the function u_h is given by the following proposition (see for example [20]):

Proposition C.3. *The unique quasi stationary distribution ν_h associated with the dynamics* (C.1) *and the domain Ω is given by:*

$$\nu_h(dx) = \frac{u_h(x)e^{-\frac{2}{h}f(x)}}{\displaystyle\int_\Omega u_h(y)e^{-\frac{2}{h}f(y)}dy}\, dx, \tag{C.8}$$

where u_h is the principal eigenfunction of $-L_{f,h}^{D,(0)}$.

The next proposition (which can be found in [20]) characterizes the law of the exit event from Ω.

Proposition C.4. *Let us consider the dynamics* (C.1) *and the quasi stationary distribution ν_h associated with the domain Ω. If X_0 is distributed according to ν_h, the random variables τ_Ω and X_{τ_Ω} are independent. Furthermore τ_Ω is exponentially distributed with parameter λ_h and the law of X_{τ_Ω} has a density with respect to the Lebesgue measure on $\partial\Omega$ given by*

$$z \in \partial\Omega \mapsto -\frac{h}{2\lambda_h}\frac{\partial_n u_h(z)e^{-\frac{2}{h}f(z)}}{\displaystyle\int_\Omega u_h(y)e^{-\frac{2}{h}f(y)}dy}. \tag{C.9}$$

Here and in the following, $\partial_n = n \cdot \nabla$ stands for the normal derivative and n is the unit outward normal on $\partial\Omega$.

C.1.3 Hypotheses and notations

This section is dedicated to the statement of the hypotheses used in this work (see Section C.1.3.1) and the notations chosen for the local minima of f and the saddle points of f (see Section C.1.3.2). In all this work, for $a \in \mathbb{R}$, the following notations will be used:

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

and

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

C.1.3.1 Hypotheses on the function f

In the following, we consider a setting that is more general than the one of Section C.1.2: $\overline{\Omega}$ is a C^∞ oriented compact and connected Riemannian manifold of dimension d with boundary $\partial\Omega$. Let us now introduce the following set of hypotheses which will be used in this work:

- **[H-Morse]** The function $f : \overline{\Omega} \to \mathbb{R}$ is a C^∞ function. The functions f and $f\big|_{\partial\Omega}$ are Morse functions and $\nabla f(x) \neq 0$ for all $x \in \partial\Omega$.
- **[H-Boundary]** The function f satisfies

$$\min_{\partial\Omega} f > \min_{\overline{\Omega}} f \text{ and } \min_{\partial\Omega} f > c_M := \sup\{f(x)\,;\, x \text{ is a local minimum of } f \text{ in } \Omega\}\,. \tag{C.10}$$

  In addition, for every connected component C of $\{f < \min_{\partial\Omega} f\}$, one has

$$\overline{C} \cap \partial\Omega \neq \emptyset.$$

- **[H-Connexity]** The function f satisfies **[H-Boundary]** and the set $\arg\min_\Omega f = \arg\min_{\overline{\Omega}} f$ is contained in one single connected component of $\{f < \min_{\partial\Omega} f\}$ denoted by C_1.
- **[H-Connexity+]** The function f satisfies **[H-Connexity]** and the closure of the connected component C_1 of $\{f < \min_{\partial\Omega} f\}$ containing $\arg\min_\Omega f$ is disjoint from the closure of any of the other connected components of $\{f < \min_{\partial\Omega} f\}$.

Let us recall that a critical point $z \in \overline{\Omega}$ of f is non degenerate if the hessian matrix of f at z, denoted by $\operatorname{Hess} f(z)$, is invertible. We refer for example to [7, Section 1.5.2] for a definition of the hessian matrix on a manifold. A non degenerate critical point $z \in \overline{\Omega}$ of f is said to have index $p \in \{0, \dots, d\}$ if $\operatorname{Hess} f(z)$ has precisely p negative eigenvalues (counted with multiplicity). In the case $p = 1$, z is called a saddle point. A function $g : \overline{\Omega} \to \mathbb{R}$ is a Morse function if all its critical points are non degenerate (which implies in particular that g has a finite number of critical points since $\overline{\Omega}$ is compact and a non degenerate critical point is isolated from the other critical points).

C.1.3.2 Notation for the local minima and saddle points of the function f

The main purpose of this section is to introduce the local minima of f and the generalized saddle points of f. These two sets are used extensively throughout this work and play a crucial role in our analysis. Roughly speaking, the set of generalized saddle points of f are the saddle points $z \in \overline{\Omega}$ of the extension of f by $-\infty$ outside $\overline{\Omega}$. Thus, when the function f satisfies the assumption **[H-Morse]**, a generalized saddle point of f (as denoted in [15]) is either a saddle point $z \in \Omega$ of f or a local minimum $z \in \partial\Omega$ of $f|_{\partial\Omega}$ with $\partial_n f(z) > 0$.

Let us assume the function f satisfies the assumption **[H-Morse]**. The set of local minima of f and the set of generalized saddle points of f are defined as follows.

<u>Definition of the local minima of f.</u>

Let us denote by:

$$\mathcal{U}_0^\Omega = \{x_1, \dots, x_{m_0^\Omega}\} \subset \Omega, \tag{C.11}$$

the set of local minima of f in Ω where $m_0^\Omega \in \mathbb{N}$ is the number of local minima of f in Ω. In addition, these critical points are labeled such that:

$$\{x_1, \ldots, x_{k_0^\Omega}\} = \arg\min_{\Omega} f, \tag{C.12}$$

where $k_0^\Omega \in \mathbb{N}$ satisfies $k_0^\Omega \leq m_0^\Omega$. Notice that when f satisfies [**H-Boundary**] in addition to [**H-Morse**], $k_0^\Omega \geq 1$ since the minimum of f is attained in Ω.

<u>Definition of the generalized saddle points of f.</u>

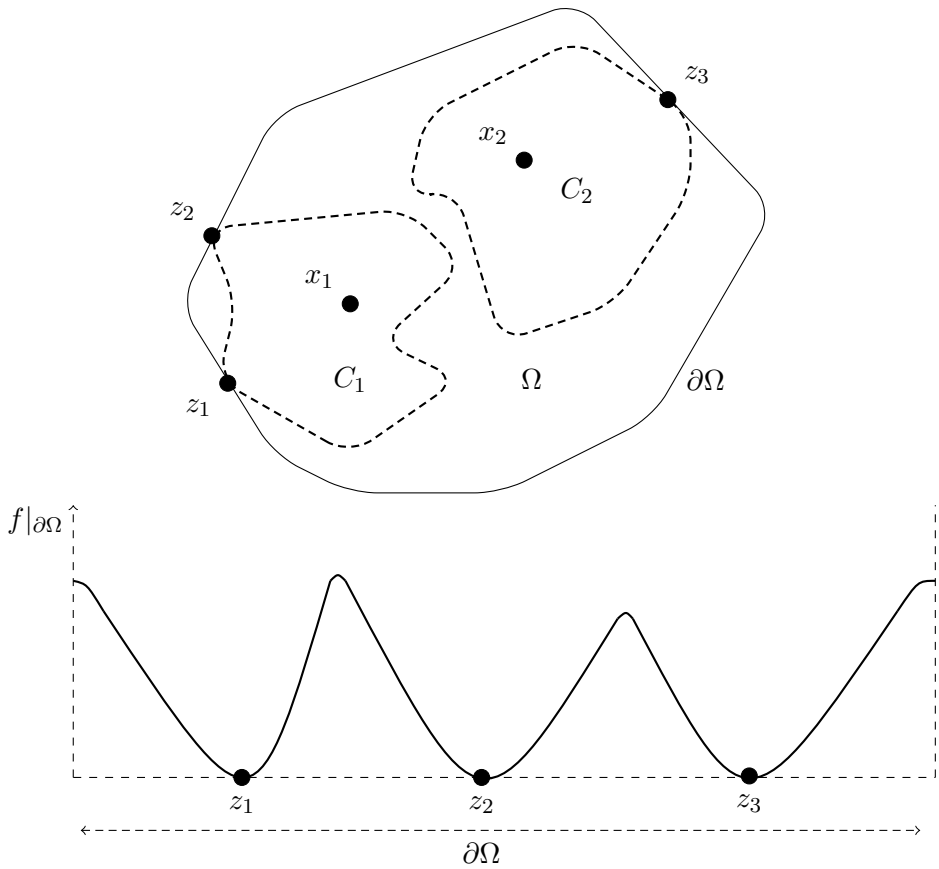

Figure C.1: Schematic representation of the connected components of $\{f < \min_{\partial\Omega} f\}$ and the function $f|_{\partial\Omega}$ when the assumptions [**H-Connexity+**] and [**H-Morse**] are satisfied. In this representation, the open sets C_1 and C_2 are the two connected components of $\{f < \min_{\partial\Omega} f\}$, $\overline{C_1} \cap \overline{C_2} = \emptyset$, $\mathcal{U}_1^{\partial\Omega} = \{z_1, z_2, z_3\}$ is the set of local minima of $f|_{\partial\Omega}$, $\partial C_1 \cap \partial\Omega = \{z_1, z_2\}$, $\mathcal{U}_1^\Omega = \emptyset$, $\mathcal{U}_0^\Omega = \{x_1, x_2\}$ and $\arg\min_{\overline{\Omega}} f = \{x_1\} \subset C_1$. Therefore, one has $k_1^{\partial C_1} = 2$, $k_1^{\partial\Omega} = 3$, $m_1^{\partial\Omega} = m_1^{\overline{\Omega}} = 3$, $m_0^\Omega = 2$ and $k_0^\Omega = 1$.

The set of saddle points of f of index 1 in Ω is denoted by $\mathcal{U}_1^\Omega$ and its cardinality by m_1^Ω. Let us define

$$\mathcal{U}_1^{\partial\Omega} := \{z \in \partial\Omega,\ z \text{ is a local minimum of } f|_{\partial\Omega} \text{ but not a local minimum of } f \text{ in } \overline{\Omega}\ \} \tag{C.13}$$

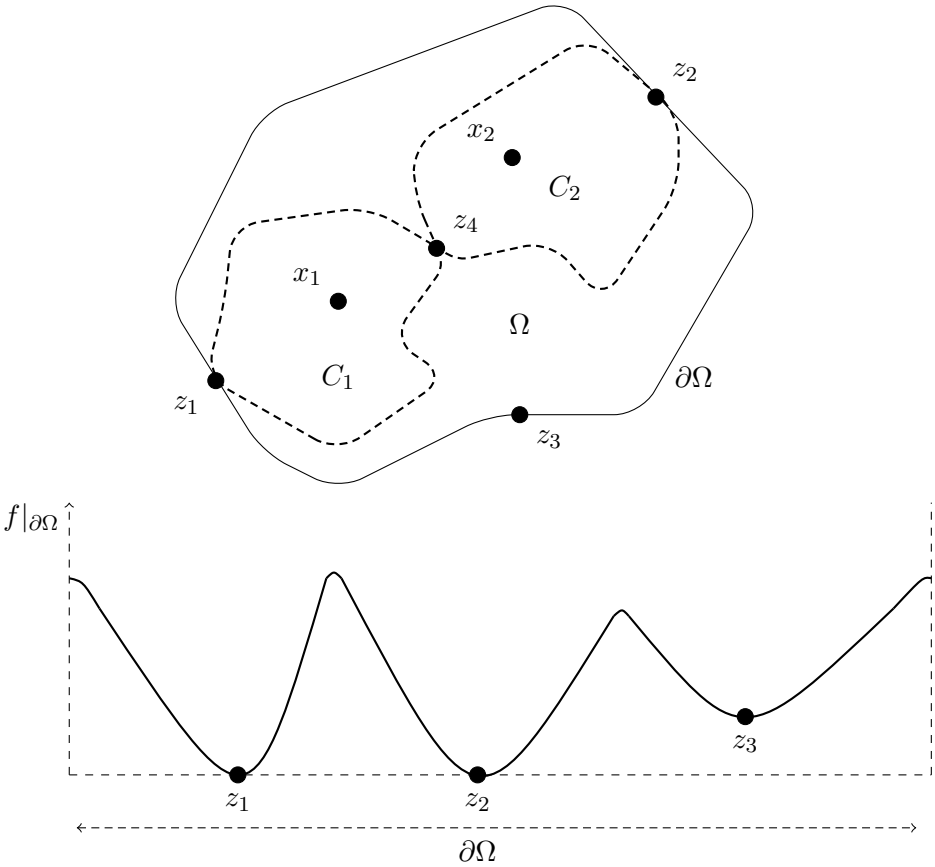

Figure C.2: Schematic representation of the connected components of $\{f < \min_{\partial\Omega} f\}$ and $f|_{\partial\Omega}$ when the assumptions [**H-Connexity**] and [**H-Morse**] are satisfied but not the assumption [**H-Connexity+**]. In this representation, the open sets C_1 and C_2 are the two connected components of $\{f < \min_{\partial\Omega} f\}$, $\mathcal{U}_1^{\partial\Omega} = \{z_1, z_2, z_3\}$ is the set of local minima of $f|_{\partial\Omega}$, $\mathcal{U}_1^{\Omega} = \{z_4\} = \overline{C}_1 \cap \overline{C}_2$, $\partial C_1 \cap \partial\Omega = \{z_1\}$, $\mathcal{U}_0^{\Omega} = \{x_1, x_2\}$ and $\arg\min_{\overline{\Omega}} f = \{x_1\} \subset C_1$. Therefore, one has $k_1^{\partial C_1} = 1$, $k_1^{\partial\Omega} = 2$, $m_1^{\partial\Omega} = 3$, $m_1^{\overline{\Omega}} = 4$, $k_0^{\Omega} = 1$ and $m_1^{\Omega} = 2$. The point z_4 is a separating saddle point as introduced in Definition C.3.

Notice that

$$\mathcal{U}_1^{\partial\Omega} = \{z \in \partial\Omega,\, z \text{ is a local minimum of } f|_{\partial\Omega}\} \cap \{z \in \partial\Omega,\, \partial_n f(z) > 0\}, \tag{C.14}$$

which follows from the fact that $\nabla f(x) \neq 0$ for all $x \in \partial\Omega$. Let us introduce

$$m_1^{\partial\Omega} := \mathrm{Card}(\mathcal{U}_1^{\partial\Omega}).$$

In addition, one defines:

$$\mathcal{U}_1^{\overline{\Omega}} := \mathcal{U}_1^{\partial\Omega} \cup \mathcal{U}_1^{\Omega} \text{ and } m_1^{\overline{\Omega}} := \mathrm{Card}(\mathcal{U}_1^{\overline{\Omega}}) = m_1^{\partial\Omega} + m_1^{\Omega}.$$

The set $\mathcal{U}_1^{\overline{\Omega}}$ is the set of generalized saddle points of f. If $\mathcal{U}_1^{\partial\Omega}$ is not empty, its elements are denoted by:

$$\mathcal{U}_1^{\partial\Omega} = \{z_1, ..., z_{m_1^{\partial\Omega}}\} \subset \partial\Omega, \tag{C.15}$$

and if $\mathcal{U}_1^{\Omega}$ is not empty, its elements are labeled such that:

$$\mathcal{U}_1^{\Omega} = \{z_{m_1^{\partial\Omega}+1}, ..., z_{m_1^{\overline{\Omega}}}\} \subset \Omega. \tag{C.16}$$

Thus, one has:

$$\mathcal{U}_1^{\overline{\Omega}} = \{z_1, ..., z_{m_1^{\partial\Omega}}, z_{m_1^{\partial\Omega}+1}, ..., z_{m_1^{\overline{\Omega}}}\}.$$

In addition, the elements of $\mathcal{U}_1^{\partial\Omega}$ are labeled such that:

$$\{z_1, ..., z_{k_1^{\partial\Omega}}\} = \mathcal{U}_1^{\partial\Omega} \cap \arg\min_{\partial\Omega} f, \tag{C.17}$$

where $k_1^{\partial\Omega} \in \mathbb{N}^*$ satisfies $k_1^{\partial\Omega} \leq m_1^{\partial\Omega}$.

Let us assume that the function f satisfies the assumption [**H-Connexity**] in addition to [**H-Morse**]. In this case, let us recall that C_1 stands for the connected component of $\{f < \min_{\partial\Omega} f\}$ which contains $\arg\min_{\Omega} f$. Notice that necessarily $\{z_1, ..., z_{k_1^{\partial\Omega}}\} \cap \partial C_1$ is not empty. We assume that $\{z_1, ..., z_{k_1^{\partial\Omega}}\}$ is ordered such that:

$$\{z_1, ..., z_{k_1^{\partial C_1}}\} = \{z_1, ..., z_{k_1^{\partial\Omega}}\} \cap \partial C_1, \tag{C.18}$$

where $k_1^{\partial C_1} \in \mathbb{N}^*$ satisfies $k_1^{\partial C_1} \leq k_1^{\partial\Omega}$. By definition,

$$\{z_1, ..., z_{k_1^{\partial C_1}}\} = \arg\min_{\partial\Omega} f \cap \partial C_1.$$

Therefore, since $\partial C_1 \subset \{f = \min_{\partial\Omega} f\}$, $\nabla f(x) \neq 0$ for all $x \in \partial\Omega$, $\partial_n f \geq 0$ on ∂C_1 and $f_{|\partial\Omega}$ is Morse, one has:

$$\{z_1, ..., z_{k_1^{\partial C_1}}\} = \partial\Omega \cap \partial C_1. \tag{C.19}$$

We provide examples in Figures C.1 and C.2 to illustrate the notations introduced in this section.

As introduced in [15, Section 5.2], $\mathcal{U}_0^{\Omega}$ is the set of critical points of f of index 0 for the Witten Laplacian acting on functions with Dirichlet boundary conditions on $\partial\Omega$, and $\mathcal{U}_1^{\overline{\Omega}}$ is the set of critical points of f of index 1 for the Witten Laplacian acting on 1-forms with tangential Dirichlet boundary conditions on $\partial\Omega$. We refer to Section C.2.2 for the definition of these Witten Laplacians .

C.1.4 Main results

This section is dedicated to the statement of the main results of this work. This section is organized as follows. In Section C.1.4.1, a sharp asymptotic estimate in the limit $h \to 0$ of the smallest eigenvalue λ_h of $-L_{f,h}^{D,(0)}$is provided in Theorem C.1 and a sharp asymptotic estimate of the normal derivative of the eigenfunction u_h associated with λ_h is provided in Theorem C.2. In Section C.1.4.2, the consequences of these results on the law of X_{τ_Ω} are stated in Corollary C.6 and Theorem C.3. Then, in Section C.1.4.3, we discuss the geometric assumptions [**H-Boundary**], [**H-Connexity**] and [**H-Connexity+**]. Finally, in Section C.1.4.4, we give an overview of the strategy of the proofs of the main results.

C.1.4.1 Main results on λ_h and $\partial_n u_h$

Theorem C.1. *Assume that* ***[H-Morse]*** *and* ***[H-Connexity]*** *hold. Let λ_h be the principal eigenvalue of $-L_{f,h}^{D,(0)}$ (see* (C.5)*). Then, one has in the limit $h \to 0$:*

$$\lambda_h = \frac{\sum_{j=1}^{k_1^{\partial C_1}} \partial_n f(z_j)\big(\det \mathrm{Hess} f\big|_{\partial\Omega}(z_j)\big)^{-\frac{1}{2}}}{\sqrt{\pi\, h}\, \sum_{k=1}^{k_0^{\Omega}} \big(\det \mathrm{Hess} f(x_k)\big)^{-\frac{1}{2}}}\, e^{-\frac{2}{h}(f(z_1)-f(x_1))}\big(1+O(\sqrt{h})\big) \tag{C.20}$$

and, denoting by $\lambda_{2,h}$ the second smallest eigenvalue of $-L_{f,h}^{D,(0)}$, there exists $c>0$ such that in the limit $h \to 0$:

$$\lambda_h = \lambda_{2,h}\; O(e^{-\frac{c}{h}}).$$

Moreover, when ***[H-Connexity+]*** *holds, the remainder term $O(\sqrt{h})$ in* (C.20) *is actually of order $O(h)$ and admits a full asymptotic expansion in h (as defined in Remark C.1 below).*

Remark C.1. *Let us recall that for $\alpha > 0$, $(r(h))_{h>0}$ admits a full asymptotic expansion in h^α if there exists a sequence $(a_k)_{k\geq 0} \in \mathbb{R}^{\mathbb{N}}$ such that for any $N \in \mathbb{N}$, it holds in the limit $h \to 0$:*

$$r(h) = \sum_{k=0}^{N} a_k h^{\alpha k} + O(h^{\alpha(N+1)}).$$

Without the assumption **[H-Connexity+]**, we are not able to prove an asymptotic expansion in $\sqrt{h}$ of the remainder term $O(\sqrt{h})$ in (C.20) except in some specific cases, see Section C.4.2.1.

Theorem C.1 is a consequence of Theorem C.4 stated in Section C.3.1.2.

Theorem C.2. *Assume that* ***[H-Morse]*** *and* ***[H-Connexity]*** *hold, and let u_h be the principal eigenfunction of $-L_{f,h}^{D,(0)}$ which satisfies* (C.6)*. Let $F \in L^\infty(\partial\Omega, \mathbb{R})$ and $(\Sigma_i)_{i\in\{1,\dots,k_1^{\partial\Omega}\}}$ be a family of disjoint open subsets of $\partial\Omega$ such that for all $i \in \{1,\dots,k_1^{\partial\Omega}\}$, $z_i \in \Sigma_i$. Then, there exists $c>0$ such that in the limit $h \to 0$,*

$$\int_{\partial\Omega} F\, \partial_n u_h\, e^{-\frac{2}{h}f} = \sum_{i=1}^{k_1^{\partial\Omega}} \int_{\Sigma_i} F\, \partial_n u_h\, e^{-\frac{2}{h}f} + O(e^{-\frac{1}{h}(2f(z_1)-f(x_1)+c)}), \tag{C.21}$$

and

$$\sum_{i=k_1^{\partial C_1}+1}^{k_1^{\partial\Omega}} \int_{\Sigma_i} F\, \partial_n u_h\, e^{-\frac{2}{h}f} = O(h^{\frac{d-5}{4}} e^{-\frac{1}{h}(2f(z_1)-f(x_1))}), \tag{C.22}$$

with the convention $\sum_{i=n}^{m} = 0$ if $n > m$. Moreover, when, for some $i \in \{1,\dots,k_1^{\partial C_1}\}$, F is C^∞ in a neighborhood of z_i, one has in the limit $h \to 0$:

$$\int_{\Sigma_i} F\, \partial_n u_h\, e^{-\frac{2}{h}f} = A_i\, \big(F(z_i) + O(h^{\frac{1}{4}})\big)\, h^{\frac{d-6}{4}}\, e^{-\frac{1}{h}(2f(z_1)-f(x_1))}, \tag{C.23}$$

where

$$A_i = -2\,\partial_n f(z_i)\,\pi^{\frac{d-2}{4}}\left(\left(\det\,\mathrm{Hess} f\big|_{\partial\Omega}(z_i)\right)\sum_{k=1}^{k_0^\Omega}\left(\det\,\mathrm{Hess} f(x_k)\right)^{-\frac{1}{2}}\right)^{-\frac{1}{2}}. \tag{C.24}$$

Lastly, when ***[H-Connexity+]*** *holds, the remainder term* $O(h^{\frac{d-5}{4}}e^{-\frac{1}{h}(2f(z_1)-f(x_1))})$ *in* (C.22) *is of the order* $O(e^{-\frac{1}{h}(2f(z_1)-f(x_1)+c)})$ *for some* $c>0$ *and the remainder term* $O(h^{\frac{1}{4}})$ *in* (C.23) *is of the order* $O(h)$ *and admits a full asymptotic expansion in* h.

According to Theorem C.2, when the function F belongs to $C^\infty(\partial\Omega,\mathbb{R})$, one has the following equivalent of (C.21) in the limit $h\to 0$:

$$\int_{\partial\Omega} F\,\partial_n u_h\,e^{-\frac{2}{h}f} = \sum_{i=1}^{k_1^{\partial C_1}} A_i\left(F(z_i)+O(h^{\frac{1}{4}})\right)h^{\frac{d-6}{4}}\,e^{-\frac{1}{h}(2f(z_1)-f(x_1))}.$$

In Section C.4.2.2, one shows that the optimal remainder term in (C.22) is $O(h^{\frac{d-4}{4}}e^{-\frac{1}{h}(2f(z_1)-f(x_1))})$ and the optimal remainder term in (C.23) is $O(\sqrt{h})$. They are obtained in some specific cases, see Proposition C.40.

Remark C.2. *Theorem C.1 and Proposition C.4 give the asymptotic estimate of the mean exit time from* Ω *in the limit* $h\to 0$ *under the assumptions* ***[H-Morse]*** *and* ***[H-Connexity]****:*

$$\mathbb{E}^{\nu_h}[\tau_\Omega] = \sqrt{\pi\,h}\,\frac{\sum_{k=1}^{k_0^\Omega}\left(\det\,\mathrm{Hess} f(x_k)\right)^{-\frac{1}{2}}}{\sum_{j=1}^{k_1^{\partial C_1}}\partial_n f(z_j)\left(\det\,\mathrm{Hess} f\big|_{\partial\Omega}(z_j)\right)^{-\frac{1}{2}}}\,e^{\frac{2}{h}(f(z_1)-f(x_1))}\left(1+O(\sqrt{h})\right).$$

In view of (C.9), the following proposition will also be needed in order to study the law of X_{τ_Ω} in the limit $h\to 0$.

Proposition C.5. *Assume that* ***[H-Morse]*** *and* ***[H-Connexity]*** *hold. One then has in the limit* $h\to 0$,

$$\int_\Omega u_h\,e^{-\frac{2}{h}f} = (h\pi)^{\frac{d}{4}}e^{-\frac{1}{h}f(x_1)}\left(\sum_{k=1}^{k_0^\Omega}\left(\det\,\mathrm{Hess} f(x_k)\right)^{-\frac{1}{2}}\right)^{1/2}\left(1+O(h)\right), \tag{C.25}$$

where u_h *is the principal eigenfunction of* $-L_{f,h}^{D,(0)}$ *which satisfies* (C.6). *Moreover, the remainder term* $O(h)$ *in* (C.25) *admits a full asymptotic expansion in* h.

C.1.4.2 Consequences on the distribution of X_{τ_Ω}

Since Proposition C.4 implies that, for any $F\in L^\infty(\partial\Omega,\mathbb{R})$,

$$\mathbb{E}^{\nu_h}\left[F(X_{\tau_\Omega})\right] = -\frac{h}{2\lambda_h}\frac{\int_{\partial\Omega}F\,\partial_n u_h\,e^{-\frac{2}{h}f}}{\int_\Omega u_h e^{-\frac{2}{h}f}},$$

one immediately gets the following corollary from Proposition C.5 and Theorem C.2.

Corollary C.6. *Assume that **[H-Morse]** and **[H-Connexity]** hold. Let $F \in L^\infty(\partial\Omega, \mathbb{R})$ and $(\Sigma_i)_{i\in\{1,\dots,k_1^{\partial\Omega}\}}$ be a family of disjoint open subsets of $\partial\Omega$ such that for all $i \in \{1,\dots,k_1^{\partial\Omega}\}$, $z_i \in \Sigma_i$. Then, there exists $c > 0$ such that in the limit $h \to 0$:*

$$\mathbb{E}^{\nu_h}\left[F\left(X_{\tau_\Omega}\right)\right] = \sum_{i=1}^{k_1^{\partial\Omega}} \mathbb{E}^{\nu_h}\left[\mathbf{1}_{\Sigma_i} F\left(X_{\tau_\Omega}\right)\right] + O(e^{-\frac{c}{h}}) \tag{C.26}$$

and

$$\sum_{i=k_1^{\partial C_1}+1}^{k_1^{\partial\Omega}} \mathbb{E}^{\nu_h}\left[\mathbf{1}_{\Sigma_i} F\left(X_{\tau_\Omega}\right)\right] = O(h^{\frac{1}{4}}). \tag{C.27}$$

Moreover, when for some $i \in \{1,\dots,k_1^{\partial C_1}\}$ F is C^∞ in a neighborhood of z_i, one has when $h \to 0$:

$$\mathbb{E}^{\nu_h}\left[\mathbf{1}_{\Sigma_i} F\left(X_{\tau_\Omega}\right)\right] = F(z_i)\, a_i + O(h^{\frac{1}{4}}), \tag{C.28}$$

where

$$a_i = \frac{\partial_n f(z_i)}{\sqrt{\det \operatorname{Hess} f\big|_{\partial\Omega}(z_i)}} \left(\sum_{j=1}^{k_1^{\partial C_1}} \frac{\partial_n f(z_j)}{\sqrt{\det \operatorname{Hess} f\big|_{\partial\Omega}(z_j)}} \right)^{-1}. \tag{C.29}$$

*Lastly, when **[H-Connexity+]** holds, the remainder term $O(h^{\frac{1}{4}})$ in (C.27) is of the order $O(e^{-\frac{c}{h}})$ for some $c > 0$ and the remainder term $O(h^{\frac{1}{4}})$ in (C.28) is of the order $O(h)$ and admits a full asymptotic expansion in h.*

Corollary C.6 implies that in the limit $h \to 0$ the law of X_{τ_Ω} when $X_0 \sim \nu_h$ concentrates on the set $\{z_1,\dots,z_{k_1^{\partial C_1}}\} = \partial\Omega \cap \partial C_1$ with an explicit repartition of the probabilities. Moreover, a consequence of Corollary C.6 is that the probability to exit through a global minimum z of $f_{|\partial\Omega}$ which satisfies $\partial_n f(z) < 0$ is exponentially small in the limit $h \to 0$ and when assuming **[H-Connexity+]**, the exit through $z_{k_1^{\partial C_1}+1},\dots,z_{k_1^{\partial\Omega}}$ is also exponentially small even though all these points belong to $\arg\min_{\partial\Omega} f$.

Corollary C.6 can be extended to other initial conditions for the process (C.1).

Theorem C.3. *Let us assume that the hypotheses **[H-Morse]** and **[H-Connexity]** hold. Let us recall that C_1 is the connected component of $\{f < \min_{\partial\Omega} f\}$ which contains all the global minima of f in Ω. Let K be a compact subset of C_1, $F \in L^\infty(\partial\Omega, \mathbb{R})$ and $(\Sigma_i)_{i\in\{1,\dots,k_1^{\partial\Omega}\}}$ be a family of disjoint open subsets of $\partial\Omega$ such that for all $i \in \{1,\dots,k_1^{\partial\Omega}\}$, $z_i \in \Sigma_i$. Then, there exists $c > 0$ such that in the limit $h \to 0$ and uniformly with respect to $x \in K$:*

$$\mathbb{E}^{x}\left[F\left(X_{\tau_\Omega}\right)\right] = \sum_{i=1}^{k_1^{\partial\Omega}} \mathbb{E}^{x}\left[\mathbf{1}_{\Sigma_i} F\left(X_{\tau_\Omega}\right)\right] + O(e^{-\frac{c}{h}}) \tag{C.30}$$

and

$$\sum_{i=k_1^{\partial C_1}+1}^{k_1^{\partial\Omega}} \mathbb{E}^{x}\left[\mathbf{1}_{\Sigma_i} F\left(X_{\tau_\Omega}\right)\right] = O(h^{\frac{1}{4}}). \tag{C.31}$$

Moreover, when for some $i \in \{1, \dots, k_1^{\partial C_1}\}$ F is C^∞ in a neighborhood of z_i, one has when $h \to 0$ and uniformly with respect to $x \in K$:

$$\mathbb{E}^x \left[\mathbf{1}_{\Sigma_i} F\left(X_{\tau_\Omega}\right)\right] = F(z_i)\, a_i + O(h^{\frac{1}{4}}), \tag{C.32}$$

where for $i \in \{1, \dots, k_1^{\partial C_1}\}$, a_i is defined in (C.29)*. Lastly, when **[H-Connexity+]** holds, the remainder term $O(h^{\frac{1}{4}})$ in* (C.31) *is, for some $c > 0$ of the order $O(e^{-\frac{c}{h}})$ and the remainder term $O(h^{\frac{1}{4}})$ in* (C.32) *is of the order $O(h)$ and admits a full asymptotic expansion in h.*

According to Theorem C.3, when the function F belongs to $C^\infty(\partial\Omega, \mathbb{R})$, one has the following equivalent of (C.21) in the limit $h \to 0$:

$$\mathbb{E}^x \left[F\left(X_{\tau_\Omega}\right)\right] = \sum_{i=1}^{k_1^{\partial C_1}} a_i F(z_i) + O(h^{\frac{1}{4}}) = \frac{\displaystyle\int_{\partial\Omega} F \partial_n f\, e^{-\frac{2}{h} f}}{\displaystyle\int_{\partial\Omega} \partial_n f\, e^{-\frac{2}{h} f}} + O(h^{\frac{1}{4}}).$$

This is reminiscent of previous results obtained in [19], [18] and [26].

Remark C.3. *In Section C.4.2.1, one shows, in some specific cases for which the assumption **[H-Connexity+]** does not hold, that the remainder terms $O(h^{\frac{1}{4}})$ in* (C.27), (C.28), (C.31) *and* (C.32) *are of the order $O(\sqrt{h})$ and in Section C.4.2.2, one shows that this $O(\sqrt{h})$ is actually optimal and thus is not in general exponentially small. One expects that the optimal remainder term in* (C.28) *and* (C.32) *is of the order $O(\sqrt{h})$ when **[H-Connexity+]** does not hold.*

Remark C.4. *In Section C.4.1.2, we show that the metastability of Ω depends on the initial distribution of the process* (C.1)*.*

Let us mention that in Section C.4.3, we generalize the results of this section to the case when f can have local minima inside Ω which do not belong to $\{f < \min_{\partial\Omega} f\}$ (i.e. when **[H-Boundary]** is not satisfied).

C.1.4.3 On the hypotheses

The goal of this section is to discuss the geometric assumptions **[H-Boundary]**, **[H-Connexity]** and **[H-Connexity+]** to obtain Theorems C.1 and C.3, Proposition C.5 and Corollary C.6.

On the assumption **[H-Boundary]**.
Let us recall that under **[H-Boundary]** it is assumed that the closure of all the connected components of $\{f < \min_{\partial\Omega} f\}$ meet $\partial\Omega$ and all the local minima of f are contained in $\{f < \min_{\partial\Omega} f\}$ (see Section C.1.3.1). Roughly speaking, this assumption ensures that in the small temperature regime, the highest energetic barrier that the process (C.1), starting from any local minimum of f, has to cross to leave Ω is $\min_{\partial\Omega} f - \min_\Omega f$. In other words, the strongest effect of metastability in Ω is caused by some of the global minima of f on the boundary and not by saddle points of f in Ω. When **[H-Boundary]** does not hold, it is possible to exhibit cases in which, there exists a connected component C of $\{f < \min_{\partial\Omega} f\}$ such that when $X_0 = x \in C$

or when $X_0 \sim \nu_h$ (see (C.8)), the law of X_{τ_Ω} does not concentrate on points belonging to $\arg\min_{\partial\Omega} f$ when $h \to 0$ and $\lim_{h\to 0} h \log \mathbb{E}[\tau_\Omega] > 2(\min_{\partial\Omega} f - \min_\Omega f)$, see Section C.4.1.1.

Although the assumption [**H-Boundary**] is sufficient in order to associate the strongest effect of metastability in Ω with its boundary, it is not necessary. The assumption [**H-Boundary**] can thus be relaxed and this is the purpose of Section C.4.3.

On the assumption [**H-Connexity**].
Let us recall that under [**H-Connexity**], the assumption [**H-Boundary**] holds and, in addition, all the global minima of f are contained in one single connected component of $\{f < \min_{\partial\Omega} f\}$ which is denoted by C_1 (see Section C.1.3.1). Hence, under these assumptions, we expect that the most metastable subdomain of Ω is C_1 and thus that the quasi stationary distribution ν_h (see (C.8)) concentrates in C_1. This explains the result given in Proposition C.5. Consequently, we expect in addition that when $X_0 \sim \nu_h$ or when $X_0 = x \in C_1$, the law of X_{τ_Ω} concentrates on points belonging to $\partial C_1 \cap \arg\min_{\partial\Omega} f$ and we expect that $\mathbb{E}[\tau_\Omega]$ is associated with $\partial C_1 \cap \arg\min_{\partial\Omega} f$ and $\arg\min_\Omega f$ ($\subset C_1$). This explains the results obtained in Theorem C.1 (since according to Proposition C.4, $\lambda_h = \frac{1}{\mathbb{E}^{\nu_h}[\tau_\Omega]}$), Theorem C.3 and Corollary C.6.

If C_1 does not contain all the global minima of f, ν_h concentrates on the connected component of $\{f < \min_{\partial\Omega} f\}$ which contain a global minimum of f. However, it is difficult to estimate the relative distribution of ν_h in the connected components of $\{f < \min_{\partial\Omega} f\}$ which contains a global minimum of f (see Remark C.17). Consequently, [**H-Connexity**] is an assumption which simplifies the analysis in concentrating ν_h in C_1.

On the assumption [**H-Connexity+**].
Let us recall that under [**H-Connexity+**], the assumption [**H-Connexity**] holds and, in addition, $\overline{C_1}$ does not intersect the closure of any other connected components of $\{f < \min_{\partial\Omega} f\}$. When [**H-Connexity+**] does not hold, it is possible to exhibit cases in which, when $X_0 \sim \nu_h$ or when $X_0 = x \in C_1$, the process (C.1) does not have a very small probability to leave Ω through a point belonging to $\partial\Omega \setminus (C_1 \cap \arg\min_{\partial\Omega} f)$ when $h \to 0$, see Section C.4.2.2. Under [**H-Connexity+**], we can show that this probability is very small (actually exponentially small), see the remainder terms obtained in Theorem C.3 and Corollary C.6 under [**H-Connexity+**].

C.1.4.4 Organization of the paper and outlines of the proofs of Theorems C.1 and C.2

The aim of this section is to give an overview of the strategy of the proofs of Theorems C.1 and C.2. Let us recall that λ_h is defined in (C.5) and u_h by (C.7). In view of (C.20), we would like to identify the asymptotic behaviour of the smallest eigenvalue of $-L_{f,h}^{D,(0)}$ as well as, in view of (C.21), the gradient of u_h on $\partial\Omega$. The first key point is to notice that the gradient of any eigenfunction associated with an eigenvalue of $-L_{f,h}^{D,(0)}$ is also a solution to an eigenvalue problem for the same eigenvalue. Let us be more precise. Let v be an eigenfunction associated with $\lambda \in \sigma(-L_{f,h}^{D,(0)})$. The

eigenvalue-eigenfunction couple (λ, v) satisfies:

$$\begin{cases} -L_{f,h}^{(0)} v = \lambda v \text{ on } \Omega, \\ \qquad v = 0 \text{ on } \partial\Omega. \end{cases}$$

By differentiating this relation, we observe that ∇v satisfies

$$\begin{cases} -L_{f,h}^{(1)} \nabla v = \lambda \nabla v \text{ on } \Omega, \\ \nabla_T v = 0 \text{ on } \partial\Omega, \\ \left(\frac{h}{2}\mathrm{div} - \nabla f \cdot\right) \nabla v = 0 \text{ on } \partial\Omega, \end{cases} \tag{C.33}$$

where

$$L_{f,h}^{(1)} = \frac{h}{2}\Delta - \nabla f \cdot \nabla - \mathrm{Hess}\, f \tag{C.34}$$

is an operator acting on 1-forms (namely on vector fields). Therefore, the vector field ∇v is an eigen-1-form of the operator $-L_{f,h}^{D,(1)}$ which is the operator $-L_{f,h}^{(1)}$ with tangential Dirichlet boundary conditions (see (C.33)), associated with the eigenvalue λ.
The second key point (see for example [15]) is that in our geometric setting, $-L_{f,h}^{D,(0)}$ admits exactly m_0^Ω eigenvalues smaller than $\frac{\sqrt{h}}{2}$ (where we recall m_0^Ω is the number of local minima of f in Ω) and that $-L_{f,h}^{D,(1)}$ admits exactly $m_1^{\overline{\Omega}}$ eigenvalues smaller than $\frac{\sqrt{h}}{2}$ (where, we recall, $m_1^{\overline{\Omega}}$ is the number generalized saddle points of f in $\overline{\Omega}$). Actually, all these small eigenvalues are exponentially small in the regime $h \to 0$, the other eigenvalues being bounded from below by a constant in this regime. This implies in particular that λ_h is a (exponentially) small eigenvalue of $-L_{f,h}^{D,(1)}$. Let us denote by $\pi_h^{(0)}$ (resp. $\pi_h^{(1)}$) the projector onto the vector space spanned by the eigenfunctions (resp. eigenforms) associated with the m_0^Ω (resp. $m_1^{\overline{\Omega}}$) smallest eigenvalue of $-L_{f,h}^{D,(0)}$ (resp. $-L_{f,h}^{D,(1)}$). To prove Theorem C.1, in view of Proposition C.2 and (C.33), the strategy consists in studying the smallest singular values of the matrix of the gradient operator ∇ which maps $\mathrm{Ran}\,\pi_h^{(0)}$ to $\mathrm{Ran}\,\pi_h^{(1)}$. To this end, the idea is then to construct an appropriate basis (with so called quasi-modes) of $\mathrm{Ran}\,\pi_h^{(0)}$ and $\mathrm{Ran}\,\pi_h^{(1)}$. Moreover, from (C.33), $\nabla u_h \in \mathrm{Ran}\,\pi_h^{(1)}$ and thus, to prove Theorem C.2, one decomposes ∇u_h along the basis of $\mathrm{Ran}\,\pi_h^{(1)}$. The terms in the decomposition are approximated using quasi-modes.

The paper is organized as follows. Section C.2 is dedicated to the construction of quasi-modes for $-L_{f,h}^{D,(0)}$ and $-L_{f,h}^{D,(1)}$. In Section C.3, we prove Theorems C.1, C.2 and C.3 and Proposition C.5. Finally, in Section C.4, we discuss the optimality of the remainder terms appearing in Theorems C.1, C.2 and C.3, and Corollary C.6 under the assumption **[H-Connexity]**, and then, we generalized the results obtained in Section C.1.4 to a larger general setting.

C.2 Construction of quasi-modes

This section is concerned with the construction of two families of quasi-modes: a family of functions which aims at approximating the vector space spanned by the eigenfunctions

associated with the m_0^Ω smallest eigenvalues of $-L_{f,h}^{D,(0)}$ and a family of 1-forms which aims at approximating the vector space spanned by the eigenforms associated with the $m_1^{\overline{\Omega}}$ smallest eigenvalues of $-L_{f,h}^{D,(1)}$.

This section is organized as follows. In Section C.2.1, we introduce the notations which are used throughout this paper. In Section C.2.2, we recall the properties of Witten Laplacians and of the operators $L_{f,h}^{D,(p)}$ needed in our analysis. In Section C.2.3, we construct two maps $\mathbf{j}$ and $\widetilde{\mathbf{j}}$ relating local minima to subsets of saddle points of f. These maps are then used to build the quasi-modes in Section C.2.4.

C.2.1 Notation for Sobolev spaces

For $p \in \{0, \dots, d\}$, one denotes by $\Lambda^p C^\infty(\overline{\Omega})$ the space of C^∞ p-forms on $\overline{\Omega}$. Moreover, $\Lambda^p C_T^\infty(\overline{\Omega})$ is the set of C^∞ p-forms v such that $\mathbf{t}v = 0$ on $\partial\Omega$, where $\mathbf{t}$ denotes the tangential trace on forms. For $p \in \{0, \dots, d\}$ and $q \in \mathbb{N}$, one denotes by $\Lambda^p H_w^q(\Omega)$ the weighted Sobolev spaces of p forms with regularity index q, for the weight $e^{-\frac{2}{h}f(x)}$ on Ω: $v \in \Lambda^p H_w^q(\Omega)$ if and only if for all multi-index α with $|\alpha| \leq p$, the α derivative of v is in $\Lambda^p L_w^2(\Omega)$ where $\Lambda^p L_w^2(\Omega)$ is the completion of the space $\Lambda^p C^\infty(\overline{\Omega})$ for the norm

$$w \in \Lambda^p C^\infty(\overline{\Omega}) \mapsto \int_\Omega |w|^2 e^{-\frac{2}{h}f}.$$

See for example [29] for an introduction to Sobolev spaces on manifolds with boundaries. For $p \in \{0, \dots, d\}$ and $q > \frac{1}{2}$, the set $\Lambda^p H_{w,T}^q(\Omega)$ is defined by

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

Notice that $\Lambda^p L_w^2(\Omega)$ is the space $\Lambda^p H_w^0(\Omega)$ and that $\Lambda^0 H_{w,T}^1(\Omega)$ is the space $H_{w,0}^1(\Omega)$ than we introduced in Proposition C.2 to define the domain of $L_{f,h}^{D,(0)}(\Omega)$. We will denote by $\|.\|_{H_w^q}$ the norm on the weighted space $\Lambda^p H_w^q(\Omega)$. Moreover $\langle \cdot, \cdot \rangle_{L_w^2}$ denotes the scalar product in $\Lambda^p L_w^2(\Omega)$.

Finally, we will also use the same notation without the index w to denote the standard Sobolev spaces defined with respect to the Lebesgue measure on Ω.

C.2.2 The Witten Laplacian and the infinitesimal generator of the diffusion (C.1)

In this section, we recall some basic properties of Witten Laplacians, as well as the link between those and the operators $L_{f,h}^{(p)}$ introduced above (see (C.4) and (C.34)).

For $p \in \{0, \dots, n\}$, one defines à la Witten the distorted exterior derivative $d_{f,h}^{(p)} : \Lambda^p \mathcal{C}^\infty(\Omega) \to \Lambda^{p+1} \mathcal{C}^\infty(\Omega)$ and its formal adjoint: $d_{f,h}^{(p)*} : \Lambda^{p+1} \mathcal{C}^\infty(\Omega) \to \Lambda^p \mathcal{C}^\infty(\Omega)$ by

$$d_{f,h}^{(p)} := e^{-\frac{1}{h}f}\, h\, d^{(p)}\, e^{\frac{1}{h}f} \text{ and } d_{f,h}^{(p)*} := e^{\frac{1}{h}f}\, h\, d^{(p)*}\, e^{-\frac{1}{h}f}.$$

The Witten Laplacian, firstly introduced in [33], is then defined similarly as the Hodge Laplacian $\Delta_H^{(p)} := (d + d^*)^2 : \Lambda^p \mathcal{C}^\infty(\Omega) \to \Lambda^p \mathcal{C}^\infty(\Omega)$ by

$$\Delta_{f,h}^{(p)} := (d_{f,h} + d_{f,h}^*)^2 = d_{f,h} d_{f,h}^* + d_{f,h}^* d_{f,h} \ : \ \Lambda^p \mathcal{C}^\infty(\Omega) \to \Lambda^p \mathcal{C}^\infty(\Omega).$$

The Dirichlet realization of $\Delta_{f,h}^{(p)}$ on $\Lambda^p L^2(\Omega)$ is denoted by $\Delta_{f,h}^{D,(p)}$ and its domain is

$$D\left(\Delta_{f,h}^{D,(p)}\right) = \left\{w \in \Lambda^p H^2(\Omega) \mid \mathbf{t}w = 0,\ \mathbf{t}d_{f,h}^{*}w = 0\right\}.$$

The operator $\Delta_{f,h}^{D,(p)}$ is self-adjoint, nonnegative, and its associated quadratic form is given by

$$\phi \in \Lambda^p H_T^1(\Omega) \ \mapsto\ \|d_{f,h}^{(p)}\phi\|_{L^2}^2 + \|d_{f,h}^{(p)*}\phi\|_{L^2}^2,$$

where

$$\Lambda^p H_T^1(\Omega) = \left\{w \in \Lambda^p H^1(\Omega) \mid \mathbf{t}w = 0\right\}.$$

We refer in particular to [15, Section 2.4] for a comprehensive definition of Witten Laplacians with Dirichlet tangential boundary conditions and statements on their properties. The link between the Witten Laplacian and the infinitesimal generator $L_{f,h}^{(0)}$ of the diffusion (C.1), which can be found for example in [22], is explained in the following: since

$$L_{f,h}^{(0)} = -\nabla f \cdot \nabla - \frac{h}{2}\,\Delta_H^{(0)} \ \text{ and } \ \Delta_{f,h}^{(0)} = h^2\Delta_H^{(0)} + |\nabla f|^2 + h\Delta_H^{(0)}, \tag{C.35}$$

one has:

$$\Delta_{f,h}^{D,(0)} = -2\,h\,U\,L_{f,h}^{D,(0)}\,U^{-1}$$

where U is the unitary operator

$$U : \begin{cases} \Lambda^p L_w^2(\Omega) \ \to\ \Lambda^p L^2(\Omega) \\ \phi \mapsto e^{-\frac{1}{h}f}\phi. \end{cases} \tag{C.36}$$

In particular, the operator $L_{f,h}^{D,(0)}$ has a natural extension to p-forms defined by the relation

$$L_{f,h}^{D,(p)} = -\frac{1}{2h}\,U^{-1}\,\Delta_{f,h}^{D,(p)}\,U. \tag{C.37}$$

The operator $L_{f,h}^{D,(p)}$ with domain

$$D\left(L_{f,h}^{D,(p)}\right) = U^{-1}\,D\left(\Delta_{f,h}^{D,(p)}\right) = \left\{w \in \Lambda^p H_w^2(\Omega) \mid \mathbf{t}w = 0,\ \mathbf{t}d_{\frac{2f}{h},1}^{*}w = 0\right\},$$

is then self-adjoint on $\Lambda^p L_w^2(\Omega)$, non positive and the associated quadratic form is

$$\Lambda^p H_T^1(\Omega) \ \ni\ \phi\ \mapsto\ -\frac{h}{2}\Big[\left\|d^{(p)}\phi\right\|_{L_w^2}^2 + \left\|d_{\frac{2f}{h},1}^{(p)*}\phi\right\|_{L_w^2}^2\Big].$$

Let us also recall that $-L_{f,h}^{D,(p)}$ (or equivalently $\Delta_{f,h}^{D,(p)}$) has a compact resolvent. From general results on elliptic operators when $p = 0$, $-L_{f,h}^{D,(0)}$ (or $\Delta_{f,h}^{D,(0)}$) admits a non degenerate smallest eigenvalue with an associated eigenfunction which has a sign on Ω. Denoting moreover by $\pi_E(L_{f,h}^{D,(p)})$ the spectral projector associated with $L_{f,h}^{D,(p)}$ and some Borel set $E \subset \mathbb{R}$, the following commutation relations hold on $\Lambda^p H_T^1(\Omega)$:

$$d^{(p)}\,\pi_E(L_{f,h}^{D,(p)}) = \pi_E(L_{f,h}^{D,(p+1)}(\Omega))\,d^{(p)} \ \text{ and } \ d_{\frac{2f}{h},1}^{(p)*}\,\pi_E(L_{f,h}^{D,(p)}) = \pi_E(L_{f,h}^{D,(p-1)})\,d_{\frac{2f}{h},1}^{(p)*}. \tag{C.38}$$

Noting now that for any bounded Borel set $E \subset \mathbb{R}$, $\operatorname{Ran} \pi_E(L_{f,h}^{D,(d)}) \subset \Lambda^p \mathcal{C}_T^\infty(\Omega)$ from the elliptic regularity of $L_{f,h}^{D,(p)}$, the relation (C.38) leads to the following complex structure:

$$\{0\} \longrightarrow \operatorname{Ran} \pi_E(L_{f,h}^{D,(0)}) \xrightarrow{d} \operatorname{Ran} \pi_E(L_{f,h}^{D,(1)}) \xrightarrow{d} \cdots \xrightarrow{d} \operatorname{Ran} \pi_E(L_{f,h}^{D,(d)}) \xrightarrow{d} \{0\}$$

and

$$\{0\} \xleftarrow{d^*_{\frac{2f}{h},1}} \operatorname{Ran} \pi_E(L_{f,h}^{D,(0)}) \xleftarrow{d^*_{\frac{2f}{h},1}} \operatorname{Ran} \pi_E(L_{f,h}^{D,(1)}) \xleftarrow{d^*_{\frac{2f}{h},1}} \cdots \xleftarrow{d^*_{\frac{2f}{h},1}} \operatorname{Ran} \pi_E(L_{f,h}^{D,(d)}) \longleftarrow \{0\}.$$

For ease of notation, one defines:

$$\forall p \in \{0, \dots, d\}, \quad \pi_h^{(p)} := \pi_{[0, \frac{\sqrt{h}}{2})}(-L_{f,h}^{D,(p)}) = \pi_{(\frac{-\sqrt{h}}{2}, 0]}(L_{f,h}^{D,(p)}). \tag{C.39}$$

The following result, instrumental in our investigation of the smallest eigenvalue λ_h of $-L_{f,h}^{D,(0)}$, is an immediate consequence of [15, Theorem 3.2.3] together with (C.37).

Lemma C.7. *Under assumption [**H-Morse**], there exists $h_0 > 0$ such that for all $h \in (0, h_0)$,*

$$\dim \operatorname{Ran} \pi_h^{(0)} = m_0^\Omega \ \text{ and } \ \dim \operatorname{Ran} \pi_h^{(1)} = m_1^{\overline{\Omega}},$$

where $m_0^\Omega = \operatorname{Card}(\mathcal{U}_0^\Omega)$ and $m_1^{\overline{\Omega}} = \operatorname{Card}(\mathcal{U}_1^{\overline{\Omega}})$ are defined in Section C.1.3.2.

In the sequel, one denotes the exterior differential d acting on functions by ∇. Note that it follows from the above considerations and Lemma C.7 that under [**H-Boundary**] and [**H-Morse**], it holds

$$u_h \in \operatorname{Ran} \pi_h^{(0)} \ \text{ and } \ \nabla u_h \in \operatorname{Ran} \pi_h^{(1)}. \tag{C.40}$$

Moreover, from (C.37), it is equivalent to study the spectrum of $L_{f,h}^{D,(0)}$ or the spectrum of $\Delta_{f,h}^{D,(0)}$. We end this section with the following lemma which will be frequently used throughout this work.

Lemma C.8. *Let $(A, D(A))$ be a non negative self adjoint operator on a Hilbert Space $(\mathcal{H}, \|\cdot\|)$ with associated quadratic form $q_A(x) = (x, Ax)$ whose domain is $Q(A)$. It then holds, for any $u \in Q(A)$ and $b > 0$,*

$$\left\|\pi_{[b,+\infty)}(A)\, u\right\|^2 \leq \frac{q_A(u)}{b},$$

where, for a Borel set $E \subset \mathbb{R}$, $\pi_E(A)$ is the spectral projector associated with A and E.

C.2.3 Association between local minima of f and saddle points of f

This section is dedicated to the construction of two maps: the map $\mathbf{j}$ which associates each local minima of f with a set of saddle points of f and the map $\widetilde{\mathbf{j}}$ which associates each local minima of f with a connected component of a sublevel set of f. This construction requires two preliminary results: Lemma C.9 and Proposition C.11 which are respectively the purposes of Section C.2.3.1 and Section C.2.3.2. Then, the constructions of the maps $\mathbf{j}$ and $\widetilde{\mathbf{j}}$ are made in Section C.2.3.3.

C.2.3.1 A topological result under the assumption [H-Boundary]

This section is concerned with Lemma C.9 which deals with topological aspects of the sublevel sets of the function f under the assumption [**H-Boundary**]. Lemma C.9 will be used several times when constructing the maps $\mathbf{j}$ and $\widetilde{\mathbf{j}}$ in Section C.2.3.3.
Lemma C.9 is stated only under the assumption [**H-Boundary**] and under this assumption, one still defines $\mathcal{U}_1^{\partial\Omega}$ by the relation (C.13) (notice that the equality between (C.13) and (C.14) does not hold in general since it is not assumed that $\nabla f(x) \neq 0$ for all $x \in \partial\Omega$).

Let us first note that under [**H-Boundary**], it holds

$$\min_{\Omega} f = \min_{\overline{\Omega}} f < \min_{\partial\Omega} f \quad \text{and} \quad \mathcal{U}_1^{\partial\Omega} \neq \emptyset. \tag{C.41}$$

Let us explain the second relation in (C.41). Since $\{f < \min_{\partial\Omega} f\}$ is not empty, it has at least one connected component, say C, whose closure meets $\partial\Omega$ (by [**H-Boundary**]), i.e. $\partial\Omega \cap \overline{C} \neq \emptyset$. Let $x \in \partial\Omega \cap \overline{C}$. Since $f(x) = \min_{\partial\Omega} f$, one has $\nabla_T f(x) = 0$ and since $x \in \partial C \cap \partial\Omega$, $\partial_n f(x) \geq 0$. Thus, by [**H-Boundary**], it holds $\partial_n f(x) > 0$ and therefore $x \in \mathcal{U}_1^{\partial\Omega}$. This justifies the second relation in (C.41) and implies

$$\{z \in \arg\min_{\partial\Omega} f, z \,\text{is a local minimum of}\, f \,\text{in}\, \overline{\Omega}\} \cap \overline{\{f < \min_{\partial\Omega} f\}} = \emptyset.$$

Note by the way that the latter relation ogether with the second part of (C.10) implies that

$$\overline{\{f < \min_{\partial\Omega} f\}} = \{f \leq \min_{\partial\Omega} f\} \setminus \{z \in \arg\min_{\partial\Omega} f, z \text{ is a local minimum of } f \text{ in } \overline{\Omega}\}. \tag{C.42}$$

Lemma C.9. *Let us assume that the function $f : \overline{\Omega} \to \mathbb{R}$ is a C^∞ function and that **[H-Boundary]** is satisfied. The following holds:*

1. *The number of connected components of $\{f < \min_{\partial\Omega} f\}$ is finite. We denote by $N_1 \in \mathbb{N}^*$ this number and by $C_1, \ldots, C_{N_1}$ these components.*

2. *The sets $C_1, \ldots, C_{N_1}$ are open sets of Ω and it holds*

$$\cup_{k=1}^{N_1} \partial C_k \subset \{f = \min_{\partial\Omega} f\}, \ \left(\cup_{k=1}^{N_1} \partial C_k\right) \cap \partial\Omega = \mathcal{U}_1^{\partial\Omega} \cap \arg\min_{\partial\Omega} f = \{z_1, ..., z_{k_1^{\partial\Omega}}\}$$

and

$$\forall k \in \{1, \ldots, N_1\}, \ \partial C_k \cap \partial\Omega \cap \mathcal{U}_1^{\partial\Omega} \neq \emptyset.$$

3. *Assume in addition that*

$$d_M := \sup\left\{f(x), \ x \in \overline{\Omega} \ \text{ st } |\nabla f(x)| \neq 0 \ \text{ and } f(x) < \min_{\partial\Omega} f\right\} < \min_{\partial\Omega} f. \tag{C.43}$$

The relation (C.43) *is in particular satisfied when **[H-Morse]** holds. Then, for all $\varepsilon \in (0, \min_{\partial\Omega} f - d_M)$, the set $\{f < \min_{\partial\Omega} f - \varepsilon\}$ has exactly N_1 connected component $C_1(\varepsilon), \ldots, C_{N_1}(\varepsilon)$ such that:*

$$\forall k \in \{1, \ldots, N_1\}, \ C_k(\varepsilon) = C_k \cap \{f < \min_{\partial\Omega} f - \varepsilon\} \subset C_k \tag{C.44}$$

and

$$\overline{\{f < \min_{\partial\Omega} f - \varepsilon\}} = \bigcup_{k=1}^{N_1} \overline{C_k(\varepsilon)} = \{f \leq \min_{\partial\Omega} f - \varepsilon\}. \tag{C.45}$$

Notice that in our geometric setting, any open subset O of $\overline{\Omega}$ is connected if and only if it is path-connected. Indeed, since O is open and $\overline{\Omega}$ is locally path-connected, O is locally path-connected.

Proof. First, the connected components $\big(C_\alpha\big)_{\alpha\in\mathcal{A}}$, of the open set $\{f < \min_{\partial\Omega} f\} \subset \Omega$ are open and connected. For any $\alpha \in \mathcal{A}$, it is moreover clear that $\partial C_\alpha \subset \{f = \min_{\partial\Omega} f\}$. Note also that for any $\alpha \in \mathcal{A}$, $\arg\min_{\overline{C_\alpha}} f$ is a subset of C_α disjoint from the open sets $C_{\alpha'}$, $\alpha' \neq \alpha$, and from $\{f > \frac{1}{2}(\min_{\partial\Omega} f + c_M)\} \subset \overline{\Omega}$, where c_M has been defined in (C.10). The cardinal of $\mathcal{A}$ is hence finite since $\overline{\Omega}$ is compact and the covering

$$\overline{\Omega} = \big(\cup_{\alpha\in\mathcal{A}} C_\alpha\big) \bigcup \Big\{f > \frac{1}{2}(\min_{\partial\Omega} f + c_M)\Big\}$$

is minimal. This proves in particular the first point. To finish the proof of the second point, note that every $z \in \mathcal{U}^{(1)}_{\partial\Omega}$ is obviously in the closure of $\{f < \min_{\partial\Omega} f\}$ and hence in some ∂C_α. Conversely, any ∂C_α meets $\partial\Omega$ according to **[H-Boundary]**, their intersection being contained in $\mathcal{U}^{(1)}_{\partial\Omega}$.

The third point of Lemma C.9 follows from the previous analysis and from Morse theory (see [24]), using the fact that from (C.43),

$$\big\{x \in \overline{\Omega},\ d_M < f(x) < \min_{\partial\Omega} f\big\} \bigcap \big(|\nabla f|\big)^{-1}(\{0\}) = \emptyset.$$

Indeed, this implies that for all $\varepsilon \in (0, \min_{\partial\Omega} f - d_M)$ and $k \in \{1, \ldots, N_1\}$, the open set

$$C_k(\varepsilon) \text{ defined by (C.44)}$$

is a deformation retract of C_k (see [24, Theorem 3.1]) and thus is connected. Note also that the relation

$$\{f < \min_{\partial\Omega} f - \varepsilon\} = \big(\cup_{k=1}^{N_1} C_k\big) \bigcap \big\{f < \min_{\partial\Omega} f - \varepsilon\big\} = \bigcup_{k=1}^{N_1} C_k(\varepsilon)$$

implies the closedness of the sets $C_k(\varepsilon)$'s in $\{f < \min_{\partial\Omega} f - \varepsilon\}$, the above union being disjoint. Hence, the sets $C_k(\varepsilon)$'s being connected and both open and closed in $\{f < \min_{\partial\Omega} f - \varepsilon\}$, they are its connected components. Lastly, it holds $\overline{\{f < \min_{\partial\Omega} f - \varepsilon\}} \subset \{f \leq \min_{\partial\Omega} f - \varepsilon\}$ and the reverse inclusion is true since $\big\{f = \min_{\partial\Omega} f - \varepsilon\big\} \cap |\nabla f|^{-1}(\{0\}) = \emptyset$. ∎

Let us now introduce some notations and a labeling of the connected components of $\{f < \min_{\partial\Omega} f\}$.

Definition C.2. *Let us assume that the function $f : \overline{\Omega} \to \mathbb{R}$ is a C^∞ function and that **[H-Boundary]** is satisfied. Let $\{C_1, ..., C_{N_1}\}$ be the connected components of $\{f <$*

$\min_{\partial\Omega} f\}$ *as introduced in item 1 of Lemma C.9. The integer* N_0 *is defined by the number of* C_k*'s which contains a global minimum of* f *in* Ω*, i.e*

$$N_0 := \mathrm{Card}\Big\{k \in \{1, ..., N_1\},\ C_k \cap \arg\min_{\Omega} f \neq \emptyset\Big\}. \tag{C.46}$$

Notice that $1 \leq N_0 \leq N_1$ *and in the case when* ***[H-Morse]*** *holds, then:*

$$N_0 \leq k_0^{\Omega}.$$

where k_0^{Ω} *is defined in* (C.12)*. The set* $\{C_1, ..., C_{N_1}\}$ *is labeled such that*

$$\forall k \in \{1, ..., N_0\},\ C_k \cap \arg\min_{\Omega} f \neq \emptyset.$$

Notice that with this labelling, C_1 *always contains a global minimum of* f *in* Ω*, and in the case when* ***[H-Connexity]*** *holds, then* $N_0 = 1$ *and* C_1 *is the unique connected components of* $\{f < \min_{\partial\Omega} f\}$ *which contains a global minimum of* f *in* Ω*. Finally, for all* $k \in \{1, ..., N_1\}$*,* C_k *is denoted by*

$$E_{1,k} := C_k. \tag{C.47}$$

C.2.3.2 Separating saddle points

This section is devoted to the proof of Proposition C.11 which will be needed when constructing the maps $\mathbf{j}$ and $\widetilde{\mathbf{j}}$ in Section C.2.3.3. Let us first prove the following lemma which will be used in the proof of Proposition C.11.

Lemma C.10. *Let us assume that the function* $f : \overline{\Omega} \to \mathbb{R}$ *is a* C^{∞} *function. Let* $x \in \overline{\Omega}$*. For all* $\mu > f(x)$*, we denote respectively by* $C_x(\mu)$ *and* $C_x^+(\mu)$ *the connected components of* $\{f < \mu\}$ *and of* $\{f \leq \mu\}$ *containing* x*. Then, it holds:*

$$C_x(\mu) = \bigcup_{\lambda < \mu} C_x(\lambda) \tag{C.48}$$

and

$$C_x^+(\mu) = \bigcap_{\lambda > \mu} C_x^+(\lambda). \tag{C.49}$$

Proof. The proof is divided into two steps.
Step 1. Let us first prove (C.48). Since $\{f < \lambda\}$ is open in the locally connected space $\overline{\Omega}$, the set $C_x(\lambda) \subset \overline{\Omega}$ is open for all $\lambda \in (f(x), \mu)$. Since moreover $C_x(\lambda) \subset C_x(\mu)$ for all $\lambda \in (f(x), \mu)$, the union $\cup_{\lambda \in (f(x),\mu)} C_x(\lambda)$ is an open subset of $C_x(\mu)$. Therefore, since $C_x(\mu)$ is connected, to obtain (C.48), it is enough to prove that the set $\cup_{\lambda \in (f(x),\mu)} C_x(\lambda)$ is closed in $C_x(\mu)$. To this end, let us show that the complement of $\cup_{\lambda \in (f(x),\mu)} C_x(\lambda)$ in $C_x(\mu)$ is open. It is obviously the case if it is empty. If $\cup_{\lambda \in (f(x),\mu)} C_x(\lambda)$ is not empty, let us choose

$$y \in C_x(\mu) \setminus \cup_{\lambda \in (f(x),\mu)} C_x(\lambda).$$

Then, since $y \in C_x(\mu)$, one has $f(y) < \mu$ and thus $y \in C_y(\lambda) \cap C_x(\mu)$ for all $\lambda \in (f(y), \mu)$. Therefore, it holds $C_y(\lambda) \subset C_x(\mu)$ and $C_y(\lambda) \cap C_x(\lambda) = \emptyset$ for all $\lambda \in (\max\{f(x), f(y)\}, \mu)$. Hence, the open set $C_y(\lambda)$ is included in $C_x(\mu)$ and disjoint from

the set $\cup_{\lambda\in(f(x),\mu)}C_x(\lambda)$ for all $\lambda \in (f(y),\mu)$. This proves that $\cup_{\lambda\in(f(x),\mu)}C_x(\lambda)$ is closed in $C_x(\mu)$. This concludes the proof of (C.48).

Step 2. Let us now prove (C.49). Since for all λ, $C_x^+(\lambda)$ is a connected component of $\{f \le \lambda\}$, it is closed in this closed set of $\overline{\Omega}$ and thus it is closed in $\overline{\Omega}$. It follows that the set $\cap_{\lambda>\mu}C_x^+(\lambda)$ is compact and connected as a decreasing intersection of compact connected sets. Since $\cap_{\lambda>\mu}C_x^+(\lambda)$ is also obviously included in $\{f \le \mu\}$ and contains x, it is then included in $C_x^+(\mu)$ by definition of $C_x^+(\mu)$. The reverse inclusion follows from the fact that $C_x^+(\mu) \subset C_x^+(\lambda)$ for all $\lambda > \mu$. This proves (C.49) and ends the proof of Lemma C.10. ∎

The constructions of the maps $\mathbf{j}$ and $\widetilde{\mathbf{j}}$ made in Section C.2.3.3 are based on the notions of separating saddle points and of sritical components as introduced in [17, Section 4.1]. Let us define and slightly adapt theses two notions in our setting. To this end, let us first recall that according to [15, Section 5.2], for any non critical point $z \in \Omega$, for $r > 0$ small enough

$$\{f < f(z)\} \cap B(z,r) \text{ is connected,} \tag{C.50}$$

and for any critical point $z \in \Omega$ of order p of the Morse function f, for $r > 0$ small enough, one has the three possible cases:

$$\begin{cases} \text{either } p = 0 \ (z \text{ is a local minimum of } f) \text{ and } \{f < f(z)\} \cap B(z,r) = \emptyset, \\ \text{or } p = 1 \text{ and } \{f < f(z)\} \cap B(z,r) \text{ has exactly two connected components,} \\ \text{or } p \ge 2 \text{ and } \{f < f(z)\} \cap B(z,r) \text{ is connected,} \end{cases} \tag{C.51}$$

where $B(z,r) := \{x \in \overline{\Omega} \text{ s.t. } |x - z| < r\}$. The separating saddle points of f and the sritical components of f are defined as follows.

Definition C.3. *Assume hypotheses **[H-Boundary]** and **[H-Morse]**.*

1. *A point $z \in U_1^{\overline{\Omega}}$ is a* separating saddle point *if*
   - *either $z \in \mathcal{U}_1^{\Omega} \cap \{f \le \min_{\partial\Omega} f\}$ and, if, for $r > 0$ small enough, the two connected components of $\{f < f(z)\} \cap B(z,r)$ are contained in different connected components of $\{f < f(z)\}$,*
   - *or $z \in \mathcal{U}_1^{\partial\Omega} \cap \arg\min_{\partial\Omega} f = \{z_1, ..., z_{k_1^{\partial\Omega}}\}$.*

   Notice that in the former case $z \in \Omega$ while in the latter case $z \in \partial\Omega$. The set of separating saddle points *is denoted by $\mathcal{U}_1^{ssp}$.*

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

In Figure C.3, one gives an example of a saddle point z which is not a separating saddle point as introduced in Definition C.3. Let us mention that according to Definition C.3, one has:

$$\mathcal{U}_1^{ssp} \cap \{f < \min_{\partial\Omega} f\} \subset \mathcal{U}_1^{\Omega} \quad \text{and} \quad \mathcal{U}_1^{ssp} \subset \mathcal{U}_1^{\overline{\Omega}} \cap \{f \le \min_{\partial\Omega} f\}.$$

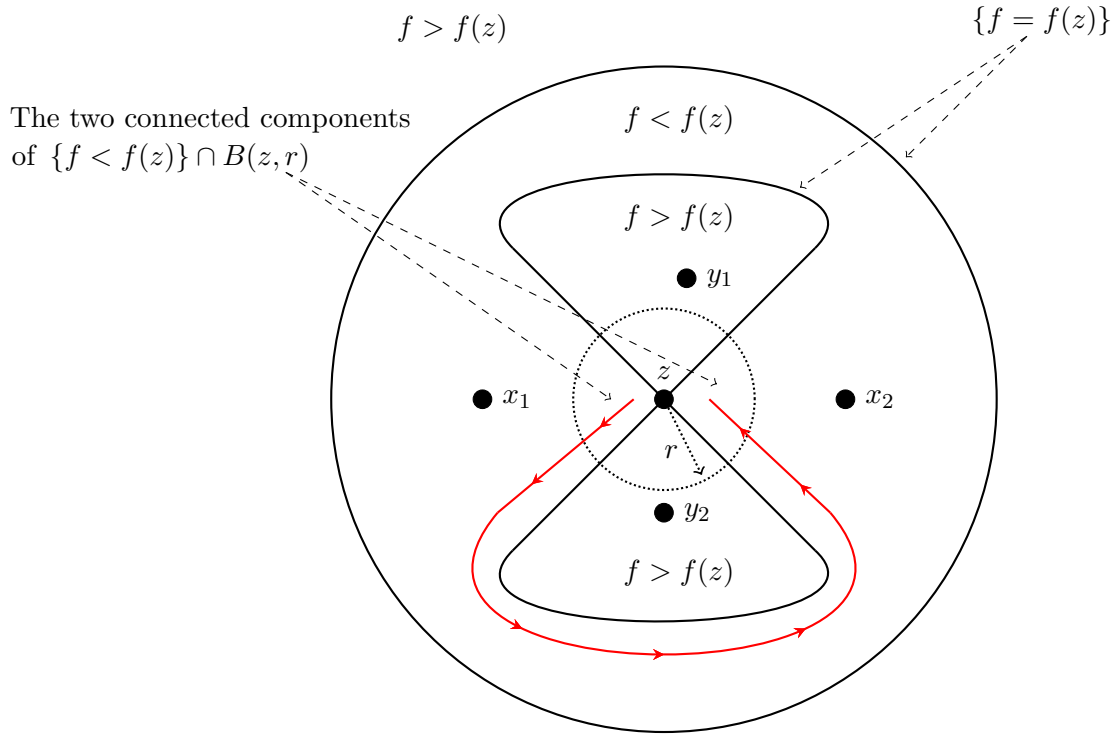

Figure C.3: Representation of a non separating saddle point z in dimension 2. The points x_1 and x_2 are two local minima of f, and the points y_1 and y_2 are two local maxima of f. The two connected components of $\{f < f(z)\} \cap B(z,r)$ are contained in the same connected components of $\{f < f(z)\}$: any two points of these two connected components can be joined by a path with values in $\{f < f(z)\}$ (see the red path on the figure).

One is now in position to prove the following proposition which will be used in the construction of the maps $\mathbf{j}$ and $\widetilde{\mathbf{j}}$ in Section C.2.3.3 .

Proposition C.11. *Let us assume that the assumptions **[H-Boundary]** and **[H-Morse]** are satisfied. Let $\lambda \in (\min_\Omega f, \min_{\partial\Omega} f]$ and C be a connected component of $\{f < \lambda\}$. Then,*

$$\left(C \cap \mathcal{U}_1^{ssp} \neq \emptyset\right) \quad \textit{iff} \quad C \cap \mathcal{U}_0^{\Omega} \textit{ contains more than one point.} \tag{C.52}$$

Moreover, let us define $\sigma := \max_{C \cap \mathcal{U}_1^{ssp}} f$ with the convention $\sigma = \min_C f$ when $C \cap \mathcal{U}_1^{ssp} = \emptyset$. Then, the following assertions hold.

1. *The set $C \cap \{f < \mu\}$ is connected for all $\mu \in (\sigma, \lambda]$,*
2. *If $C \cap \mathcal{U}_1^{ssp} \neq \emptyset$, one has $C \cap \mathcal{U}_0^{\Omega} \subset \{f < \sigma\}$ and the connected components of $C \cap \{f < \sigma\}$ belong to $\mathcal{C}_{crit}$.*

Proof. Notice that from the assumption **[H-Boundary]** and since $\lambda \in (\min_\Omega f, \min_{\partial\Omega} f]$, the set C is an open subset of Ω (since Ω is locally connected). The proof of Proposition C.11 is divided into three steps.

Step 1. Proof of (C.52).
The fact that

$$\left(C \cap \mathcal{U}_1^{ssp} \neq \emptyset\right) \quad \text{implies} \quad C \cap \mathcal{U}_0^{\Omega} \text{ contains more than one point} \tag{C.53}$$

is straightforward. Indeed, let $z \in C \cap \mathcal{U}_1^{ssp}$. Since $f(z) < \lambda \leq \min_{\partial\Omega} f$, $z \in \mathcal{U}_1^{\Omega} \cap \{f < \min_{\partial\Omega} f\}$ and for $r > 0$ small enough, the two connected components of $\{f < f(z)\} \cap B(z,r)$ are contained in different connected components of $\{f < f(z)\}$ (see item 1 in Definition C.3). Then, since the set C is a connected component of $\{f < \lambda\}$, C contains at least two open connected components C_1 and C_2 of $\{f < f(z)\}$. Moreover, for $k \in \{1,2\}$, $\partial C_k \subset \{f = f(z)\}$. Thus, for $k \in \{1,2\}$, the global minimum of f on $\overline{C_k}$ is reached in C_k and hence at some $x_k \in C_k \cap \mathcal{U}_0^{\partial\Omega}$. This implies that $C \cap \mathcal{U}_0^{\Omega}$ contains at least two elements, x_1 and x_2.
Let us now prove the reverse implication in (C.53). To this end, let us assume that there exist two points $x \neq y$ in $C \cap \mathcal{U}_0^{\Omega}$. Let

$$x \in \arg\min_{\overline{C}} f = \arg\min_{C} f \in \mathcal{U}_0^{\Omega} \quad \text{and} \quad y \in C \cap \mathcal{U}_0^{\Omega} \setminus \{x\}.$$

Let us define for $\mu > f(y)$,

$$C(\mu, y) \quad \text{as the connected component of } \{f < \mu\} \text{ containing } y \tag{C.54}$$

as well as,

$$\lambda(y) := \sup\{\mu > f(y) \text{ s.t. } x \notin C(\mu, y)\}, \quad \text{and} \quad C(y) := C(\lambda(y), y). \tag{C.55}$$

Let us show that

$$f(y) < \lambda(y) < \lambda. \tag{C.56}$$

Notice first that $\lambda(y)$ is well defined since $\{\mu > f(y) \text{ s.t. } x \notin C(\mu, y)\}$ is non empty and bounded. Indeed, since y is a non degenerate local minimum of f, for $\beta > 0$ sufficiently small, $f(w) > f(y)$ for all $w \in C(f(y) + \beta, y)$, $w \neq y$. Therefore, $x \notin C(f(y) + \beta, y)$ (because $x \neq y$ and $f(x) \leq f(y)$). Moreover for all $\eta \in \{\mu > f(y) \text{ s.t. } x \notin C(\mu, y)\}$, $\eta < \lambda$ (because $x, y \in C$ implies $C(\lambda, y) = C$ since $C(\lambda, y)$ and C are both connected components of $\{f < \lambda\}$). Therefore, $\lambda(y)$ is well defined and satisfies $f(y) < \lambda(y) \leq \lambda$ (which proves the first inequality in (C.56)). Since $\mu \mapsto C(\mu, y)$ is increasing on $(f(y), +\infty)$, it holds $x \notin C(\mu, y)$ for all $\mu \in (f(y), \lambda(y))$ by definition of $\lambda(y)$. Thus, since according to Lemma C.10 (see (C.48)),

$$C(\lambda(y), y) = \bigcup_{\mu \in (f(y), \lambda(y))} C(\mu, y),$$

the set $C(\lambda(y), y)$ does not contain x and hence $\lambda(y) < \lambda$. This proves (C.56). Notice that (C.56) implies

$$\overline{C(\lambda(y), y)} \subset C \tag{C.57}$$

Let us now prove that $\partial C(\lambda(y), y) \cap \mathcal{U}_1^{ssp} \neq \emptyset$ which will conclude the proof of (C.53). Let us prove it by contradiction and let us assume that $\partial C(\lambda(y), y) \cap \mathcal{U}_1^{ssp} = \emptyset$. Then, using in addition the fact the function f is Morse and the fact that

$$\partial C(\lambda(y), y) \subset \{f = \lambda(y)\} \subset \Omega, \tag{C.58}$$

(where the second inclusion follows from (C.56)), for all $z \in \partial C(\lambda(y), y)$,

- either $z \notin \mathcal{U}_1^\Omega$ in which case there exists $r_z > 0$ such that $B(z, r_z) \cap \{f < \lambda(y)\}$ is connected (see (C.50)) and thus $B(z, r_z) \cap \{f < \lambda(y)\}$ is included in $C(\lambda(y), y)$,
- or $z \in \mathcal{U}_1^\Omega$ in which case there exists $r_z > 0$ such that $B(z, r_z) \cap \{f < \lambda(y)\}$ has two connected components both included in $C(\lambda(y), y)$ (because we assume that there is no separating saddle point on $\partial C(\lambda(y), y)$).

In all cases, one can assume, choosing r_z smaller, that $B(z, r_z) \subset \Omega$ and $B(z, r_z) \cap \mathcal{U}_0^\Omega = \emptyset$. Let us now consider

$$\mathcal{V} := \Big(\cup_{z \in \partial C(\lambda(y), y)} B(z, r_z) \Big) \bigcup C(\lambda(y), y).$$

Then, the set $\mathcal{V}$ is an open subset of Ω such that $\overline{C(\lambda(y), y)} \subset \mathcal{V}$ and $\mathcal{V} \cap \{f \leq \lambda(y)\} = \overline{C(\lambda(y), y)}$. Therefore, the connected set $\overline{C(\lambda(y), y)}$ is closed and open in $\{f \leq \lambda(y)\}$, and thus

$$\overline{C(\lambda(y), y)} \text{ is a connected component of } \{f \leq \lambda(y)\}. \tag{C.59}$$

Let us now denote, for $\mu \geq \lambda(y)$, by $C^+(\mu, y)$ the connected component of $\{f \leq \mu\}$ containing $\overline{C(\lambda(y), y)}$. It then holds, according to Lemma C.10 (see (C.49)),

$$\bigcap_{\mu > \lambda(y)} C^+(\mu, y) = C^+(\lambda(y), y) = \overline{C(\lambda(y), y)}. \tag{C.60}$$

In addition, for all $\mu > \lambda(y)$, $x \in C(\mu, y)$ by definition of $\lambda(y)$, and $C(\mu, y) \subset C^+(\mu, y)$. Thus, using (C.60), $x \in \overline{C(\lambda(y), y)}$ and hence, since $x \notin C(\lambda(y), y)$, it holds $f(x) = \lambda(y) > f(y)$. This contradicts the fact that that $x \in \arg\min_{\overline{C}} f$. Therefore, we have proven that

$$\partial C(\lambda(y), y) \cap \mathcal{U}_1^{ssp} \neq \emptyset. \tag{C.61}$$

Using (C.57), this implies that $C \cap \mathcal{U}_1^{ssp} \neq \emptyset$ which concludes the proof of the reverse implication in (C.53) and thus the proof of (C.52).

Step 2. Proof of item 1 in Proposition C.11.
Let us first deal with the case $\mathcal{U}_1^{ssp} \cap C = \emptyset$. In that case, the set $C \cap \mathcal{U}_0^\Omega$ is reduced to one element. This implies that for all $\lambda \in (\min_C f, \lambda]$, the set $C \cap \{f < \lambda\}$ is connected since each of its connected components necessarily contains at least one element of $\mathcal{U}_0^\Omega$. Let us now deal with the case $\mathcal{U}_1^{ssp} \cap C \neq \emptyset$. Let us then consider $x \in \arg\min_C f \subset \mathcal{U}_0^\Omega$ and, for every $y \in C \cap \mathcal{U}_0^\Omega \setminus \{x\}$, let $\lambda(y)$ be as defined in (C.55). Let us also define

$$\sigma := \max\{\lambda(y); y \in C \cap \mathcal{U}_0^\Omega \setminus \{x\}\}, \tag{C.62}$$

which is well defined since the set $\{y \in C \cap \mathcal{U}_0^\Omega \setminus \{x\}\}$ is non empty (by (C.52)) and contains a finite number of elements (since f is Morse). Then, from (C.56), (C.61) and the first inclusion in (C.58), one has

$$\sigma \in (\min_C f, \lambda) \cap \{f(z),\, z \in \mathcal{U}_1^{ssp}\}. \tag{C.63}$$

Then, since for all $\mu \in (\sigma, \lambda]$ and for all $y \in C \cap \big(\mathcal{U}_0^\Omega \setminus \{x\}\big)$, $x \in C(\mu, y)$ (because $\mu > \lambda(y)$ and by definition of $\lambda(y)$, see (C.55)) and since the $C(\mu, y)$'s are connected

components of $\{f < \mu\}$, one obtains that $C(\mu, y) = C(\mu, w)$ for all $y, w \in C \cap \big(\mathcal{U}_0^\Omega \setminus \{x\}\big)$. Thus, one has

$$\text{for all } \mu \in (\sigma, \lambda] \text{ and for all } y \in C \cap \big(\mathcal{U}_0^\Omega \setminus \{x\}\big), \quad C \cap \mathcal{U}_0^\Omega \subset C(\mu, y). \tag{C.64}$$

This implies that for any $y \in C \cap \big(\mathcal{U}_0^\Omega \setminus \{x\}\big)$, $\{f < \mu\} \cap C$ is equal to $C(\mu, y)$ (since every connected component of $\{f < \mu\} \cap C$ contains at least one element of $\mathcal{U}_0^\Omega$).

$$\forall \mu \in (\sigma, \lambda], \ \{f < \mu\} \cap C \text{ is connected.} \tag{C.65}$$

Moreover, it holds

$$\sigma = \max_{x \in \mathcal{U}_1^{ssp} \cap C} f(x). \tag{C.66}$$

Indeed, if it is not the case, then from (C.63), one has $\sigma < \max_{x \in \mathcal{U}_1^{ssp} \cap C} f(x)$ and thus C contains at least two connected components of $\{f < \max_{\mathcal{U}_1^{ssp} \cap C} f\}$ with $\max_{\mathcal{U}_1^{ssp} \cap C} f > \sigma$, which contradicts (C.65). Item 1 in Proposition C.11 follows from (C.65) and (C.66).

Step 3. Proof of item 2 in Proposition C.11. Let us assume that $\mathcal{U}_1^{ssp} \cap C \neq \emptyset$. Then, using (C.52), $C \cap \mathcal{U}_0^\Omega$ contains at least two elements. Let $x \in \arg\min_C f$ and $y \in C \cap \mathcal{U}_0^\Omega \setminus \{x\}$. Then $f(x) \leq f(y)$ and according to (C.56), it holds $f(y) < \lambda(y)$. From (C.66) and (C.62), it holds moreover

$$\sigma := \max_{\mathcal{U}_1^{ssp} \cap C} f \geq \lambda(y).$$

Therefore $f(x) \leq f(y) < \sigma$ and thus

$$C \cap \mathcal{U}_0^\Omega \subset \{f < \sigma\}. \tag{C.67}$$

This proves the first statement of item 2 in Proposition C.11.
Let us now prove that each connected component of $C \cap \{f < \sigma\}$ is a critical connected component (as introduced in item 2 in Definition C.3). Let us first notice that $C \cap \mathcal{U}_0^\Omega \subset \{f < \sigma\}$ implies

$$C \cap \{f < \sigma\} = \bigcup_{w \in \mathcal{U}_0^\Omega \cap C} C(\sigma, w), \tag{C.68}$$

where $C(\sigma, w)$ is defined in (C.54) (since every connected component of $C \cap \{f < \sigma\}$ contains at least one element of $\mathcal{U}_0^\Omega$). Let us consider a connected component of $C \cap \{f < \sigma\}$. From (C.68), this component has the form $C(\sigma, y)$ for some $y \in \mathcal{U}_0^\Omega$. Since $\sigma \in f(\mathcal{U}_1^{ssp})$ (see (C.63)), $C \cap \{f < \sigma\}$ contains at least two connected components, and thus $(C \cap \mathcal{U}_0^\Omega) \setminus C(\sigma, y) \neq \emptyset$. Let $w \in (C \cap \mathcal{U}_0^\Omega) \setminus C(\sigma, y)$. Let us assume that $C(\sigma, y)$ is not a critical connected component, i.e that $\partial C(\sigma, y) \cap \mathcal{U}_1^{ssp} = \emptyset$. Then, the arguments used to prove (C.59) imply that $\overline{C(\sigma, y)}$ is a connected component of $\{f \leq \sigma\}$. Thus, using Lemma C.10 (see (C.49)), it holds

$$\cap_{\lambda > \sigma} C^+(\lambda, y) = \overline{C(\sigma, y)}.$$

Moreover, since for all $\lambda > \sigma$, $w \in C(\lambda, y)$ (see (C.64)) and $C(\lambda, y) \subset C^+(\lambda, y)$, it holds $w \in \overline{C(\sigma, y)}$. Therefore, since $f(w) < \sigma$ (see (C.67)), one has $w \in C(\sigma, y)$ which contradicts the fact that $w \in (C \cap \mathcal{U}_0^\Omega) \setminus C(\sigma, y)$. This ends the proof of Proposition C.11. ∎

C.2.3.3 Construction of the maps $\mathbf{j}$ and $\widetilde{\mathbf{j}}$

In this section we construct, under [**H-Boundary**] and [**H-Morse**], two maps $\mathbf{j}$ and $\widetilde{\mathbf{j}}$ which rely on an association between the local minima of f and its (generalized) saddle points $\mathcal{U}_1^{\overline{\Omega}}$. Associations between the local minima of f and the saddle points of f have been introduced in [1, 2] and [14, 17] in the boundaryless case in order to give sharp asymptotic estimates of the eigenvalues of the involved operators. This association has been generalized in [15] in the boundary case (in which the authors introduced the notion of generalized saddle points for $\Delta_{f,h}^{D,(0)}$).

Let us recall that from Lemma C.7, $L_{f,h}^{D,(0)}$ has exactly m_0^{Ω} smaller than $\sqrt{h}$ in the limit h to 0. Actually, from [15, 16], it can be shown that these m_0^{Ω} eigenvalues are exponentially small. The goal of the map $\mathbf{j}$ is to associate each local minimum x of f with a set of generalized saddle points $\mathbf{j}(x) \subset \mathcal{U}_1^{\overline{\Omega}}$ such that

$$\forall z, y \in \mathbf{j}(x),\ f(z) = f(y),$$

and such that, in the limit $h \to 0$, there exists at least one eigenvalue of $-L_{f,h}^{D,(0)}$ whose exponential rate of decay is $2\big(f(\mathbf{j}(x)) - f(x)\big)$ i.e.

$$\exists \lambda \in \sigma\big(L_{f,h}^{D,(0)}\big) \text{ such that } \lim_{h\to 0} h \log \lambda = -2\big(f(\mathbf{j}(x)) - f(x)\big).$$

The aim of the map $\widetilde{\mathbf{j}}$ is to associate each local minimum x of f with the connected component of $\{f < f(\mathbf{j}(x))\}$ which contains x. To make the link with the metastability of the process (C.1), the saddle points $\mathbf{j}(x)$ are the points through which the process (C.1) leaves $\widetilde{\mathbf{j}}(x)$ in the limit $h \to 0$. To construct the maps $\mathbf{j}$ and $\widetilde{\mathbf{j}}$, the procedure one uses in this work relies on the analysis of the sublevel sets of f which follows from the general analysis of the sublevel sets of a Morse function on a manifold without boundary which is done in [17, Section 4.1], where the authors generalize the procedure described in [14]. To build the maps $\mathbf{j}$ and $\widetilde{\mathbf{j}}$, the procedure consists in detecting the connected components of $\{f \leq \lambda\} \cap \mathcal{U}_1^{ssp}$ when λ is decreasing from $\min_{\partial\Omega} f$ to $-\infty$. In each new connected component, we pick arbitrarily a local minima and then, we associate this local minima with the separating saddle points on the boundary of this new connected component. The construction of $\mathbf{j}$ and $\widetilde{\mathbf{j}}$ is made recursively and each step of the recurrence corresponds an intersection between $\{f \leq \lambda\}$ and the set of separating saddle points $\mathcal{U}_1^{ssp}$.

Let assume that the assumptions [**H-Boundary**] and [**H-Morse**] hold. The construction of the maps $\mathbf{j}$ and $\widetilde{\mathbf{j}}$ is made recursively as follows:

1. Step 1. Let us consider $\{f = \min_{\partial\Omega} f\}$.
   For $k \in \{1, \ldots, N_1\}$, let $x_{1,k}$ denote one point in $\arg\min_{\overline{E_{1,k}}} f(x) = \arg\min_{E_{1,k}} f$, where $E_{1,k}$ is defined in (C.47). In addition, let us define

   $$\sigma_1 := \min_{x\in\partial\Omega} f(x),\ \ \widetilde{\mathbf{j}}(x_{1,k}) := E_{1,k} \in \mathcal{C}_{crit},\ \text{ and }\ \mathbf{j}(x_{1,k}) := \partial E_{1,k} \cap \mathcal{U}_1^{ssp}.$$

   Note that according to Lemma C.9, it holds

   $$\big(\cup_{k=1}^{N_1} \mathbf{j}(x_{1,k})\big) \cap \partial\Omega = \mathcal{U}_1^{\partial\Omega} \cap \arg\min_{\partial\Omega} f = \mathcal{U}_1^{ssp} \cap \partial\Omega = \{z_1, ..., z_{k_1^{\partial\Omega}}\}.$$

Moreover, one has under [**H-connexity**] (see (C.18) and (C.19))

$$\mathbf{j}(x_{1,1}) \cap \partial\Omega = \{z_1, ..., z_{k_1^{\partial C_1}}\} = \partial\Omega \cap \partial C_1. \tag{C.69}$$

According to the labelling introduced in Definition C.2, $E_{1,1} \cap \arg\min_\Omega f \neq \emptyset$ implies $x_{1,1} \in \arg\min_\Omega f$. Moreover, one has (see indeed (C.51) and Definition C.3),

$$\forall k \neq l \in \{1, \dots, N_1\},\ \partial E_{1,k} \cap \partial E_{1,l} \subset \mathcal{U}_1^{ssp} \cap \mathcal{U}_1^\Omega \cap \{f = \min_{\partial\Omega} f\}. \tag{C.70}$$

2. Step 2. Let us now consider $\{f < \lambda\}$ for $\lambda < \sigma_1$.

From Proposition C.11, for each $k \in \{1, \dots, N_1\}$, $C_k \cap \mathcal{U}_0^\Omega \neq \{x_{1,k}\}$ if and only if $\mathcal{U}_1^{ssp} \cap C_k \neq \emptyset$. As a consequence, one has:

$$\mathcal{U}_1^{ssp} \cap \{f < \min_{\partial\Omega} f\} \neq \emptyset \ \text{ iff } \ \{x_{1,1}, \dots, x_{1,N_1}\} \neq \mathcal{U}_0^\Omega.$$

If $\mathcal{U}_1^{ssp} \cap \{f < \min_{\partial\Omega} f\} \neq \emptyset$, one defines

$$\sigma_2 := \max_{x \in \mathcal{U}_1^{ssp} \cap \{f < \min_{\partial\Omega} f\}} f(x) \ \in \ (\min_\Omega f, \min_{\partial\Omega} f).$$

The sublevel set $\{f < \sigma_2\}$ is then the union of finitely many connected components and we denote by $E_{2,1}, \dots, E_{2,N_2}$ (with $N_2 \geq 1$) the ones which do not contain any of the minima $x_{1,l}$, $l \in \{1, \dots, N_1\}$. Let us associate with each $E_{2,k}$, $1 \leq k \leq N_2$, one point $x_{2,k}$ arbitrarily chosen in $\arg\min_{\overline{E_{2,k}}} f = \arg\min_{E_{2,k}} f$ (the last equality follows from the fact that $\partial E_{2,k} \subset \{f = \sigma_2\}$). From Proposition C.11,

$$\forall k \in \{1, ..., N_2\},\ E_{2,k} \in \mathcal{C}_{crit},$$

while the other connected components (i.e. those containing the $x_{1,i}$) may be non critical. Let us define, for $1 \leq k \leq N_2$,

$$\widetilde{\mathbf{j}}(x_{2,k}) := E_{2,k} \text{ and } \mathbf{j}(x_{2,k}) := \partial E_{2,k} \cap \mathcal{U}_1^{ssp} \subset \{f = \sigma_2\}.$$

Notice that from Proposition C.11, it holds

$$\forall k \in \{1, \dots, N_1\} \text{ s.t. } C_k \cap \mathcal{U}_0^\Omega \neq \{x_{1,k}\},\ \ C_k \cap \mathcal{U}_0^\Omega \subset \{f < \sigma_2\}.$$

3. Step 3. Let us now consider $\{f < \lambda\}$ for $\lambda < \sigma_2$.

From Proposition C.11, if all the minima of f have not been yet considered at the previous step, it holds

$$\mathcal{U}_1^{ssp} \cap \{f < \sigma_2\} \neq \emptyset.$$

In that case, we define

$$\sigma_3 := \max_{x \in \mathcal{U}_1^{ssp} \cap \{f < \sigma_2\}} f(x).$$

Then, one denotes by $E_{3,1}, \dots, E_{3,N_3}$ (with $N_3 \geq 1$) the connected components of $\{f < \sigma_3\}$ which do not contain any of the already labeled minima $x_{1,k}, x_{2,l}$, $1 \leq k \leq N_1$, $1 \leq l \leq N_2$. These components belong to $\mathcal{C}_{crit}$. Proceeding now as in the previous step, let $x_{3,k}$ be one point in $\arg\min_{E_{3,k}} f$ and let us define, for $1 \leq k \leq N_3$,

$$\widetilde{\mathbf{j}}(x_{3,k}) := E_{3,k} \text{ and } \mathbf{j}(x_{3,k}) := \partial E_{3,k} \cap \mathcal{U}_1^{ssp} \subset \{f = \sigma_3\}.$$

4. <u>End of the recurrence.</u>
One continues this procedure until all the values of $f(\mathcal{U}_1^{ssp})$ have been considered. Let us emphasize that according to Proposition C.11, all the local minima of f are labeled after the last step. This defines two mappings:

$$\widetilde{\mathbf{j}} \,:\, \mathcal{U}_0^{\Omega} \longrightarrow \mathcal{C}_{crit} \quad \text{and} \quad \mathbf{j} \,:\, \mathcal{U}_0^{\Omega} \longrightarrow \mathcal{P}(\mathcal{U}_1^{\overline{\Omega}}) \tag{C.71}$$

which are clearly injective. Notice that the $\mathbf{j}(x)$, $x \in \mathcal{U}_0^{\Omega}$, are not disjoint in general. Note lastly that for all $x \in \mathcal{U}_0^{\Omega}$, $f(\mathbf{j}(x))$ contains exactly one value, which will be denoted by $f(\mathbf{j}(x))$, and that $\mathbf{j}(x) \in \mathcal{U}_1^{\Omega} \cap \{f < \min_{\partial\Omega} f\}$ when $x \notin \{x_{1,1}, \ldots, x_{1,N_1}\}$.
Let us now give important features of the map $\mathbf{j}$ which follows directly from its construction. First, one has $\forall x \in \mathcal{U}_0^{\Omega},\ f(\mathbf{j}(x)) - f(x) > 0$ and

$$\forall k \in \{1, ..., N_1\} \text{ and } \forall x \in \mathbf{j}(x_k),\ f(x) = f(z_1) \tag{C.72}$$

Secondly, from the definition of N_0 introduced in Definition C.2, one has for all $(k, l) \in \{1, ..., N_0\}^2$

$$f(\mathbf{j}(x_{1,k})) - f(x_{1,k}) = f(\mathbf{j}(x_{1,l})) - f(x_{1,l}) = f(z_1) - f(x_{1,1}), \tag{C.73}$$

and

$$\forall x \in \mathcal{U}_0^{\Omega} \setminus \{x_{1,1}, \ldots, x_{1,N_0}\},\ f(\mathbf{j}(x)) - f(x) < f(\mathbf{j}(x_{1,1})) - f(x_{1,1}) = f(z_1) - f(x_{1,1}), \tag{C.74}$$

since $f(\mathbf{j}(x_{1,1})) = f(z_1) = \min_{\partial\Omega} f$, see (C.17) for the definition of z_1. Finally, one has

$$\cup_{k=1}^{N_1} \mathbf{j}(x_{1,k}) \cap \partial\Omega = \{z_1, ..., z_{k_1^{\partial\Omega}}\}, \tag{C.75}$$

where $\{z_1, ..., z_{k_1^{\partial\Omega}}\}$ is defined in (C.17) and

$$\forall x \in \mathcal{U}_0^{\Omega} \setminus \{x_{1,1}, \ldots, x_{1,N_1}\},\ \mathbf{j}(x_k) \subset \Omega. \tag{C.76}$$

In Figure C.4, the construction of the maps $\mathbf{j}$ and $\widetilde{\mathbf{j}}$ is given for a one dimensional example. Since, one can pick a minimum rather than an other in a critical connected component at each step of the construction of $\mathbf{j}$ and $\widetilde{\mathbf{j}}$, it can occur that several constructions are possible. The results of Theorem C.1, Theorem C.2, Proposition C.5, Corollary C.6 and Theorem C.3 do not depend on a particular choice of the maps $\mathbf{j}$ and $\widetilde{\mathbf{j}}$. In Figure C.5, we give an example for which two equivalent constructions of the maps $\mathbf{j}$ and $\widetilde{\mathbf{j}}$ are possible.

Remark C.5. *In the case when for all local minima x of f, $\mathbf{j}(x)$ is a point, $\mathbf{j}(x) \cap \mathbf{j}(y) = \emptyset$ for all $x \neq y$ and when all the heights $(f(\mathbf{j}(x)) - f(x))_{x \in \mathcal{U}_1^{\overline{\Omega}}}$ are distinct, the map $\mathbf{j}$ is exactly the one constructed in [15].*

C.2.4 Construction of the quasi-modes for $-L_{f,h}^{D,(p)}$, $p \in \{0, 1\}$

Let us recall that from Lemma C.7, one has for any h small enough

$$\dim \operatorname{Ran} \pi_h^{(0)} = m_0^{\Omega} \text{ and } \dim \operatorname{Ran} \pi_h^{(1)} = m_1^{\overline{\Omega}},$$

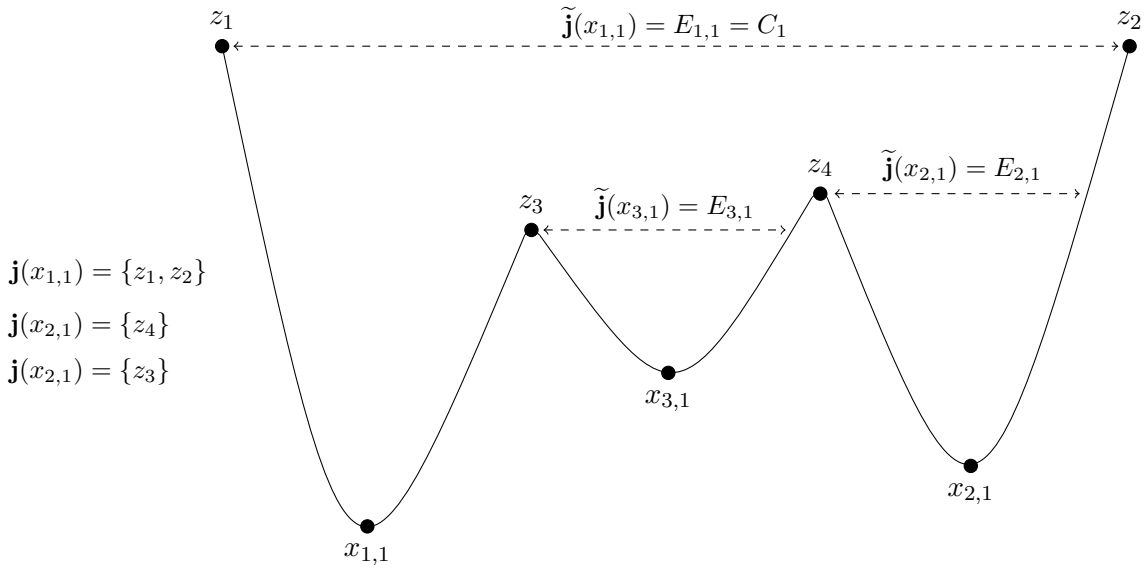

Figure C.4: The maps $\mathbf{j}$ and $\widetilde{\mathbf{j}}$ in a one dimensional example. The construction required three steps.

where we recall, m_0^Ω is the number of local minima of f in Ω and $m_1^{\overline{\Omega}}$ is the number generalized saddle points of f in $\overline{\Omega}$, see Section C.1.3.2. To prove Theorem C.1 and Theorem C.2, the strategy consists in constructing a family of quasi-modes of size m_0^Ω in order to approximate $\operatorname{Ran} \pi_h^{(0)}$ and a family of quasi-modes of size m_1^Ω in order to approximate $\operatorname{Ran} \pi_h^{(1)}$, see (C.39).

Since the construction of the quasi-modes rely on the one made for Witten Laplacians in [14,15,17], we first construct quasi-modes for the Witten Laplacians $\Delta_{f,h}^{D,(0)}$ and $\Delta_{f,h}^{D,(1)}$. The quasi-modes for $-L_{f,h}^{D,(0)}$ and $-L_{f,h}^{D,(1)}$ are then obtained using (C.37).

C.2.4.1 Quasi-modes for the Witten Laplacian $\Delta_{f,h}^{D,(0)}$

Let us assume that the assumptions **[H-Boundary]** and **[H-Morse]** hold. Let us recall that from Lemma C.7 and (C.37), there exists $h_0 > 0$ such that for any $h \in (0, h_0)$:

$$\dim \operatorname{Ran} \pi_{[0,h^{\frac{3}{2}})} \big(\Delta_{f,h}^{D,(0)}\big) = m_0^\Omega,$$

where we recall m_0^Ω is the number of local minima of f in Ω. In this section, one constructs using the maps $\mathbf{j}$ and $\widetilde{\mathbf{j}}$ constructed in Section C.2.3.3, a family of functions of size m_0^Ω which aims at approximating $\operatorname{Ran} \pi_{[0,h^{\frac{3}{2}})} \big(\Delta_{f,h}^{D,(0)}\big)$. The properties of this family which are listed in this section will be useful to prove Propositions C.20 and C.21 in the next section. Following [14, 15, 17], we associate each critical point $x \in \mathcal{U}_0^\Omega$ with a quasi-mode for $\Delta_{f,h}^{D,(0)}$. The notation is the one adopted in the Section C.2.3.3.

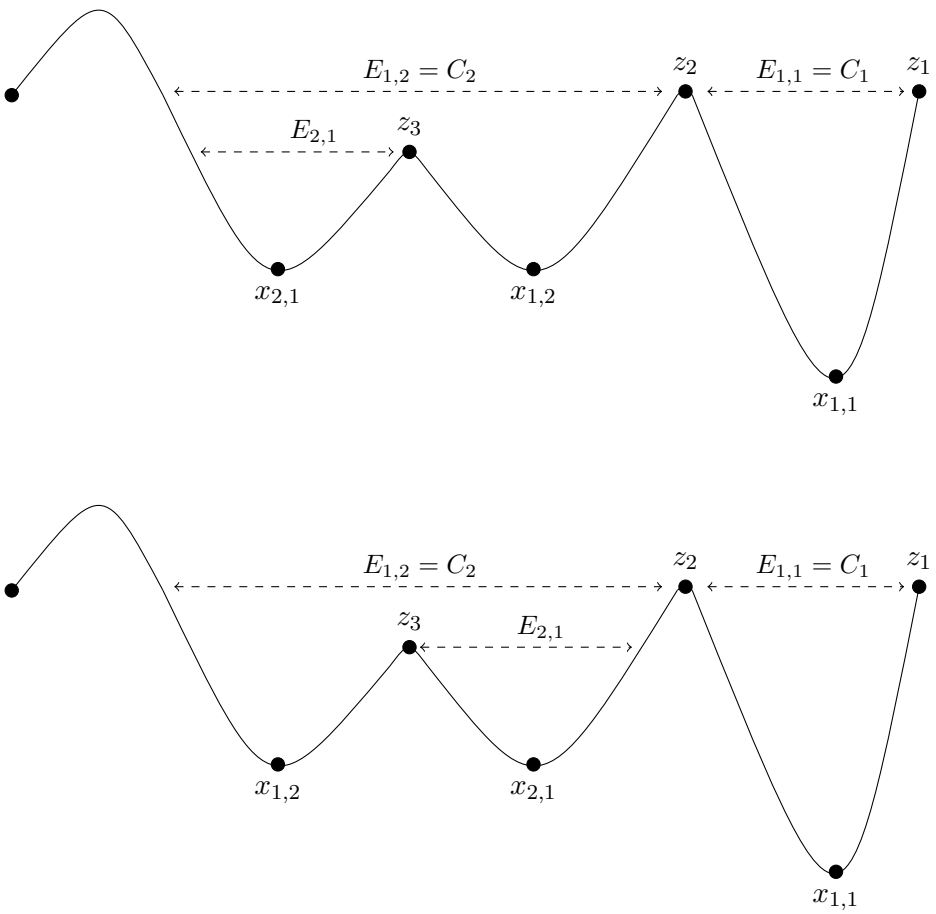

Figure C.5: One dimensional example for which two equivalent constructions of the maps $\mathbf{j}$ and $\widetilde{\mathbf{j}}$ are possible. This is due to the fact that two choices for $x_{1,2}$ can be made in $E_{1,2}$ at the first step of the construction since the two local minima which differ from the global minimum $x_{1,1} \in E_{1,1}$ are at the same height. Both constructions required two steps.

Let us first introduce two parameters $\varepsilon_1 > 0$ and $\varepsilon > 0$. In the following, d is the geodesic distance on $\overline{\Omega}$ for the initial metric. Let us consider $\varepsilon_1 > 0$ small enough such that

$$\forall z, z' \in \mathcal{U}_1^{\overline{\Omega}},\ z \neq z' \text{ implies } d(z, z') \geq 6\varepsilon_1 \tag{C.77}$$

and for all $z \in \mathcal{U}_1^{\overline{\Omega}}$,

$$z \in \mathcal{U}_1^{\Omega} \text{ and } \{f < f(z)\} \cap B(z, 2\varepsilon_1) \text{ has two connected components (see (C.51))}, \tag{C.78}$$

or

$$z \in \mathcal{U}_1^{\partial\Omega} \text{ and } \{f < f(z)\} \cap B(z, 2\varepsilon_1) \text{ is connected.} \tag{C.79}$$

The parameter $\varepsilon_1 > 0$ will be reduced a finite number of times in this section and in

Section C.2.4.2, and it will be kept fixed at the end of Section C.2.4.2. Let $\varepsilon > 0$ be such that

$$\varepsilon \in \Big(0, \frac{1}{2}\big(\min_{\partial\Omega} f - d_M\big)\Big),$$

where d_M is defined in (C.43). The parameters ε_1 and ε are used to define the quasi-modes for $\Delta_{f,h}^{D,(0)}$. Let us now define the m_0^Ω quasi-modes for $\Delta_{f,h}^{D,(0)}$.

Definition C.4. *Let us assume that the assumptions **[H-Boundary]** and **[H-Morse]** hold. The quasi-modes associated with the $x_{1,k}$, $k \in \{1, \dots, N_1\}$ are defined by:*

$$\forall k \in \{1, \dots, N_1\},\ \widetilde{v}_{1,k} := \frac{\chi_{1,k}^{\varepsilon,\varepsilon_1}\, e^{-\frac{1}{h}f}}{\|\chi_{1,k}^{\varepsilon,\varepsilon_1}\, e^{-\frac{1}{h}f}\|_{L^2}}, \tag{C.80}$$

where the functions $\chi_{1,k}^{\varepsilon,\varepsilon_1} \in C_c^\infty(\Omega, \mathbb{R}^+)$. Choosing if necessary $\varepsilon_1 > 0$ small enough, the functions $\chi_{1,k}^{\varepsilon,\varepsilon_1}$ are chosen such that the following properties hold for all $\varepsilon > 0$ small enough:

a) it holds

$$\overline{C_k(2\varepsilon)} \subset \{\chi_{1,k}^{\varepsilon,\varepsilon_1} = 1\} \quad \text{and} \quad \operatorname{supp} \chi_{1,k}^{\varepsilon,\varepsilon_1} \subset \Omega \cap \{x \in \overline{\Omega}, d(x, \overline{C_k}) \le 3\varepsilon_1\} \setminus \mathbf{j}(x_{1,k}), \tag{C.81}$$

see item 3 in Lemma C.9 for the definition of $C_k(2\varepsilon)$,

b) for all $y \in \operatorname{supp} \chi_{1,k}^{\varepsilon,\varepsilon_1}$,

$$f(y) \ \le\ f(\mathbf{j}(x_{1,k})) \text{ implies } y \in \overline{C_k}$$

and hence, according to (C.81),

$$\operatorname*{arg\,min}_{\operatorname{supp} \chi_{1,k}^{\varepsilon,\varepsilon_1}} f = \operatorname*{arg\,min}_{C_k} f \quad \text{and} \quad \min_{\operatorname{supp} \nabla\chi_{1,k}^{\varepsilon,\varepsilon_1}} f \ge \min_{\partial\Omega} f - 2\varepsilon = f(\mathbf{j}(x_{1,k})) - 2\varepsilon, \tag{C.82}$$

c) for all $z \in \mathbf{j}(x_{1,k}) \cap \Omega$, it holds

$$\operatorname{supp} \chi_{1,k}^{\varepsilon,\varepsilon_1} \cap B(z, 2\varepsilon_1) \subset C_k, \tag{C.83}$$

d) for all $z \in \mathcal{U}_1^{\overline{\Omega}} \setminus \mathbf{j}(x_{1,k})$, it holds

$$\big(z \in \overline{C_k} \text{ and } \overline{B(z, 2\varepsilon_1)} \subset \{\chi_{1,k}^{\varepsilon,\varepsilon_1} = 1\}\big) \text{ or } \big(z \notin \overline{C_k} \text{ and } \overline{B(z, 2\varepsilon_1)} \subset \{\chi_{1,k}^{\varepsilon,\varepsilon_1} = 0\}\big), \tag{C.84}$$

e) for all $\ell \in \{1, \dots, N_1\} \setminus \{\ell\}$, it holds $\operatorname{supp} \chi_{1,k}^{\varepsilon,\varepsilon_1} \cap \operatorname{supp} \chi_{1,\ell}^{\varepsilon,\varepsilon_1} = \emptyset$.

For $\ell \ge 2$ and $k \in \{1, \dots, N_\ell\}$, the quasi-mode associated with $x_{\ell,k}$ is defined by

$$\widetilde{v}_{\ell,k} := \frac{\chi_{\ell,k}^{\varepsilon,\varepsilon_1}\, e^{-\frac{1}{h}f}}{\|\chi_{\ell,k}^{\varepsilon,\varepsilon_1}\, e^{-\frac{1}{h}f}\|_{L^2}}, \tag{C.85}$$

where the functions $\chi_{\ell,k}^{\varepsilon,\varepsilon_1} \in C_c^\infty(\Omega, \mathbb{R}^+)$. Choosing if necessary $\varepsilon_1 > 0$ small enough, the functions $\chi_{\ell,k}^{\varepsilon,\varepsilon_1}$ are chosen such that the following properties hold for all $\varepsilon > 0$ small enough:

a) it holds

$$\overline{\{f < \min_{\partial\Omega} f - 2\varepsilon\} \cap E_{\ell,k}} \subset \{\chi_{\ell,k}^{\varepsilon,\varepsilon_1} = 1\} \quad \textit{and}$$
$$\operatorname{supp} \chi_{\ell,k}^{\varepsilon,\varepsilon_1} \subset \Omega \cap \left\{x \in \overline{\Omega}, d(x, \overline{E_{\ell,k}}) \leq 3\varepsilon_1\right\} \setminus \mathbf{j}(x_{\ell,k}), \tag{C.86}$$

(notice that $\{f < \min_{\partial\Omega} f - \delta\}$ is connected for all $\delta > 0$ small enough by the same analysis as the one leading to item 3 in Lemma C.9),

b) for all $y \in \operatorname{supp} \chi_{\ell,k}^{\varepsilon,\varepsilon_1}$,

$$f(y) \ \leq \ f(\mathbf{j}(x_{\ell,k})) \textit{ implies } y \in \overline{E_{\ell,k}}$$

and hence, according to (C.86)*,*

$$\underset{\operatorname{supp} \chi_{\ell,k}^{\varepsilon,\varepsilon_1}}{\arg\min} f = \underset{E_{\ell,k}}{\arg\min} f \quad \textit{and} \quad \min_{\operatorname{supp} \nabla \chi_{\ell,k}^{\varepsilon,\varepsilon_1}} f \geq f(\mathbf{j}(x_{\ell,k})) - 2\varepsilon, \tag{C.87}$$

c) for any $(\ell', k') \in \{1, \ldots, \ell - 1\} \times \{1, \ldots, N_{\ell'}\}$ such that $E_{\ell,k} \subset E_{\ell',k'}$, it holds

$$\operatorname{supp} \chi_{\ell,k}^{\varepsilon,\varepsilon_1} \subset \{\chi_{\ell',k'}^{\varepsilon,\varepsilon_1} = 1\} \tag{C.88}$$

(note that by a connexity argument, it holds $E_{\ell,k} \subset E_{\ell',k'}$ or $E_{\ell,k} \cap E_{\ell',k'} = \emptyset$ for any $(\ell', k') \in \{1, \ldots, \ell - 1\} \times \{1, \ldots, N_{\ell'}\}$),

d) for all $z \in \mathbf{j}(x_{\ell,k}) \subset \Omega$, it holds

$$\operatorname{supp} \chi_{\ell,k}^{\varepsilon,\varepsilon_1} \cap B(z, 2\varepsilon_1) \subset E_{\ell,k}, \tag{C.89}$$

e) for all $z \in \mathcal{U}_1^{\overline{\Omega}} \setminus \mathbf{j}(x_{\ell,k})$, it holds

$$\left(z \in \overline{E_{\ell,k}} \textit{ and } \overline{B(z, 2\varepsilon_1)} \subset \{\chi_{\ell,k}^{\varepsilon,\varepsilon_1} = 1\}\right) \textit{ or } \left(z \notin \overline{E_{\ell,k}} \textit{ and } \overline{B(z, 2\varepsilon_1)} \subset \{\chi_{\ell,k}^{\varepsilon,\varepsilon_1} = 0\}\right). \tag{C.90}$$

For the ease of notation, we do not indicate the dependance on the parameters ε and ε_1 in the notation of the functions $\widetilde{v}_{l,k}$ for $l \geq 1$, $k \in \{1, ..., N_l\}$, introduced in Definition C.4. In Figures C.6-C.7-C.8 are given the schematic representations of the cut of function $\chi_{1,k}^{\varepsilon,\varepsilon_1}$ respectively near $z \in \mathbf{j}(x_{1,k}) \cap \Omega$, $z \in \mathbf{j}(x_{1,k}) \cap \partial\Omega$ and $z \in \left(\mathcal{U}_1^{\overline{\Omega}} \setminus \mathbf{j}(x_{1,k})\right) \cap \partial C_k$ for $k \in \{1, ..., N_1\}$. Notice that Figures C.6 and C.8 also give schematic representations of $\chi_{\ell,k}^{\varepsilon,\varepsilon_1}$ near $z \in \mathbf{j}(x_{\ell,k}) \cap \Omega$ and $z \in \left(\mathcal{U}_1^{\overline{\Omega}} \setminus \mathbf{j}(x_{\ell,k})\right) \cap \partial E_{\ell,k}$ for $\ell \geq 2$ and $k \in \{1, ..., N_\ell\}$.

Remark C.6. *The construction of quasi-modes introduced in Definition C.4 is similar to the one made in [14, Section 4], [15, Section 6] and [17, Sections 4.2 and 5.1].*

Lemma C.12. *Let us assume that the assumptions **[H-Boundary]** and **[H-Morse]** hold. Then, for $\ell \geq 1$ and $k \in \{1, \ldots, N_\ell\}$, there exist $c > 0$, $C > 0$ and $h_0 > 0$ such that for all $h \in (0, h_0)$,*

$$\left\|d_{f,h}\widetilde{v}_{\ell,k}\right\|_{L^2} = \frac{\left\|h\, e^{-\frac{1}{h}f}\, d\chi_{\ell,k}^{\varepsilon,\varepsilon_1}\right\|_{L^2}}{\left\|e^{-\frac{1}{h}f}\, \chi_{\ell,k}^{\varepsilon,\varepsilon_1}\right\|_{L^2}} \leq C\, e^{-\frac{f(\mathbf{j}(x_{\ell,k})) - f(x_{\ell,k}) - c\varepsilon}{h}}, \tag{C.91}$$

where the function $\widetilde{v}_{\ell,k}$ is introduced in Definition C.4.

Proof. This estimate follows from (C.80)–(C.82), (C.85)–(C.87), and Laplace's method applied to $\|\chi_{\ell,k}^{\varepsilon,\varepsilon_1}\, e^{-\frac{1}{h}f}\|_{L^2}$. ∎

According to Lemma C.8, Lemma C.12 indicates how accurate are the projections onto $\operatorname{Ran}\pi_{[0,h^{\frac{3}{2}})}\left(\Delta_{f,h}^{D,(0)}\right)$ of the m_0^Ω functions $(\widetilde{v}_{\ell,k})_{\ell\geq 1,\, k\in\{1,\dots,N_\ell\}}$ introduced in Definition C.4. The following lemma ensures that the family $(\widetilde{v}_{\ell,k})_{\ell\geq 1,\, k\in\{1,\dots,N_\ell\}}$ is linearly independent for any h small enough.

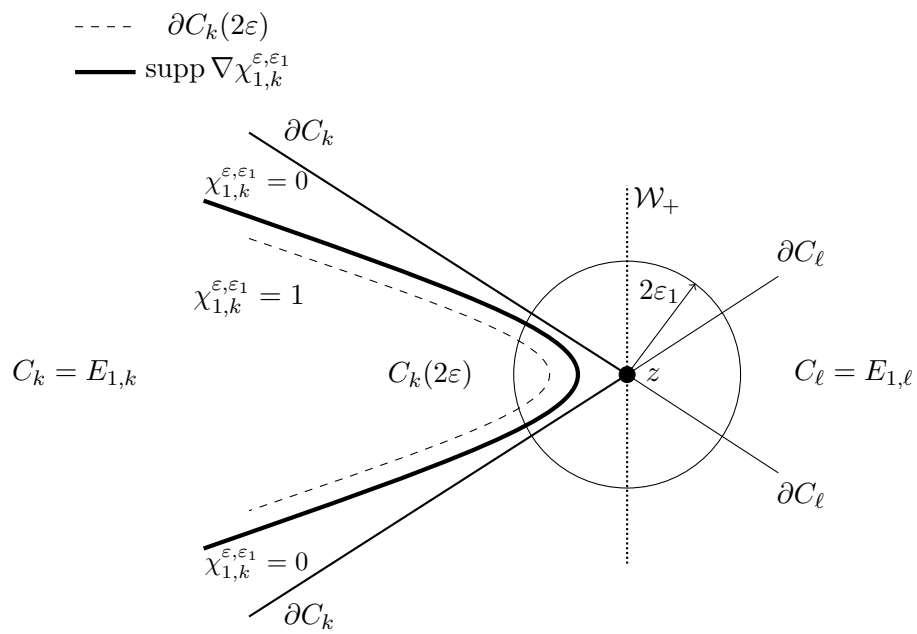

Figure C.6: Schematic representation of the cut of function $\chi_{1,k}^{\varepsilon,\varepsilon_1}$ near $z\in\mathbf{j}(x_{1,k})\cap\Omega\subset\mathcal{U}_1^\Omega$ for $k\in\{1,...,N_1\}$ (z is a separating saddle point as introduced in Definition C.3). In the figure, $\ell\neq k$ and C_ℓ is another connected component of $\{f<\min_{\partial\Omega} f\}$. The set $\mathcal{W}_+$ is the stable manifold of the saddle point z.

Lemma C.13. *Let us assume that the assumptions **[H-Boundary]** and **[H-Morse]** hold. The family $\mathcal{B}_v=(\widetilde{v}_{\ell,k})_{\ell\geq 1,\, k\in\{1,\dots,N_\ell\}}$, introduced in Definition C.4, is linearly independant, uniformly with respect to h. This means that for some (and hence for any) orthonormal family $\mathcal{B}_o$ spanning* $\operatorname{Span}(\mathcal{B}_v)$*, there exist $C>0$ and $h_0>0$ such that for all $h\in(0,h_0)$,*

$$\|Mat_{\mathcal{B}_o}\mathcal{B}_v\|\leq C \quad \textit{and} \quad \|Mat_{\mathcal{B}_v}\mathcal{B}_o\|\leq C. \tag{C.92}$$

Proof. The proof of Lemma C.13 is made in [17, Section 4.2]. ∎

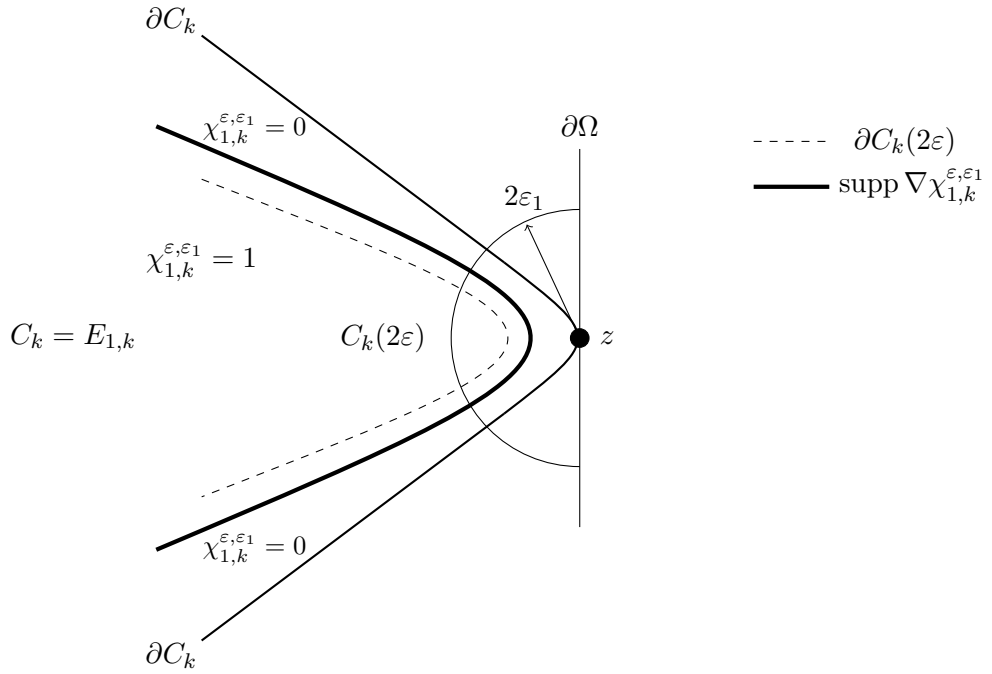

Figure C.7: Schematic representation of the cut of function $\chi_{1,k}^{\varepsilon,\varepsilon_1}$ near $z \in \mathbf{j}(x_{1,k}) \cap \partial\Omega \subset \mathcal{U}_1^{\partial\Omega}$ for $k \in \{1, ..., N_1\}$.

C.2.4.2 Quasi-modes for the Witten Laplacian $\Delta_{f,h}^{D,(1)}$

Let us assume that the assumptions **[H-Boundary]** and **[H-Morse]** hold. Let us recall that from Lemma C.7 and (C.37), there exists $h_0 > 0$ such that for any $h \in (0, h_0)$:

$$\dim \operatorname{Ran} \pi_{[0,h^{\frac{3}{2}})}\big(\Delta_{f,h}^{D,(1)}\big) = m_1^{\overline{\Omega}},$$

where we recall, $m_1^{\overline{\Omega}}$ is the number of generalized saddle points of f in $\overline{\Omega}$. In this section, one constructs a family of 1-forms $(\widetilde{\phi}_j)_{j\in\{1,...,m_1^{\overline{\Omega}}\}}$ which aims at approximating $\operatorname{Ran} \pi_{[0,h^{\frac{3}{2}})}\big(\Delta_{f,h}^{D,(1)}\big)$. To this end, for each $z \in \mathcal{U}_1^{\overline{\Omega}}$, one constructs a 1-form locally supported in a neighborhood of z in $\overline{\Omega}$. More precisely, one proceeds as follows:

1. for each $z \in \mathcal{U}_1^{\Omega}$, the 1-form associated with z is constructed exactly as in [14, 17] and,
2. for each $z \in \mathcal{U}_1^{\partial\Omega}$, the 1-form associated with z is constructed exactly as in [15].

Let us recall these constructions and some estimates which will be used throughout this work.

<u>Quasi-mode associated with $z \in \mathcal{U}_1^{\Omega}$</u>

Let us recall that from (C.16),

$$\mathcal{U}_1^{\Omega} = \{z_{m_1^{\partial\Omega}+1}, ..., z_{m_1^{\overline{\Omega}}}\} \subset \Omega,$$

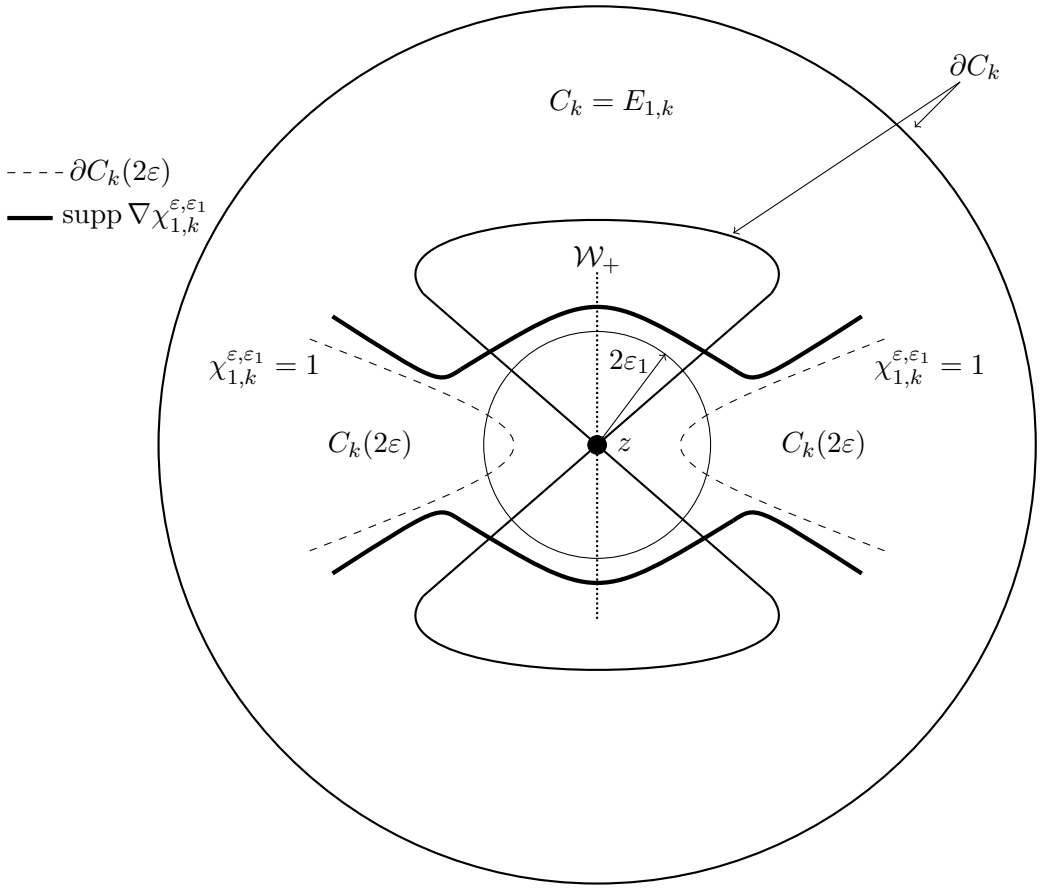

Figure C.8: Schematic representation of the cut of function $\chi_{1,k}^{\varepsilon,\varepsilon_1}$ near $z \in \left(\mathcal{U}_1^{\overline{\Omega}} \backslash \mathbf{j}(x_{1,k})\right) \cap \partial C_k$ (z is a saddle point on ∂C_k but is not a separating saddle point as introduced in Definition C.3).

is the set of saddle points of f in Ω. Let $j \in \{m_1^{\partial\Omega}+1, \ldots, m_1^{\overline{\Omega}}\}$ and $z_j \in \mathcal{U}_1^{\Omega}$. Let $\mathcal{V}_j$ be some small smooth neighborhood of z_j such that $\overline{\mathcal{V}_j} \cap \partial\Omega = \emptyset$ and for $x \in \overline{\mathcal{V}_j}$, $|\nabla f(x)| = 0$ if and only if $x = z_j$. Let us now consider the full Dirichlet realization $\Delta_{f,h}^{FD,(1)}(\mathcal{V}_j)$ of the Witten Laplacian $\Delta_{f,h}^{(1)}$ in $\mathcal{V}_j$ whose domain is

$$D(\,\Delta_{f,h}^{FD,(1)}(\mathcal{V}_j)\,) = \left\{ w \in \Lambda^1 H^2\left(\mathcal{V}_j\right),\, w\big|_{\partial\mathcal{V}_j} = 0 \right\},$$

where the superscript FD stands for full Dirichlet boundary conditions. Let us recall that according to [16, Section 2], there exists, choosing if necessary $\mathcal{V}_j$ smaller, a C^∞ non negative solution $\Phi_j : \mathcal{V}_j \to \mathbb{R}^+$ to the eikonal equation

$$|\nabla\Phi_j| = |\nabla f| \text{ in } \mathcal{V}_j \quad \text{such that } \Phi_j(y) = 0 \text{ iff } y = z_j. \tag{C.93}$$

Moreover, Φ_j is the unique non negative solution to (C.93) in the sense that if $\widetilde{\Phi}_j : \widetilde{\mathcal{V}_j} \to \mathbb{R}^+$ is another non negative C^∞ solution to (C.93) on a neighborhood $\widetilde{\mathcal{V}_j}$ of z_j, then $\widetilde{\Phi}_j = \Phi_j$ on $\widetilde{\mathcal{V}_j} \cap \mathcal{V}_j$.

Remark C.7. *The function Φ_j actually equals the Agmon distance to z_j, see [16, Section 1].*

The next proposition, which follows from [16, Theorem 1.4 and Lemma 1.6], gathers all the estimates one needs in the following on the operator $\Delta_{f,h}^{FD,(1)}(\mathcal{V}_j)$.

Proposition C.14. *Let us assume that the assumptions **[H-Boundary]** and **[H-Morse]** hold. Then, the operator $\Delta_{f,h}^{FD,(1)}(\mathcal{V}_j)$ is self-adjoint, has compact resolvent and is positive. Moreover:*

- *There exist $\varepsilon_0 > 0$ and $h_0 > 0$ such that for all $h \in (0, h_0)$:*

$$\dim \operatorname{Ran} \pi_{[0,\varepsilon_0 h)}\big(\Delta_{f,h}^{FD,(1)}(\mathcal{V}_j)\big) = 1. \tag{C.94}$$

- *The smallest eigenvalue $\lambda_h(\mathcal{V}_j)$ of $\Delta_{f,h}^{FD,(1)}(\mathcal{V}_j)$ is exponentially small: there exist $C > 0$, $c > 0$ and $h_0 > 0$ such that for any $h \in (0, h_0)$:*

$$\lambda_h(\mathcal{V}_j) \leq C e^{-\frac{c}{h}}. \tag{C.95}$$

- *Any L^2-normalized eigenform w_j associated with the smallest eigenvalue $\lambda_h(\mathcal{V}_j)$ of $\Delta_{f,h}^{FD,(1)}(\mathcal{V}_j)$ satisfies the following Agmon estimates: for all $\varepsilon > 0$, there exist $C_\varepsilon > 0$ and $h_0 > 0$ such that for any $h \in (0, h_0)$, it holds:*

$$\|e^{\frac{1}{h}\Phi_j} w_j\|_{H^1(\mathcal{V}_j)} \leq C_\varepsilon\, e^{\frac{\varepsilon}{h}}. \tag{C.96}$$

Choosing ε_1 smaller if necessary, one assumes that there exists $\alpha > 0$ such that

$$B(z_j, 2\varepsilon_1 + \alpha) \subset \mathcal{V}_j.$$

Let us now define the quasi-mode associated with $z_j \in \mathcal{U}_1^\Omega$.

Definition C.5. *Let us assume that the assumptions **[H-Boundary]** and **[H-Morse]** hold. Let $j \in \{m_1^{\partial\Omega} + 1, \ldots, m_1^{\overline{\Omega}}\}$ and $z_j \in \mathcal{U}_1^\Omega$. The quasi-mode associated with z_j is defined by*

$$\widetilde{\phi}_j := \frac{\theta_j\, w_j}{\|\theta_j\, w_j\|_{L^2}} \in \Lambda^1 C_c^\infty(\Omega), \tag{C.97}$$

where w_j be a L^2-normalized eigenform associated with the smallest eigenvalue $\lambda_h(\mathcal{V}_j)$ of $\Delta_{f,h}^{FD,(1)}(\mathcal{V}_j)$ and θ_j is a smooth non negative cut-off function satisfying, $\operatorname{supp} \theta_j \subset B(z_j, 2\varepsilon_1) \subset \mathcal{V}_j$ *and $\theta_j = 1$ on $B(z_j, \varepsilon_1)$.*

Notice that both w_j and $-w_j$ can be used to build a quasi-mode and the choice of the sign is determined in Proposition C.16. Using Proposition C.14, one deduces the following estimate on the quasi-mode $\widetilde{\phi}_j$ introduced in Definition C.5.

Corollary C.15. *Let us assume that the assumptions **[H-Boundary]** and **[H-Morse]** hold. Let $\widetilde{\phi}_j$ be the quasi-mode associated with $z_j \in U_1^\Omega$ ($j \in \{m_1^{\partial\Omega} + 1, \ldots, m_1^{\overline{\Omega}}\}$), see Definition C.5. Then, there exist $C > 0$, $c > 0$ and $h_0 > 0$ such that for any $h \in (0, h_0)$:*

$$\big\|d_{f,h}\widetilde{\phi}_j\big\|_{L^2} + \big\|d_{f,h}^*\widetilde{\phi}_j\big\|_{L^2} \leq C e^{-\frac{c}{h}}. \tag{C.98}$$

Let us now be more specific in prevision of later computations. Let us denote by $\mathcal{W}_+(z_j)$ and $\mathcal{W}_-(z_j)$ respectively the stable and unstable manifolds of z_j associated with the flow of $-\nabla f$. In other words, denoting by $\varphi_t(y)$ the solution of $\frac{d}{dt}\varphi_t(y) = -\nabla f(\varphi_t(y))$ with initial condition $\varphi_0(y) = y$,

$$\mathcal{W}_\pm(z_j) := \left\{ y \in \Omega, \varphi_t(y) \underset{t\to\pm\infty}{\longrightarrow} z_j \right\}. \tag{C.99}$$

It then holds (see indeed [16, Section 2] and [14, Section 4.2]): $\dim \mathcal{W}_+(z_j) = d-1$, $\dim \mathcal{W}_-(z_j) = 1$, and for all $y \in \mathcal{V}_j$ (assuming $\mathcal{V}_j$ small enough),

$$|f(y) - f(z_j)| \leq \Phi_j(y) \text{ and } |f(y) - f(z_j)| = \Phi_j(y) \text{ iff } y \in \mathcal{W}_+(z_j) \cup \mathcal{W}_-(z_j) \tag{C.100}$$

with moreover

$$\Phi_j = \pm(f - f(z_j)) \text{ on } \mathcal{W}_\pm(z_j) \text{ and } \det \mathrm{Hess}\, \Phi_j(z_j) = |\det \mathrm{Hess}\, f(z_j)|. \tag{C.101}$$

Additionnaly, there exists by [16, Theorem 1.4, Lemma 1.6, Proposition 1.3 and Proposition 2.3] a $C^\infty(\overline{\mathcal{V}_j})$ 1-form $a_j(x,h) = \widetilde{a}_j(x) + O(h)$ where $n(z_j)$ a unit normal to $\mathcal{W}_+(z_j)$, and with $a_j(z_j,h) = \widetilde{a}_j(z_j) = n(z_j)$ and such that the 1-form $u^{(1)}_{j,wkb} = a_j e^{-\frac{1}{h}\Phi_j}$ satisfies

$$\Delta^{(1)}_{f,h} u^{(1)}_{j,wkb} = O(h^\infty) e^{-\frac{1}{h}\Phi_j} \text{ in } \mathcal{V}_j. \tag{C.102}$$

Moreover, one has in the limit $h \to 0$ (see [16, Section 2]):

$$\|\theta_j u^{(1)}_{j,wkb}\|_{L^2} = \frac{(\pi h)^{\frac{d}{4}}}{\left|\det \mathrm{Hess}\, f(z_j)\right|^{\frac{1}{4}}} \big(1 + O(h)\big). \tag{C.103}$$

Remark C.8. *Let us explain how to get* (C.102) *from [16]. In [16, Proposition 1.3], it is actually stated that there exists $\mu(h)$ such that $\mu(h) \sim h^2 \sum_{k=1}^\infty \mu_k h^k$ and*

$$\big(\Delta^{(1)}_{f,h} - \mu(h)\big) u^{(1)}_{j,wkb} = O(h^\infty) e^{-\frac{1}{h}\Phi_j} \text{ in } \mathcal{V}_j.$$

Using in addition (C.114)*, one obtains that $\Delta^{FD,(1)}_{f,h}(\mathcal{V}_j)$ admits an eigenvalue which equals $\mu(h) + O(h^\infty)$. From* (C.94) *and* (C.95)*, one deduces that $\mu(h) = O(h^\infty)$. This leads to* (C.102)*.*

The following proposition deals with the comparison between w_j and $u^{(1)}_{j,wkb}$.

Proposition C.16. *Let us assume that the assumptions **[H-Boundary]** and **[H-Morse]** hold. Let w_j be a L^2-normalized eigenform associated with the smallest eigenvalue $\lambda_h(\mathcal{V}_j)$ of $\Delta^{FD,(1)}_{f,h}(\mathcal{V}_j)$. Then, there exists $h_0 > 0$ such that for all $h \in (0, h_0)$ one has:*

$$\left\| \theta_j (w_j - c_j(h) u^{(1)}_{j,wkb}) \right\|_{H^1} = O(h^\infty) \tag{C.104}$$

where

$$c_j(h)^{-1} = \langle w_j, \theta_j u^{(1)}_{j,wkb} \rangle_{L^2}.$$

Moreover, in the limit $h \to 0$, one has:

$$c_j(h) = \frac{\left|\det \mathrm{Hess}\, f(z_j)\right|^{\frac{1}{4}}}{(\pi h)^{\frac{d}{4}}} \big(1 + O(h)\big). \tag{C.105}$$

In addition, one can assume, up to replacing w_j by $-w_j$, that $c_j(h) \geq 0$.

Proof. Let us define $k_j(h) := \langle w_j, \theta_j u^{(1)}_{j,wkb} \rangle_{L^2}$. If $k_j(h) < 0$, then one changes w_j to $-w_j$ so that one can suppose without loss of generality that $k_j(h) \geq 0$. For h small enough, one has from (C.94):

$$\pi_{[0,\varepsilon_0 h)}\big(\Delta^{FD,(1)}_{f,h}(\mathcal{V}_j)\big)(\theta_j u^{(1)}_{j,wkb}) = k_j(h) w_j.$$

Let us define the following 1-form

$$\alpha_j := \theta_j\big(u^{(1)}_{j,wkb} - k_j(h)\, w_j\big).$$

Thus, the following identity holds for h small enough

$$\alpha_j = k_j(h)\,(1-\theta_j)\, w_j + \pi_{[\varepsilon_0 h,+\infty)}\big(\Delta^{FD,(1)}_{f,h}(\mathcal{V}_j)\big)(\theta_j u^{(1)}_{j,wkb}).$$

Notice that, from (C.114), there exist $C > 0$ and $h_0 > 0$ such that for all $h \in (0, h_0)$

$$|k_j(h)| \leq C h^{\frac{d}{4}}.$$

Therefore, using Lemma C.8, (C.96) and (C.102), for any $\varepsilon > 0$ there exists $C > 0$ such that

$$\begin{aligned}
\|\alpha_h\|^2_{L^2} &\leq 2k_j(h)^2 \|\,(1-\theta_j)\, w_j\|^2_{L^2} \;+\; 2\left\|\pi_{[\varepsilon_0 h,+\infty)}\big(\Delta^{FD,(1)}_{f,h}(\mathcal{V}_j)\big)(\theta_j u^{(1)}_{j,wkb})\right\|^2_{L^2} \\
&\leq C h^{\frac{d}{2}} \left\|(1-\theta_j)\, w_j e^{\frac{\Phi_j}{h}} e^{\frac{-\Phi_j}{h}}\right\|^2_{L^2} + C h^{-1} O(h^\infty) \\
&\leq C h^{\frac{d}{2}} e^{-\frac{c-\varepsilon}{h}} + O(h^\infty) = O(h^\infty),
\end{aligned}$$

with $c := \inf_{\mathrm{supp}(1-\theta_j)} \Phi_j > 0$ (since $\theta_j = 1$ near z_j) and for any $\varepsilon < c$. Moreover, since $d_{f,h} = hd + df\wedge$ and $d^*_{f,h} = hd^* + \mathbf{i}_{\nabla f}$, one obtains using the Gaffney inequality (see [29]), the fact that from (C.98)

$$\big\|d_{f,h}(\theta_j w_j)\big\|_{L^2} \;+\; \big\|d^*_{f,h}(\theta_j w_j)\big\|_{L^2} \leq C e^{-\frac{c}{h}}$$

and from (C.102)

$$\big\|d_{f,h}(\theta_j u^{(1)}_{j,wkb})\big\|_{L^2} \;+\; \big\|d^*_{f,h}(\theta_j u^{(1)}_{j,wkb})\big\|_{L^2} = O(h^\infty),$$

there exists $C > 0$ such that:

$$\begin{aligned}
\|\alpha_j\|^2_{H^1} &\leq C(\|d\alpha_j\|^2_{L^2} + \|d^*\alpha_j\|^2_{L^2} + \|\alpha_j\|^2_{L^2}) \\
&\leq C h^{-2}\left(\big\|d_{f,h}\alpha_j\big\|^2_{L^2} \;+\; \big\|d^*_{f,h}\alpha_j\big\|^2_{L^2} + \|\alpha_j\|^2_{L^2}\right) = O(h^\infty).
\end{aligned}$$

Moreover since $\|\theta_j w_j\|_{L^2} = 1 + O(e^{-\frac{c}{h}})$ (from (C.96)), by considering $\|\theta_j(u^{(1)}_{j,wkb} - k_j(h) w_j)\|^2_{L^2} = O(h^\infty)$, one gets using (C.114):

$$k_j(h)^2 = \frac{\|\theta_j u^{(1)}_{j,wkb}\|^2_{L^2} + O(h^\infty)}{2 - \|\theta_j w_j\|^2_{L^2}} = \frac{(\pi h)^{\frac{d}{2}}}{\big|\det \mathrm{Hess}\, f(z_j)\big|^{\frac{1}{2}}}\,\big(1 + O(h)\big).$$

Since $k_j(h) \geq 0$, one has $k_j(h) = \frac{(\pi h)^{\frac{d}{4}}}{\big|\det \mathrm{Hess}\, f(z_j)\big|^{\frac{1}{4}}}\,\big(1 + O(h)\big)$. This concludes the proof by choosing $c_j(h) := k_j(h)^{-1}$. ∎

Quasi-mode associated with $z \in \mathcal{U}_1^{\partial\Omega}$

Let us recall that from (C.15),

$$\mathcal{U}_1^{\partial\Omega} = \{z_1, ..., z_{m_1^{\partial\Omega}}\} \subset \partial\Omega.$$

Let $j \in \{1, \dots, m_1^{\partial\Omega}\}$ and $z_j \in \mathcal{U}_1^{\partial\Omega}$. To construct a 1-form locally supported in a neighborhood of z_j in $\overline{\Omega}$, one proceeds in the same way as in [15, Section 4.3]. Let $\mathcal{V}_j$ be a small neighborhood of z_j in $\overline{\Omega}$ as defined in [15, Section 4.3]. Let us recall that from [15, Section 4.3], $\mathcal{V}_j$ satisfies: $|\nabla f| > 0$ on $\overline{\mathcal{V}_j}$, for all $x \in \overline{\mathcal{V}_j}$, $|\nabla_T f(x)| = 0$ if and only if $x = z_j$, and $\partial_n f > 0$ on $\partial\Omega \cap \mathcal{V}_j$. As in [15, Section 4.3], let us now consider the mixed full Dirichlet–tangential Dirichlet realization $\Delta_{f,h}^{MD,(1)}(\mathcal{V}_j)$ of the Witten Laplacian $\Delta_{f,h}^{(1)}$ in $\mathcal{V}_j$ whose domain is

$$D\big(\Delta_{f,h}^{MD,(1)}(\mathcal{V}_j)\big) = \big\{w \in \Lambda^1 H^2(\mathcal{V}_j)\,,\, w|_{V_j\cap\Omega} = 0,\ \mathbf{t}w|_{V_j\cap\partial\Omega} = 0 \text{ and } \mathbf{t}d_{f,h}^* w|_{V_j\cap\partial\Omega} = 0\big\}\,,$$

where the superscript MD stands for mixed full Dirichlet–tangential Dirichlet boundary conditions (see [15, Remark 4.3.1] for the characterization of its domain). Since $\partial_n f > 0$ on $\partial\Omega \cap \mathcal{V}_j$, from [15, Section 4.2], one has that, choosing $\mathcal{V}_j$ small enough, there exists a $C^\infty(\mathcal{V}_j, \mathbb{R}^+)$ non negative solution Φ_j to the eikonal equation

$$\left.\begin{array}{l} |\nabla\Phi_j| = |\nabla f| \text{ in } \Omega\cap\mathcal{V}_j \\ \Phi_j = f - f(z_j) \text{ on } \partial\Omega\cap\mathcal{V}_j \\ \partial_n\Phi_j = -\partial_n f \text{ on } \partial\Omega\cap\mathcal{V}_j \end{array}\right\} \quad \text{and such that } \Phi_j(y) = 0 \text{ iff } y = z_j. \tag{C.106}$$

Moreover, Φ_j is the unique non negative solution to (C.106) in the sense that if $\widetilde{\Phi}_j : \widetilde{\mathcal{V}_j} \to \mathbb{R}^+$ is another non negative C^∞ solution to (C.106) on a neighborhood $\widetilde{\mathcal{V}_j}$ of z_j, then $\widetilde{\Phi}_j = \Phi_j$ on $\widetilde{\mathcal{V}_j} \cap \mathcal{V}_j$.

Remark C.9. *The function Φ_j actually equals the Agmon distance to z_j, see [7, Section 3].*

Choosing ε_1 smaller if necessary, one assumes that there exists $\alpha > 0$ such that

$$B(z_j, 2\varepsilon_1 + \alpha) \cap \overline{\Omega} \subset \mathcal{V}_j.$$

The next proposition, which follows from [15, Proposition 4.3.2], gathers all the estimates one needs in the following on the operator $\Delta_{f,h}^{MD,(1)}(\mathcal{V}_j)$.

Proposition C.17. *Let us assume that the assumptions **[H-Boundary]** and **[H-Morse]** hold. Then, the operator $\Delta_{f,h}^{MD,(1)}(\mathcal{V}_j)$ is self-adjoint, has compact resolvent and is positive. Moreover:*

- *There exists $h_0 > 0$ such that for all $h \in (0, h_0)$:*

$$\dim \operatorname{Ran} \pi_{[0,h^{\frac{3}{2}})}\big(\Delta_{f,h}^{MD,(1)}(\mathcal{V}_j)\big) = 1. \tag{C.107}$$

- *The smallest eigenvalue $\lambda_h(\mathcal{V}_j)$ of $\Delta_{f,h}^{MD,(1)}(\mathcal{V}_j)$ is exponentially small: there exist $C > 0$, $c > 0$ and $h_0 > 0$ such that for any $h \in (0, h_0)$:*

$$\lambda_h(\mathcal{V}_j) \le C e^{-\frac{c}{h}}. \tag{C.108}$$

- *Any L^2-normalized eigenform w_j associated with the smallest eigenvalue $\lambda_h(\mathcal{V}_j)$ of $\Delta_{f,h}^{MD,(1)}(\mathcal{V}_j)$ satisfies the following Agmon estimates: there exist $C>0$, $n\in\mathbb{N}$ and $h_0>0$ such that for any $h\in(0,h_0)$, it holds:*

$$\left\|e^{\frac{1}{h}\Phi_j}w_j\right\|_{H^1(B(z_j,2\varepsilon_1)\cap\Omega)}\leq Ch^{-n}. \tag{C.109}$$

Let us now define the quasi-mode associated with $z_j\in U_1^{\partial\Omega}$.

Definition C.6. *Let us assume that the assumptions **[H-Boundary]** and **[H-Morse]** hold. Let $j\in\{1,\dots,m_1^{\partial\Omega}\}$ and $z_j\in\mathcal{U}_1^{\partial\Omega}$. The quasi-mode associated with z_j is defined by*

$$\widetilde{\phi}_j\ :=\ \frac{\theta_j\,w_j}{\|\theta_j\,w_j\|_{L^2}}\in\Lambda^1H_T^1(\Omega)\cap\Lambda^1C^\infty\left(\overline{\Omega}\right), \tag{C.110}$$

where w_j a L^2-normalized eigenform associated with the first eigenvalue $\lambda_h(\mathcal{V}_j)$ of $\Delta_{f,h}^{(1),MD}(\mathcal{V}_j)$ and θ_j is a smooth non negative cut-off function satisfying $\operatorname{supp}\theta_j\subset B(z_j,2\varepsilon_1)\cap\overline{\Omega}\subset\mathcal{V}_j$, $\{z_j\}=\arg\min_{\operatorname{supp}\theta_j\cap\partial\Omega}f$, and $\theta_j=1$ on $B(z_j,\varepsilon_1)\cap\overline{\Omega}$.

Notice that both w_j and $-w_j$ can be used to build a quasi-mode and the choice of the sign is determined in Proposition C.19. Notice also that the fact that $\widetilde{\phi}_j\in\Lambda^1H^2(\Omega)$ follows from standard results on elliptic regularity. Using Proposition C.17, one deduces the following estimate on the quasi-mode $\widetilde{\phi}_j$ introduced in Definition C.5.

Corollary C.18. *Let us assume that the assumptions **[H-Boundary]** and **[H-Morse]** hold. Let $\widetilde{\phi}_j$ be the quasi-mode associated with $z_j\in U_1^{\partial\Omega}$ ($j\in\{1,\dots,m_1^{\partial\Omega}\}$), see Definition C.6. Then, there exist $C>0$, $c>0$ and $h_0>0$ such that for any $h\in(0,h_0)$:*

$$\left\|d_{f,h}\widetilde{\phi}_j\right\|_{L^2}\ +\ \left\|d_{f,h}^*\widetilde{\phi}_j\right\|_{L^2}\leq Ce^{-\frac{c}{h}}. \tag{C.111}$$

For further computations, let us give the corresponding versions of (C.102)–(C.105) when $z_j\in\mathcal{U}_1^{\partial\Omega}$. From [15, Section 4.2], there exists a $C^\infty(\overline{\mathcal{V}_j})$ function $a_j(x,h)=\widetilde{a}_j(x)+O(h)$ with $a_j\equiv\widetilde{a}_j\equiv1$ on $\partial\Omega\cap\overline{\mathcal{V}_j}$ such that the 1-form

$$u_{j,wkb}^{(1)}=d_{f,h}\left(a_j(x,h)e^{-\frac{1}{h}\Phi_j}\right)=\big(\widetilde{a}_j\,d(f-\Phi_j)+O(h)\big)e^{-\frac{1}{h}\Phi_j}, \tag{C.112}$$

satisfies

$$\begin{cases}\Delta_{f,h}^{(1)}u_{j,wkb}^{(1)}=O(h^\infty)e^{-\frac{1}{h}\Phi_j}\text{ in }\mathcal{V}_j\\ \mathbf{t}u_{j,wkb}^{(1)}=0\text{ on }\partial\Omega\cap\overline{\mathcal{V}_j}\\ \mathbf{t}d_{f,h}^*u_{j,wkb}^{(1)}=O(h^\infty)\,e^{-\frac{1}{h}\Phi_j}\text{ on }\partial\Omega\cap\overline{\mathcal{V}_j}.\end{cases} \tag{C.113}$$

Moreover, one has in the limit $h\to0$ (see [15, Section 4.2]):

$$\|\theta_ju_{j,wkb}^{(1)}\|_{L^2}=\frac{\pi^{\frac{d-1}{4}}\sqrt{2\partial_nf(z_j)}}{\big(\det\operatorname{Hess}f\big|_{\partial\Omega}(z_j)\big)^{\frac14}}\,h^{\frac{d+1}{4}}\big(1+O(h)\big). \tag{C.114}$$

The following proposition deals with the comparison between w_j and $u_{j,wkb}^{(1)}$.

Proposition C.19. *Let us assume that the assumptions **[H-Boundary]** and **[H-Morse]** hold. Let w_j be a L^2-normalized eigenform associated with the smallest eigenvalue $\lambda_h(\mathcal{V}_j)$ of $\Delta_{f,h}^{FD,(1)}(\mathcal{V}_j)$. Then, there exists $h_0 > 0$ such that for all $h \in (0, h_0)$ one has:*

$$\left\| \theta_j (w_j - c_j(h) u_{j,wkb}^{(1)}) \right\|_{H^1} = O(h^\infty) \tag{C.115}$$

where

$$c_j(h)^{-1} = \langle w_j, \theta_j u_{j,wkb}^{(1)} \rangle_{L^2}.$$

Moreover, in the limit $h \to 0$, one has:

$$c_j(h) = \frac{\left(\det \operatorname{Hess} f\big|_{\partial\Omega}(z_j)\right)^{\frac{1}{4}}}{\pi^{\frac{d-1}{4}} \sqrt{2\partial_n f(z_j)}} \, h^{-\frac{d+1}{4}} \big(1 + O(h)\big). \tag{C.116}$$

In addition, one can assume, up to replacing w_j by $-w_j$, that $c_j(h) \geq 0$. Proposition C.19 can be proved exactly as Proposition C.16.

In conclusion, one constructed in this section a family of 1-forms $(\widetilde{\phi}_j)_{j \in \{1,\dots,m_1^{\overline{\Omega}}\}}$. Since (C.77) guarantees $\overline{B(z, 2\varepsilon_1)} \cap \overline{B(z', 2\varepsilon_1)} = \emptyset$ for all $z \neq z' \in \mathcal{U}_1^{\overline{\Omega}}$, the family $(\widetilde{\phi}_j)_{j \in \{1,\dots,m_1^{\overline{\Omega}}\}}$ is orthonormal. From now on, the parameter ε_1 used to construct $(\widetilde{\phi}_j)_{j \in \{1,\dots,m_1^{\overline{\Omega}}\}}$ is fixed while $\varepsilon < \varepsilon_1$ will be fixed later on.

For upcoming computations, one needs the following definition.

Definition C.7. *Let us assume that the assumptions **[H-Boundary]** and **[H-Morse]** hold. For all $j \in \{1, ..., m_1^{\overline{\Omega}}\}$, one defines:*

$$\widetilde{\phi}_{j,wkb} := c_j(h) \, \theta_j \, u_{j,wkb}^{(1)}, \tag{C.117}$$

where for $j \in \{1, \dots, m_1^{\partial\Omega}\}$, w_j satisfies (C.113) *and θ_j is introduced in Definition C.6 and, for $j \in \{m_1^{\partial\Omega} + 1, \dots, m_1^{\overline{\Omega}}\}$, w_j satisfies* (C.102) *and θ_j is introduced in Definition C.5.*

C.2.4.3 Quasi-modes for $-L_{f,h}^{D,(p)}$, $p \in \{0, 1\}$

Before defining the quasi-modes for for $L_{f,h}^{D,(0)}$ and $L_{f,h}^{D,(1)}$, let us label the quasi-modes for $\Delta_{f,h}^{D,(0)}$ and the local minima of f using the lexicographical order.

Definition C.8. *Let us assume that the assumptions **[H-Boundary]** and **[H-Morse]** hold. Then, the family of the critical connected components $(E_{\ell,k})_{\ell \geq 1,\, k \in \{1,\dots,N_\ell\}}$ introduced in Section C.2.3.3, the local minima $(x_{\ell,k})_{\ell \geq 1,\, k \in \{1,\dots,N_\ell\}}$ of f labeled in Section C.2.3.3, the family of cut-off functions $(\chi_{\ell,k}^{\varepsilon,\varepsilon_1})_{\ell \geq 1,\, k \in \{1,\dots,N_\ell\}}$ introduced in Definition C.4 and the family of quasi-modes $(\widetilde{v}_{\ell,k})_{\ell \geq 1,\, k \in \{1,\dots,N_\ell\}}$ introduced in Definition C.4 are labeled in the lexicographical order:*

$$(E_k)_{k \in \{1,\dots,m_0^\Omega\}}, \ (\chi_k^{\varepsilon,\varepsilon_1})_{k \in \{1,\dots,m_0^\Omega\}}, \ (\widetilde{v}_k)_{k \in \{1,\dots,m_0^\Omega\}} \ \textit{and} \ (x_k)_{k \in \{1,\dots,m_0^\Omega\}}.$$

Let us recall that the lexicographic order is defined by $(i,j) < (k,l)$ if and only if $i < k$ or if $i = k$, $j < l$. From now on, one uses the labeling introduced in Definition C.8. Notice that from Definition C.2 and the first step of the construction of the maps $\mathbf{j}$ and $\widetilde{\mathbf{j}}$, it holds with the labeling introduced in Definition C.8:

$$\forall i \in \{1, \dots, N_1\},\ x_i \in C_i, \tag{C.118}$$

and $\forall i \in \{1, \dots, N_0\}$ it holds $x_i \in \arg\min_\Omega f \cap C_i$, where we recall N_0 is defined in (C.46). According to (C.37), the quasi-modes for $-L_{f,h}^{D,(0)}$ and $-L_{f,h}^{D,(1)}$ are obtained from those constructed previously for $\Delta_{f,h}^{D,(0)}$ and $\Delta_{f,h}^{D,(1)}$ using the unitary transformation U^{-1} defined in (C.36).

Definition C.9. *Let us assume that the assumptions **[H-Boundary]** and **[H-Morse]** hold. Let $(\widetilde{v}_k)_{k\in\{1,\dots,m_0^\Omega\}}$ be the family of quasi-modes for $\Delta_{f,h}^{D,(0)}$ introduced in Definition C.4 (and labeled in the lexicographical order, see Definition C.8) and let $(\widetilde{\phi}_j)_{j\in\{1,\dots,m_1^{\overline{\Omega}}\}}$ be the family of quasi-modes for $\Delta_{f,h}^{D,(1)}$ introduced in Definitions C.5 and C.6. The family of quasi-modes $(\widetilde{u}_k)_{k\in\{1,\dots,m_0^\Omega\}}$ for $-L_{f,h}^{D,(0)}$ and the family of quasi-modes $(\widetilde{\psi}_j)_{j\in\{1,\dots,m_1^{\overline{\Omega}}\}}$ for $-L_{f,h}^{D,(1)}$ are defined by: for $k \in \{1, ..., m_0^\Omega\}$, and for $j \in \{1, \dots, m_1^{\overline{\Omega}}\}$:*

$$\widetilde{u}_k := e^{\frac{1}{h}f}\,\widetilde{v}_k \in \Lambda^0 H^1_{w,T}(\Omega) \quad \textit{and} \quad \widetilde{\psi}_j := e^{\frac{1}{h}f}\,\widetilde{\phi}_j \in \Lambda^1 H^1_{w,T}(\Omega)\,. \tag{C.119}$$

Notice that, according to (C.80), (C.85) and (C.119), for all $k \in \{1, ..., m_0^\Omega\}$,

$$\widetilde{u}_k \in C_c^\infty(\Omega)\,,$$

and according to (C.97) and (C.110), for all $j \in \{1, \dots, m_1^{\overline{\Omega}}\}$,

$$\widetilde{\psi}_j \in \Lambda^1 C^\infty\left(\overline{\Omega}\right).$$

C.3 Proofs of Theorems C.1, C.2 and C.3

This section is dedicated to the proof of Theorems C.1, C.2 and C.3 and is divided into three parts. In Section C.3.1 one proves Theorem C.4 which is a more general result than Theorem C.1 (Theorem C.1 is a consequence of Theorem C.4). Theorem C.4 is concerned with the asymptotic expansions of the smallest eigenvalues of $-L_{f,h}^{D,(0)}$ when assuming [**H-Morse**] and [**H-Boundary**] but not [**H-Connexity**]. In Section C.3.2, one proves Theorem C.2. Finally, in Section C.3.3.2 one proves Theorem C.3.

C.3.1 Proof of Theorem C.1

In the whole section, one assumes that [**H-Morse**] and [**H-Boundary**] hold.

C.3.1.1 Quasi-modal estimates in the weighted space $L^2_w(\Omega)$

Let us define the following constants for all $j \in \left\{1, \dots, m_1^{\overline{\Omega}}\right\}$,

$$B_j := \begin{cases} \pi^{\frac{d-1}{4}} \sqrt{2\,\partial_n f(z_j)}\left(\det \operatorname{Hess} f\big|_{\partial\Omega}(z_j)\right)^{-1/4} & \text{if } z_j \in \partial\Omega \\ \pi^{\frac{d-2}{4}} \sqrt{|\lambda_-(z_j)|}\left|\det \operatorname{Hess} f(z_j)\right|^{-1/4} & \text{if } z_j \in \Omega \end{cases}, \tag{C.120}$$

where $\lambda_-(z_j)$ is the negative eigenvalue of Hess $f(z_j)$. The following boundary estimates will be used several times in the sequel.

Proposition C.20. *Let us assume that the assumptions **[H-Morse]** and **[H-Boundary]** hold. Let us consider $i \in \{1, \dots, m_1^{\overline{\Omega}}\}$, an open set Σ of $\partial\Omega$, and $F \in L^\infty(\partial\Omega, \mathbb{R})$. Then, there exists $c > 0$ such that one has in the limit $h \to 0$:*

$$\int_\Sigma F\, \widetilde{\psi}_i \cdot n\ e^{-\frac{2}{h}f} = \begin{cases} O\big(e^{-\frac{1}{h}(f(z_1)+c)}\big) & \text{if } i \in \big\{k_1^{\partial\Omega}+1, \dots, m_1^{\overline{\Omega}}\big\} \\ O\big(e^{-\frac{1}{h}(f(z_1)+c)}\big) & \text{if } i \in \big\{1, \dots, k_1^{\partial\Omega}\big\} \text{ and } z_i \notin \overline{\Sigma} \\ O\big(h^{\frac{d-3}{4}} e^{-\frac{1}{h}f(z_1)}\big) & \text{if } i \in \big\{1, \dots, k_1^{\partial\Omega}\big\} \text{ and } z_i \in \Sigma, \end{cases}$$

where $\widetilde{\psi}_i$ is introduced in Definition C.9, see (C.119)*. Moreover, when $i \in \big\{1, \dots, k_1^{\partial\Omega}\big\}$, $z_i \in \Sigma$, and F is C^∞ in a neighborhood of z_i, it holds*

$$\int_\Sigma F\, \widetilde{\psi}_i \cdot n\ e^{-\frac{2}{h}f} = h^{\frac{d-3}{4}}\, e^{-\frac{1}{h}f(z_1)} \big(B_i F(z_i) + O(h)\big),$$

where the constant B_i is defined in (C.120)*.*

Proof. Let $F \in L^\infty(\partial\Omega, \mathbb{R})$. From (C.119) and (C.97), the quasi-mode $\widetilde{\psi}_i$ is supported in Ω for $i \in \{m_1^{\partial\Omega}+1 \dots m_1^{\overline{\Omega}}\}$ and thus:

$$\forall i \in \big\{m_1^{\partial\Omega}+1, \dots, m_1^{\overline{\Omega}}\big\}, \int_\Sigma F\, \widetilde{\psi}_i \cdot n\ e^{-\frac{2}{h}f} = 0. \tag{C.121}$$

Take then $i \in \{1, \dots, m_1^{\partial\Omega}\}$ and note that we have for all h small enough, from the trace theorem, (C.119), (C.110), and (C.109),

$$\begin{aligned} \int_\Sigma F\, \widetilde{\psi}_i \cdot n\ e^{-\frac{2}{h}f} &= \int_{\operatorname{supp}\theta_i \cap \Sigma} F\, \widetilde{\phi}_i \cdot n\ e^{-\frac{1}{h}f} \\ &= O(\|\widetilde{\phi}_i\|_{H^1}) \Big(\int_{\operatorname{supp}\theta_i \cap \Sigma} e^{-\frac{2}{h}f} \Big)^{\frac{1}{2}} \\ &= O\big(h^{-p}\big) \Big(\int_{\operatorname{supp}\theta_i \cap \Sigma} e^{-\frac{2}{h}f} \Big)^{\frac{1}{2}}, \end{aligned} \tag{C.122}$$

where p is independent of h. Moreover, since z_i is the only minimum of f on $\operatorname{supp}\theta_i \cap \partial\Omega$ and $f(z_1) = f(z_j) < f(z_k)$ for all $j \in \big\{1, \dots, k_1^{\partial\Omega}\big\}$ and $k \in \big\{k_1^{\partial\Omega}+1, \dots, m_1^{\partial\Omega}\big\}$, one has in the limit $h \to 0$:

$$\int_{\operatorname{supp}\theta_i \cap \Sigma} e^{-\frac{2}{h}f} = \begin{cases} O\big(e^{-\frac{2}{h}(f(z_1)+c)}\big) & \text{if } i \in \big\{1, \dots, k_1^{\partial\Omega}\big\} \text{ and } z_i \notin \overline{\Sigma} \\ O\big(e^{-\frac{2}{h}(f(z_1)+c)}\big) & \text{if } i \in \big\{k_1^{\partial\Omega}+1, \dots, m_1^{\partial\Omega}\big\} \end{cases} \tag{C.123}$$

for some $c > 0$ independent of h.

Let us now assume that $i \in \big\{1, \dots, k_1^{\partial\Omega}\big\}$. One has:

$$\begin{aligned} \int_\Sigma F\, \widetilde{\psi}_i \cdot n\ e^{-\frac{2}{h}f} &= \int_\Sigma F\, \widetilde{\phi}_i \cdot n\ e^{-\frac{1}{h}f} \\ &= \int_\Sigma F\, \widetilde{\phi}_{i,wkb} \cdot n\ e^{-\frac{1}{h}f} + \int_\Sigma F\, \big(\widetilde{\phi}_i - \widetilde{\phi}_{i,wkb}\big) \cdot n\ e^{-\frac{1}{h}f}, \end{aligned} \tag{C.124}$$

where $\widetilde{\phi}_{i,wkb} = c_i(h)\theta_i u^{(1)}_{i,wkb}$ is defined in (C.117). From (C.112), let us recall that one has in the limit $h \to 0$:

$$u^{(1)}_{i,wkb} = e^{-\frac{1}{h}\Phi_i}\left(\widetilde{a}_i\, d(f-\Phi_i) + O(h)\right) \text{ on } \operatorname{supp}\theta_i$$

with $\widetilde{a}_i = 1$ on $\partial\Omega \cap \operatorname{supp}\theta_i$. Thus on $\partial\Omega \cap \operatorname{supp}\theta_i$, using also (C.106),

$$n \cdot u^{(1)}_{i,wkb} = e^{-\frac{1}{h}\Phi_i}\big|_{\partial\Omega}\, \partial_n(f-\Phi_i)\left(1+O(h)\right) = 2\partial_n f\, e^{-\frac{1}{h}(f-f(z_i))}\left(1+O(h)\right).$$

Thus, the term $\int_\Sigma F\,\widetilde{\phi}_{i,wkb}\cdot n\; e^{-\frac{1}{h}f}$ appearing in the right hand side of (C.124) satisfies in the limit $h \to 0$:

$$\begin{aligned}
\int_\Sigma F\,\widetilde{\phi}_{i,wkb}\cdot n\; e^{-\frac{1}{h}f} &= c_i(h)\int_{\Sigma\cap\operatorname{supp}\theta_i} F\,\theta_i\, u^{(1)}_{i,wkb}\cdot n\; e^{-\frac{1}{h}f} \\
&= c_i(h)\int_{\Sigma\cap\operatorname{supp}\theta_i} 2\partial_n f\, F\,\theta_i\, e^{-\frac{1}{h}(2f-f(z_i))}\left(1+O(h)\right) \qquad \text{(C.125)}\\
&= O\Big(c_i(h)\int_{\partial\Omega\cap\operatorname{supp}\theta_i} 2\partial_n f\,\theta_i\, e^{-\frac{1}{h}(2f-f(z_i))}\Big) \\
&= O\Big(c_i(h)\, h^{\frac{d-1}{2}}\, e^{-\frac{1}{h}f(z_1)}\Big) = O\big(h^{\frac{d-3}{4}}\, e^{-\frac{1}{h}f(z_1)}\big), \qquad \text{(C.126)}
\end{aligned}$$

where the last line follows from $\{z_i\} = \arg\min_{\partial\Omega\cap\operatorname{supp}\theta_i} f$, $\theta_i(z_i) = 1$, Laplace's method, and $c_i(h) = O(h^{-\frac{d+1}{4}})$ according to (C.116). When $z_i \in \Sigma$ and F is C^∞ in a neighborhood of z_i, the same arguments applied to (C.125) yield, in the limit $h \to 0$:

$$\int_\Sigma F\,\widetilde{\phi}_{i,wkb}\cdot n\; e^{-\frac{1}{h}f} = c_i(h)\, F(z_i)\,\frac{2\,\partial_n f(z_i)\,\pi^{\frac{d-1}{2}}}{\sqrt{\det\operatorname{Hess} f\big|_{\partial\Omega}(z_i)}}\, h^{\frac{d-1}{2}}\; e^{-\frac{1}{h}f(z_1)}\big(1+O(h)\big). \tag{C.127}$$

Besides, from the trace theorem, (C.110), (C.109), and (C.115), the second term in the right hand side of (C.124) satisfies in the limit $h \to 0$:

$$\int_\Sigma F\,(\widetilde{\phi}_i - \widetilde{\phi}_{i,wkb})\cdot n\; e^{-\frac{1}{h}f} = O(h^\infty)\; e^{-\frac{1}{h}f(z_1)}. \tag{C.128}$$

The first part of Proposition C.20 then results from (C.121)–(C.124), (C.126), and (C.128), and its second part from (C.124), (C.127)–(C.128), and from the precise asymptotic estimate of $c_i(h)$ given in (C.116) which yields, when $h \to 0$

$$\int_\Sigma F\,\widetilde{\psi}_i\cdot n\, e^{-\frac{2}{h}f} = F(z_i)\frac{\pi^{\frac{d-1}{4}}\sqrt{2\,\partial_n f(z_i)}}{\big(\det\operatorname{Hess} f\big|_{\partial\Omega}(z_i)\big)^{1/4}}\; h^{\frac{d-3}{4}}\; e^{-\frac{1}{h}f(z_1)}\big(1+O(h)\big).$$

This ends the proof of Proposition C.20 ∎

We are now in position to prove the following proposition which will be crucial to prove Theorem C.1 and Theorem C.2. It allows indeed to study accurately the small singular values of the restricted differential $\nabla : \operatorname{Ran}\pi^{(0)}_h \to \operatorname{Ran}\pi^{(1)}_h$, the square of the

smallest one being $\frac{2}{h}\lambda_h$, where λ_h is smallest eigenvalue of $-L_{f,h}^{D,(0)}$ (see Proposition C.2). Let us recall, that from (C.39), one defined:

$$\pi_h^{(0)} = \pi_{[0,\frac{\sqrt{h}}{2})}(-L_{f,h}^{D,(0)}) \text{ and } \pi_h^{(1)} = \pi_{[0,\frac{\sqrt{h}}{2})}(-L_{f,h}^{D,(1)}).$$

In the following, the finite dimensional spaces $\operatorname{Ran}\pi_h^{(0)}$ and $\operatorname{Ran}\pi_h^{(1)}$ are endowed with the scalar product $\langle\cdot,\cdot\rangle_{L^2_w}$.

Proposition C.21. *Let us assume that the assumptions **[H-Morse]** and **[H-Boundary]** hold. Let $(\widetilde{u}_k)_{k\in\{1,\dots,m_0^\Omega\}}$ be the family of quasi-modes for $-L_{f,h}^{D,(0)}$ and let $(\widetilde{\psi}_j)_{j\in\{1,\dots,m_1^{\overline{\Omega}}\}}$ be the family of quasi-modes for $-L_{f,h}^{D,(1)}$ introduced in Definition C.9. Let $N_1 \geq 1$ the integer introduced in item 1 of Lemma C.9.*

1. *for all $k \in \{1,\dots,m_0^\Omega\}$ and $j \in \{1,\dots,m_1^{\overline{\Omega}}\}$, $\widetilde{u}_k \in \Lambda^0 H^1_{w,T}(\Omega)$, $\widetilde{\psi}_j \in \Lambda^1 H^1_{w,T}(\Omega)$ and*

$$\|\widetilde{u}_k\|_{L^2_w} = \|\widetilde{\psi}_j\|_{L^2_w} = 1 \quad \text{and} \quad \forall i \in \{1,\dots,m_1^{\overline{\Omega}}\}\setminus\{j\}, \quad \langle\widetilde{\psi}_j,\widetilde{\psi}_i\rangle_{L^2_w} = 0\,.$$

   The family $(\widetilde{u}_k)_{k=1,\dots,m_0^\Omega}$ is moreover uniformly linearly independent (as defined in Lemma C.13) and:

$$\forall (k,l) \in \{1,\dots,N_1\}^2,\ \langle\widetilde{u}_k,\widetilde{u}_l\rangle_{L^2_w} = \delta_{k,l}.$$

2. *a) For any $\delta > 0$, one can choose the parameter ε appearing in* (C.80) *and in* (C.85) *(see also* (C.119)*) small enough such that for all $k \in \{1,\dots,m_0^\Omega\}$, in the limit $h \to 0$:*

$$\|(1-\pi_h^{(0)})\widetilde{u}_k\|^2_{L^2_w} \leq h^{\frac{1}{2}}\|\nabla\widetilde{u}_k\|^2_{L^2_w} = O\left(e^{-\frac{2}{h}(f(\mathbf{j}(x_k))-f(x_k)-\delta)}\right).$$

   b) There exist $c > 0$ such that for all $j \in \{1,\dots,m_1^{\overline{\Omega}}\}$, one has in the limit $h \to 0$:

$$\|(1-\pi_h^{(1)})\widetilde{\psi}_j\|^2_{H^1_w} = O\big(e^{-\frac{c}{h}}\big).$$

3. *There exist $c > 0$ such that for all $k \in \{1,\dots,m_0^\Omega\}$, one has in the limit $h \to 0$:*

$$\pi_h^{(0)}\widetilde{u}_k = \widetilde{u}_k + O\big(e^{-\frac{c}{h}}\big) \text{ in } L^2_w(\Omega).$$

   Moreover for all $(k,l) \in \{1,\dots,N_1\}^2$, it holds in the limit $h \to 0$:

$$\langle\pi_h^{(0)}\widetilde{u}_k,\pi_h^{(0)}\widetilde{u}_l\rangle_{L^2_w} = \delta_{k,l} + O\big(e^{-\frac{c}{h}}\big),$$

   and for all $(i,j) \in \{1,\dots,m_1^{\overline{\Omega}}\}^2$,

$$\langle\pi_h^{(1)}\widetilde{\psi}_i,\pi_h^{(1)}\widetilde{\psi}_j\rangle_{L^2_w} = \delta_{i,j} + O(e^{-\frac{c}{h}}).$$

4. *for all* $k \in \{1, \dots, m_0^\Omega\}$ *and* $j \in \{1, \dots, m_1^{\overline{\Omega}}\}$, *there exist a real constant* $C_{j,k} > 0$ *and* $\varepsilon_{j,k} \in \{-1, 1\}$ *independent of* h *such that in the limit* $h \to 0$,

$$\langle \nabla \widetilde{u}_k, \widetilde{\psi}_j \rangle_{L^2_w} = \begin{cases} \varepsilon_{i,k} C_{j,k}\ h^{p_{j,k}}\, e^{-\frac{1}{h}(f(\mathbf{j}(x_k)) - f(x_k))}\ \big(1 + O(h)\big) & \text{if } z_j \in \mathbf{j}(x_k) \\ 0 & \text{if } z_j \notin \mathbf{j}(x_k), \end{cases}$$

where

$$p_{j,k} = \begin{cases} -\frac{1}{2} & \text{if } z_j \in \mathbf{j}(x_k) \cap \Omega \\ -\frac{3}{4} & \text{if } z_j \in \mathbf{j}(x_k) \cap \partial\Omega. \end{cases}$$

Moreover, for all $k \in \{1, \dots, N_1\}$ *and* $j \in \{1, \dots, m_1^{\overline{\Omega}}\}$ *such that* $z_j \in \mathbf{j}(x_k)$, *one has*

$$C_{j,k} = \frac{B_j\, \pi^{-\frac{d}{4}}}{\Big(\sum\limits_{x \in \arg\min_{C_k} f} \big(\det \operatorname{Hess} f(x)\big)^{-\frac{1}{2}} \Big)^{1/2}}, \tag{C.129}$$

where the constant B_j *is defined in* (C.120) *and if* $z_j \in \mathbf{j}(x_k) \cap \partial\Omega$, $\varepsilon_{j,k} = -1$.

Remark C.10. *From the proof of item 4 of Proposition C.21, all the* $\varepsilon_{j,k}$ *and* $C_{j,k}$ *are computed for* $k \in \{1, \dots, m_0^\Omega\}$ *and for* $j \in \left\{1, \dots, m_1^{\overline{\Omega}}\right\}$. *Moreover, all the remainder terms* $O(h)$ *in item 4 of Proposition C.21 admits a full asymptotic expansion in* h *as defined in Remark C.1 (this follows from the fact that the Laplace's method actually yields a full asymptotic expansion in* h*).*

As a direct consequence of the items 1 and 3 of Proposition C.21, one obtains the following result.

Corollary C.22. *Let us assume that the assumptions* ***[H-Morse]*** *and* ***[H-Boundary]*** *hold. Let* $(\widetilde{u}_k)_{k \in \{1,\dots,m_0^\Omega\}}$ *and* $(\widetilde{\psi}_j)_{j \in \{1,\dots,m_1^{\overline{\Omega}}\}}$ *be the families introduced in Definition C.9. Then,*

1. *the family* $(\pi_h^{(0)} \widetilde{u}_k)_{k \in \{1,\dots,m_0^\Omega\}}$ *is linearly independant uniformly with respect to* h, *as defined in Lemma C.13.*

2. *the Gramian matrix of family* $(\pi_h^{(1)} \widetilde{\psi}_j)_{j \in \{1,\dots,m_1^{\overline{\Omega}}\}}$ *satisfies for some* $c > 0$, *in the limit* $h \to 0$*:*

$$\big(\langle \pi_h^{(1)} \widetilde{\psi}_i, \pi_h^{(1)} \widetilde{\psi}_j \rangle_{L^2_w}\big)_{(i,j)^2 \in \{1,\dots,m_1^{\overline{\Omega}}\}^2} = \mathrm{Id}_{m_1^{\overline{\Omega}}} + O(e^{-\frac{c}{h}}).$$

In particular, from Lemma C.7, there exists $h_0 > 0$ *such that for all* $h \in (0, h_0)$*:*

$$\operatorname{Ran} \pi_h^{(0)} = \operatorname{Span}\big(\pi_h^{(0)} \widetilde{u}_k,\ k = 1, \dots, m_0^\Omega\big) \text{ and } \operatorname{Ran} \pi_h^{(1)} = \operatorname{Span}\big(\pi_h^{(1)} \widetilde{\psi}_i,\ i = 1, \dots, m_1^{\overline{\Omega}}\big).$$

Let us now prove Proposition C.21.

Proof. The proof of Proposition C.21 is divided into three steps.

Step 1: Proofs of items 1 and 3. The first item is immediate according to the definition of the families $(\widetilde{u}_k)_{k=1,\dots,m_0^\Omega}$ and $(\widetilde{\psi}_i)_{i=1,\dots,m_1^{\overline{\Omega}}}$ introduced in Definition C.9. The fact that $\forall (k,l) \in \{1, \dots, N_1\}^2$

$$\big\langle \widetilde{u}_k, \widetilde{u}_l \big\rangle_{L^2_w} = \delta_{k,l},$$

follows from $\operatorname{supp}\widetilde{u}_k \cap \operatorname{supp}\widetilde{u}_l = \emptyset$ if $k \neq l$, see Definition C.9, Definition C.8 and item e) in Definition C.4. . The first equality in item 3, involving $\{\widetilde{u}_1, \dots, \widetilde{u}_{m_0^\Omega}\}$, is an easy consequence of 2.a) while the two last ones, involving $\{\widetilde{u}_1, \dots, \widetilde{u}_{N_1}\}$ and $\{\widetilde{\psi}_1, \dots, \widetilde{\psi}_{m_1^{\overline{\Omega}}}\}$, follow from 1 and 2 together with the relation

$$\langle \pi_h^{(\ell)} f, \pi_h^{(\ell)} g \rangle_{L^2_w} = -\langle (\pi_h^{(\ell)} - 1) f, (\pi_h^{(\ell)} - 1) g \rangle_{L^2_w} + \langle f, g \rangle_{L^2_w} \tag{C.130}$$

holding for f, g in $\Lambda^\ell L^2_w(\Omega)$ and $\ell \in \{1, 2\}$. Item 3 in Proposition C.21 is thus a consequence of the next step.

Step 2: Proof of item 2. The first inequality appearing in 2.a) is a direct consequence of Lemma C.8 applied to $A = -L^{D,(0)}_{f,h}$ whose associated quadratic form is given by $\frac{h}{2}\langle \nabla\cdot, \nabla\cdot \rangle_{L^2_w}$ on $H^1_{w,T}(\Omega)$. The second inequality in 2.a) follows from Laplace's methods and from the properties of the cut-off functions used to define the quasi-modes $\widetilde{u}_k$'s (see Definition C.4 and Definition C.9). Indeed, it is just a rewriting of (C.91) using Definition C.9 and the labeling introduced in Definition C.8.

Let us now deal with 2.b). First, Lemma C.8 together with (C.98) and (C.111) implies the existence of some $c > 0$ such that for all $i \in \{1, \dots, m_1^{\overline{\Omega}}\}$ and h small enough,

$$\Big\| \big(1 - \pi_{[0, h^{\frac{3}{2}})}(\Delta^{D,(1)}_{f,h}) \big) \widetilde{\phi}_i \Big\|_{L^2} = O(e^{-\frac{c}{h}}). \tag{C.131}$$

Consequently, using again (C.98) and (C.111), and owing to the following relations on $\Lambda^1 H^1_T(\Omega)$,

$$d_{f,h}\Big(1 - \pi_{[0,h^{\frac{3}{2}})}\big(\Delta^{D,(1)}_{f,h}\big)\Big) = \Big(1 - \pi_{[0,h^{\frac{3}{2}})}\big(\Delta^{D,(2)}_{f,h}\big)\Big) d_{f,h},$$
$$d^*_{f,h}\Big(1 - \pi_{[0,h^{\frac{3}{2}})}\big(\Delta^{D,(1)}_{f,h}\big)\Big) = \Big(1 - \pi_{[0,h^{\frac{3}{2}})}\big(\Delta^{D,(0)}_{f,h}\big)\Big) d^*_{f,h},$$

$d^*_{f,h} = hd^* + \mathbf{i}_{\nabla f}$, and $d_{f,h} = hd + \nabla f \wedge$, one obtains the existence of $c > 0$ such that in the limit $h \to 0$:

$$\Big\| d\big(1 - \pi_{[0,h^{\frac{3}{2}})}(\Delta^{D,(1)}_{f,h}) \big) \widetilde{\phi}_i \Big\|_{L^2} + \Big\| d^*\big(1 - \pi_{[0,h^{\frac{3}{2}})}(\Delta^{D,(1)}_{f,h}) \big) \widetilde{\phi}_i \Big\|_{L^2} = O(e^{-\frac{c}{h}}). \tag{C.132}$$

Since $\widetilde{\phi}_i \in \Lambda^1 H^1_T(\Omega)$, the estimates (C.131) and (C.132) then lead, owing to Gaffney's inequality (see [29, Corollary 2.1.6]), to

$$\Big\| \big(1 - \pi_{[0,h^{\frac{3}{2}})}(\Delta^{D,(1)}_{f,h}) \big) \widetilde{\phi}_i \Big\|_{H^1} = O(e^{-\frac{c}{h}}).$$

Therefore, we deduce from the relation $\|u\|_{H^1_w} \leq \frac{C}{h} \|u\, e^{-\frac{1}{h}f}\|_{H^1}$, valid for all $u \in \Lambda^p H^1(\Omega)$ and $h > 0$, and from

$$\pi_{[0,h^{\frac{3}{2}})}\big(\Delta^{D,(1)}_{f,h}\big) = e^{-\frac{1}{h}f} \pi_h^{(1)} e^{\frac{1}{h}f},$$

resulting from (C.37) and (C.39), that there exists $c > 0$ such that for all $i \in \{1, \dots, m_1^{\overline{\Omega}}\}$ and h small enough,

$$\Big\| (1 - \pi_h^{(1)}) \widetilde{\psi}_i \Big\|_{H^1_w} \leq \frac{C}{h} \Big\| \big(1 - \pi_{[0,h^{\frac{3}{2}})}(\Delta^{D,(1)}_{f,h}) \big) \widetilde{\phi}_i \Big\|_{H^1} = O(e^{-\frac{c}{h}}),$$

which proves 2.b).

Step 3: Proof of item 4. The proof of item 4 is divided into two steps.

Step 3a. Let us deal with the computation of the terms $\langle \nabla \widetilde{u}_k, \widetilde{\psi}_i \rangle_{L^2_w}$ for $k \in \{1, \dots, N_1\}$ and $i \in \{1, \dots, m_1^{\overline{\Omega}}\}$. Let us recall that from Definition C.2, N_1 denotes the number of connected components of $\{f < \min_{\partial\Omega} f\}$. Moreover, from the construction of the map $\mathbf{j}$ in Section C.2.3.3 and according to the lexicographical labeling of the local minima of f introduced in Definition C.8, one has for any $k \in \{1, ..., m_0^{\Omega}\}$:

$$k \in \{1, ..., N_1\} \text{ iff } \mathbf{j}(x_k) \cap \partial\Omega \neq \emptyset.$$

Moreover, one has for any $k \in \{1, ..., N_1\}$:

$$f(\mathbf{j}(x_k)) = \min_{\partial\Omega} f = f(z_1).$$

Let us deal with the case $k = 1$ (the cases $k \in \{2, ..., N_1\}$ for $i \in \{2, \dots, N_1\}$ are treated similarly). According to Definitions C.5, C.6 and C.9, one has that for all $i \in \{1, \dots, m_1^{\overline{\Omega}}\}$, the quasi-mode $\widetilde{\psi}_i$ is supported in $B(z_i, 2\varepsilon_1)$. It then follows from (C.80), (C.84), and Definition C.9 that for any $i \in \{1, \dots, m_1^{\overline{\Omega}}\}$ such that $z_i \notin \mathbf{j}(x_1)$, $\operatorname{supp} \nabla \widetilde{u}_1 \cap \operatorname{supp} \widetilde{\psi}_i = \emptyset$ and thus

$$\left\langle \nabla \widetilde{u}_1, \widetilde{\psi}_i \right\rangle_{L^2_w} = 0.$$

Let us now consider the case $z_i \in \mathbf{j}(x_1) \cap \partial\Omega$. Notice that in that case $i \in \{1, \dots, k_1^{\partial C_1}\}$. According to Definition C.9 and (C.80) and by definition of lexicographical labeling introduced in Definition C.8, one has

$$\langle \nabla \widetilde{u}_1, \widetilde{\psi}_i \rangle_{L^2_w} = \int_\Omega \nabla \widetilde{u}_1 \cdot \widetilde{\phi}_i \; e^{-\frac{1}{h} f} = \frac{\displaystyle\int_\Omega \nabla \chi_1^{\varepsilon,\varepsilon_1} \cdot \widetilde{\phi}_i \; e^{-\frac{1}{h} f}}{\sqrt{\displaystyle\int_\Omega (\chi_1^{\varepsilon,\varepsilon_1})^2 e^{-\frac{2}{h} f}}}. \tag{C.133}$$

The asymptotic behaviour of the denominator of the right hand side of (C.133) can be computed, using Laplace's method and (C.81)–(C.82):

$$\int_\Omega (\chi_1^{\varepsilon,\varepsilon_1})^2 e^{-\frac{2}{h} f} = (\pi\, h)^{\frac{d}{2}} \, e^{-\frac{2}{h} f(x_1)} \sum_{x \in \arg\min_{C_1} f} \left(\det \operatorname{Hess} f(x)\right)^{-\frac{1}{2}} \left(1 + O(h)\right). \tag{C.134}$$

Since $\operatorname{supp} \widetilde{\phi}_i \subset B(z_i, 2\varepsilon_1)$, the numerator of the right hand side of (C.133) can be rewritten as

$$\begin{aligned}
\int_\Omega \nabla \chi_1^{\varepsilon,\varepsilon_1} \cdot \widetilde{\phi}_i \; e^{-\frac{1}{h} f} &= -\int_{B(z_i, 2\varepsilon_1)} \nabla (1 - \chi_1^{\varepsilon,\varepsilon_1}) \cdot \widetilde{\phi}_i \; e^{-\frac{1}{h} f} \\
&= -\int_{B(z_i, 2\varepsilon_1)} \left(1 - \chi_1^{\varepsilon,\varepsilon_1}\right) \, d^*\left(\widetilde{\phi}_i \; e^{-\frac{1}{h} f}\right) - \int_{\partial B(z_i, 2\varepsilon_1)} \left(1 - \chi_1^{\varepsilon,\varepsilon_1}\right) \widetilde{\phi}_i \cdot n \; e^{-\frac{1}{h} f} \\
&= -\frac{1}{h} \int_{B(z_i, 2\varepsilon_1)} \left(1 - \chi_1^{\varepsilon,\varepsilon_1}\right) e^{-\frac{1}{h} f} \, d^*_{f,h} \widetilde{\phi}_i \\
&\quad - \int_{\partial B(z_i, 2\varepsilon_1) \cap \partial\Omega} \widetilde{\phi}_i \cdot n \; e^{-\frac{1}{h} f}.
\end{aligned} \tag{C.135}$$

From (C.111), there exists $c > 0$ such that for h small enough, $d^*_{f,h}\widetilde{\phi}_i = O(e^{-\frac{c}{h}})$ in $L^2(\Omega)$. Since $f \geq f(z_1) - 2\varepsilon$ on $B(z_i, 2\varepsilon_1) \cap \mathrm{supp}(1 - \chi_1^{\varepsilon,\varepsilon_1})$ by (C.79) and (C.81), there exist $c' > 0$ and $\varepsilon_0 > 0$ such that for all $\varepsilon \in (0, \varepsilon_0)$, one has in the limit $h \to 0$:

$$\frac{1}{h}\int_{B(z_i,2\varepsilon_1)} \left(1 - \chi_1^{\varepsilon,\varepsilon_1}\right) e^{-\frac{1}{h}f}\, d^*_{f,h}\widetilde{\phi}_i = O\big(e^{-\frac{1}{h}(f(z_1)+c')}\big). \tag{C.136}$$

Furthermore, applying Proposition C.20 with $\Sigma = \partial\Omega$ and $F = 1_{\partial B(z_i,2\varepsilon_1)\cap\partial\Omega}$, one has at the limit $h \to 0$:

$$\int_{\partial B(z_i,2\varepsilon_1)\cap\partial\Omega} \widetilde{\phi}_i \cdot n\; e^{-\frac{1}{h}f} = \frac{\pi^{\frac{d-1}{4}}\sqrt{2\,\partial_n f(z_i)}}{\big(\det \mathrm{Hess} f\big|_{\partial\Omega}(z_i)\big)^{1/4}}\; h^{\frac{d-3}{4}} e^{-\frac{1}{h}f(z_1)}\big(1 + O(h)\big). \tag{C.137}$$

Therefore, injecting the estimates (C.134)–(C.137) into (C.133), one obtains in the limit $h \to 0$:

$$\langle \nabla\widetilde{u}_1, \widetilde{\psi}_i\rangle_{L^2_w} = -\frac{\pi^{-\frac{1}{4}}\sqrt{2\,\partial_n f(z_i)}\, h^{-\frac{3}{4}} e^{-\frac{1}{h}(f(z_1)-f(x_1))}}{\big(\det \mathrm{Hess} f\big|_{\partial\Omega}(z_i)\big)^{\frac{1}{4}}\left(\sum_{x\in\arg\min_{C_1} f}\big(\det \mathrm{Hess} f(x)\big)^{-\frac{1}{2}}\right)^{\frac{1}{2}}}\big(1 + O(h)\big),$$

which is the desired estimate according to (C.129)–(C.120).

It thus remains to estimate $\langle \nabla\widetilde{u}_1, \widetilde{\psi}_i\rangle_{L^2_w}$ when $z_i \in \mathbf{j}(x_1) \cap \Omega$. Actually, the computation of the term $\langle \nabla\widetilde{u}_1, \widetilde{\psi}_i\rangle_{L^2_w}$ when $z_i \in \mathbf{j}(x_1) \cap \Omega$ is identical to the one made in Step 3b below when $k \in \{N_1 + 1, ..., m_0^\Omega\}$.

Step 3b. Let us deal with the computation of the terms $\langle \nabla\widetilde{u}_k, \widetilde{\psi}_i\rangle_{L^2_w}$ for $k \in \big\{N_1 + 1, ..., m_0^\Omega\big\}$ and $i \in \big\{1, \ldots, m_1^{\overline{\Omega}}\big\}$. Let us recall that from the construction of the map $\mathbf{j}$ in Section C.2.3.3 and according to the lexicographic labeling of the local minima of f introduced in Definition C.8, one has for any $k \in \{1, ..., m_0^\Omega\}$:

$$k \in \{N_1 + 1, ..., m_0^\Omega\} \text{ iff } \mathbf{j}(x_k) \subset \Omega.$$

Moreover for any $k \in \{1, ..., m_0^\Omega\}$,

$$f(\mathbf{j}(x_k)) < f(z_1) = \min_{\partial\Omega} f.$$

The estimates of $\langle \nabla\widetilde{u}_k, \widetilde{\psi}_i\rangle_{L^2_w}$ for $k \in \big\{N_1 + 1, ..., m_0^\Omega\big\}$ and $i \in \big\{1, \ldots, m_1^{\overline{\Omega}}\big\}$ here follows from the analysis led in the proof of [14, Proposition 6.4], the only difference arising from the fact $\mathbf{j}(x_k)$ and $\arg\min_{\mathrm{supp}\,\chi_k^{\varepsilon,\varepsilon_1}} f$ were both reduced to one single point there. Let us give a proof for the sake of completeness.

Let $k \in \big\{N_1 + 1, ..., m_0^\Omega\big\}$ and $i \in \big\{1, \ldots, m_1^{\overline{\Omega}}\big\}$. If $z_i \notin \mathbf{j}(x_k)$, then, using (C.90) which guarantees that $\mathrm{supp}\,\nabla\chi_k^{\varepsilon,\varepsilon_1} \cap \overline{B(z_i, 2\varepsilon_1)} = \emptyset$, one obtains

$$\big\langle \nabla\widetilde{u}_k, \widetilde{\psi}_i\big\rangle_{L^2_w} = 0.$$

Let us then consider the case $z_i \in \mathbf{j}(x_k) \subset \Omega$. One wants to precisely compute:

$$\big\langle \nabla\widetilde{u}_k, \widetilde{\psi}_i\big\rangle_{L^2_w} = \int_\Omega \nabla\widetilde{u}_k \cdot \widetilde{\phi}_i\; e^{-\frac{1}{h}f} = \frac{\displaystyle\int_\Omega \nabla\chi_k^{\varepsilon,\varepsilon_1} \cdot \widetilde{\phi}_i\; e^{-\frac{1}{h}f}}{\sqrt{\displaystyle\int_\Omega (\chi_k^{\varepsilon,\varepsilon_1})^2 e^{-\frac{2}{h}f}}} = \frac{\displaystyle\int_{B(z_i,2\varepsilon_1)} \nabla\chi_k^{\varepsilon,\varepsilon_1} \cdot \widetilde{\phi}_i\; e^{-\frac{1}{h}f}}{\sqrt{\displaystyle\int_\Omega (\chi_k^{\varepsilon,\varepsilon_1})^2 e^{-\frac{2}{h}f}}}. \tag{C.138}$$

Using Laplace's method together with (C.86)–(C.87), one obtains in the limit $h \to 0$:

$$\int_\Omega (\chi_k^{\varepsilon,\varepsilon_1})^2 e^{-\frac{2}{h}f} = (\pi\, h)^{\frac{d}{2}} e^{-\frac{2}{h}f(x_k)} \sum_{x \in \arg\min_{\operatorname{supp}\chi_k^{\varepsilon,\varepsilon_1}} f} \big(\det \operatorname{Hess} f(x)\big)^{-\frac{1}{2}} \, \big(1 + O(h)\big)\,. \tag{C.139}$$

Let us now give the estimate of the numerator of the right hand side of (C.138).

To prepare this computation, let us first recall that the set $B(z_i, 2\varepsilon_1) \cap \{f < f(z_i)\}$ has, according to (C.78), two connected components and, since $z_i \in \mathcal{U}_1^{ssp}$ (see Definition C.3), exactly one of them intersects – and is then included in – the critical connected component $\widetilde{\mathbf{j}}(x_k) = E_k$ associated with x_k (see Definition C.3 and (C.71)). Moreover, the set $B(z_i, 2\varepsilon_1) \setminus \mathcal{W}_+(z_i)$, where the stable manifold $\mathcal{W}_+(z_i)$ has been defined in (C.99), has also two connected components and one of them contains the connected component of $B(z_i, 2\varepsilon_1) \cap \{f < f(z_i)\}$ which intersects E_k, namely $B(z_i, 2\varepsilon_1) \cap E_k$ (see for instance Figure C.6). Denoting this connected component of $B(z_i, 2\varepsilon_1) \setminus \mathcal{W}_+(z_i)$ by $B_i^{\varepsilon_1}$, on can conclude using an integration by parts as in the lines following (C.134) above (using $\operatorname{supp} \widetilde{\phi}_i \subset B(z_i, 2\varepsilon_1)$ and then $\operatorname{supp}(\nabla \chi_k^{\varepsilon,\varepsilon_1} \cdot \widetilde{\phi}_i) \subset B(z_i, 2\varepsilon_1) \cap E_k \subset B_i^{\varepsilon_1}$ by (C.89)):

$$\begin{aligned}
\int_\Omega \nabla \chi_k^{\varepsilon,\varepsilon_1} \cdot \widetilde{\phi}_i \; e^{-\frac{1}{h}f} &= -\int_{B_i^{\varepsilon_1}} \nabla(1 - \chi_k^{\varepsilon,\varepsilon_1}) \cdot \widetilde{\phi}_i \; e^{-\frac{1}{h}f} \\
&= -\frac{1}{h} \int_{B_i^{\varepsilon_1}} \big(1 - \chi_k^{\varepsilon,\varepsilon_1}\big) \, e^{-\frac{1}{h}f} \, d^*_{f,h} \widetilde{\phi}_i - \int_{\partial B_i^{\varepsilon_1}} \big(1 - \chi_k^{\varepsilon,\varepsilon_1}\big) \widetilde{\phi}_i \cdot n \; e^{-\frac{1}{h}f} \\
&= -\frac{1}{h} \int_{B_i^{\varepsilon_1}} \big(1 - \chi_k^{\varepsilon,\varepsilon_1}\big) \, e^{-\frac{1}{h}f} \, d^*_{f,h} \widetilde{\phi}_i \\
&\quad - \int_{\partial B_i^{\varepsilon_1} \cap \mathcal{W}_+(z_i)} \widetilde{\phi}_i \cdot n \; e^{-\frac{1}{h}f}.
\end{aligned} \tag{C.140}$$

From (C.98), it holds for h small enough, choosing $c > 0$ smaller if necessary, $d^*_{f,h} \widetilde{\phi}_i = O(e^{-\frac{c}{h}})$ in $L^2(\Omega)$. Since moreover $f \geq f(z_i) - 2\varepsilon$ on $B(z_i, 2\varepsilon_1) \cap \operatorname{supp}(1 - \chi_1^{\varepsilon,\varepsilon_1})$ by (C.86), there exist $c' > 0$ and $\varepsilon_0 > 0$ such that for all $\varepsilon \in (0, \varepsilon_0)$ one has in the limit $h \to 0$:

$$\frac{1}{h} \int_{B_i^{\varepsilon_1}} (1 - \chi_1^{\varepsilon,\varepsilon_1}) \; e^{-\frac{1}{h}f} \, d^*_{f,h} \widetilde{\phi}_i = O\big(e^{-\frac{1}{h}(f(z_i) + c')}\big). \tag{C.141}$$

Lastly, using (C.97), (C.96), (C.104), and the trace theorem, one obtains in the limit $h \to 0$:

$$\begin{aligned}
\int_{\partial B_i^{\varepsilon_1} \cap \mathcal{W}_+(z_i)} \widetilde{\phi}_i \cdot n \; e^{-\frac{1}{h}f} &= \int_{\partial B_i^{\varepsilon_1} \cap \mathcal{W}_+(z_i)} c_i(h) \, \theta_i \, u^{(1)}_{i,wkb} \cdot n \; e^{-\frac{1}{h}f} + O(h^\infty e^{-\frac{1}{h}f(z_i)}) \\
&= \pm \frac{c_i(h) (\pi h)^{\frac{d-1}{2}}}{\big(\det \operatorname{Hess} f\big|_{\mathcal{W}_+(z_i)}(z_i)\big)^{\frac{1}{2}}} e^{-\frac{1}{h}f(z_i)} \big(1 + O(h)\big) \\
&= \pm \frac{(\pi h)^{\frac{d-2}{4}} |\lambda_-(z_i)|^{\frac{1}{2}}}{\big|\det \operatorname{Hess} f(z_i)\big|^{\frac{1}{4}}} e^{-\frac{1}{h}f(z_i)} \big(1 + O(h)\big)\,,
\end{aligned}$$

where $\lambda_-(z_i)$ denotes the negative eigenvalue of $\operatorname{Hess} f(z_i)$. The second equality follows from Laplace's method and from the fact that

$$u^{(1)}_{i,wkb} \cdot n = e^{-\frac{1}{h}\Phi_i}\big|_{\mathcal{W}_+(z_i)} \big(\widetilde{a}_i \cdot n + O(h)\big) = e^{-\frac{1}{h}(f - f(z_i))}\big|_{\mathcal{W}_+(z_i)} \big(\widetilde{a}_i \cdot n + O(h)\big)$$

and $\widetilde{a}_i(z_i)\cdot n=\pm 1$, see indeed the lines between (C.101) and (C.102). The last line follows from (C.105). The asymptotic estimate of the term $\langle\nabla\widetilde{u}_k,\widetilde{\psi}_i\rangle_{L^2_w}$ is a consequence of the latter estimate together with (C.138)–(C.141) which gives in the limit $h\to 0$:

$$\langle\nabla\widetilde{u}_k,\widetilde{\psi}_i\rangle_{L^2_w}=\pm\frac{\pi^{-\frac{1}{2}}|\lambda_-(z_i)|^{\frac{1}{2}}\,h^{-\frac{1}{2}}e^{-\frac{1}{h}(f(z_i)-f(x_k))}}{\big|\det\,\mathrm{Hess}f(z_i)\big|^{\frac{1}{4}}\Big(\sum_{x\in\arg\min_{\mathrm{supp}\,\chi_k^{\varepsilon,\varepsilon_1}}f}\big(\det\,\mathrm{Hess}f(x)\big)^{-\frac{1}{2}}\Big)^{\frac{1}{2}}}\big(1+O(h)\big).$$

This proves item 4 in Proposition C.21 for all $k\in\big\{N_1+1,...,m_0^\Omega\big\}$ and $i\in\big\{1,\dots,m_1^{\overline{\Omega}}\big\}$. To conclude the proof of Proposition C.21, it remains, as announced at the end of Step 3a, to estimate the term $\langle\nabla\widetilde{u}_k,\widetilde{\psi}_i\rangle_{L^2_w}$ when $k\in\{1,...,N_1\}$ and $i\in\big\{1,\dots,m_1^{\overline{\Omega}}\big\}$ is such that $z_i\in\mathbf{j}(x_1)\cap\Omega$. It can be checked that the same computations as those made for $k\in\big\{N_1+1,...,m_0^\Omega\big\}$ yield for $k\in\{1,...,N_1\}$ and $i\in\big\{1,\dots,m_1^{\overline{\Omega}}\big\}$ such that $z_i\in\mathbf{j}(x_1)\cap\Omega$

$$\langle\nabla\widetilde{u}_k,\widetilde{\psi}_i\rangle_{L^2_w}=\pm\frac{\pi^{-\frac{1}{2}}|\lambda_-(z_i)|^{\frac{1}{2}}\,h^{-\frac{1}{2}}e^{-\frac{1}{h}(f(z_i)-f(x_k))}}{\big|\det\,\mathrm{Hess}f(z_i)\big|^{\frac{1}{4}}\Big(\sum_{x\in\arg\min_{\mathrm{supp}\,\chi_k^{\varepsilon,\varepsilon_1}}f}\big(\det\,\mathrm{Hess}f(x)\big)^{-\frac{1}{2}}\Big)^{\frac{1}{2}}}\big(1+O(h)\big).$$

This ends the proof of Proposition C.21. ∎

C.3.1.2 Restricted differential $\nabla:\mathrm{Ran}\,\pi_h^{(0)}\to\mathrm{Ran}\,\pi_h^{(1)}$ and proof of Theorem C.1

This section is concerned with Theorem C.4 which aims at estimating in the limit $h\to 0$ the m_0^Ω first eigenvalues of $-L_{f,h}^{D,(0)}$. According to Lemma C.7 and Proposition C.2, the square of the m_0^Ω singular values of the restricted differential $\nabla:\mathrm{Ran}\,\pi_h^{(0)}\to\mathrm{Ran}\,\pi_h^{(1)}$ are the first m_0^Ω first eigenvalues of $-L_{f,h}^{D,(0)}$ times $\frac{2}{h}$. Therefore, the strategy consists in estimating in the limit $h\to 0$ the m_0^Ω singular values of the restricted differential $\nabla:\mathrm{Ran}\,\pi_h^{(0)}\to\mathrm{Ran}\,\pi_h^{(1)}$. To this end, let us first introduce the matrix of the restricted differential $\nabla:\mathrm{Ran}\,\pi_h^{(0)}\to\mathrm{Ran}\,\pi_h^{(1)}$.

Definition C.10. *Let us assume that the assumptions **[H-Morse]** and **[H-Boundary]** hold. Let $(\widetilde{u}_k)_{k\in\{1,\dots,m_0^\Omega\}}$ be the family of quasi-modes for $-L_{f,h}^{D,(0)}$ and let $(\widetilde{\psi}_j)_{j\in\{1,\dots,m_1^{\overline{\Omega}}\}}$ be the family of quasi-modes for $-L_{f,h}^{D,(1)}$, both introduced in Definition C.9. Let us denote by $S=(S_{j,k})_{j,k}$ the real value $m_1^{\overline{\Omega}}\times m_0^\Omega$ matrix defined by: for all $k\in\{1,...,m_0^\Omega\}$ and for all $j\in\{1,\dots,m_1^{\overline{\Omega}}\}$*

$$S_{j,k}:=\big\langle\nabla\pi_h^{(0)}\widetilde{u}_k,\pi_h^{(1)}\widetilde{\psi}_j\big\rangle_{L^2_w}. \tag{C.142}$$

Notice that from (C.38), it holds for all $k\in\{1,...,m_0^\Omega\}$ and for all $j\in\{1,...,m_1^{\overline{\Omega}}\}$:

$$S_{j,k}=\big\langle\nabla\pi_h^{(0)}\widetilde{u}_k,\pi_h^{(1)}\widetilde{\psi}_j\big\rangle_{L^2_w}=\big\langle\nabla\pi_h^{(0)}\widetilde{u}_k,\pi_h^{(1)}\widetilde{\psi}_j\big\rangle_{L^2_w}.$$

Using the identity

$$\big\langle\nabla\pi_h^{(0)}\widetilde{u}_k,\pi_h^{(1)}\widetilde{\psi}_j\big\rangle_{L^2_w}=\big\langle\nabla\widetilde{u}_k,\widetilde{\psi}_j\big\rangle_{L^2_w}+\big\langle\nabla\widetilde{u}_k,\big(\pi_h^{(1)}-1\big)\widetilde{\psi}_j\big\rangle_{L^2_w}$$

together with Proposition C.21, one gets the following estimates of the coefficients of S:

Proposition C.23. *Let us assume that the hypotheses **[H-Morse]** and **[H-Boundary]** hold. Let S be the matrix introduced in Definition C.10. Fixing the parameter $\varepsilon > 0$ appearing in* (C.80) *and in* (C.85) *small enough, there exists $c > 0$ such that in the limit $h \to 0$:*

$$S_{j,k} = \begin{cases} \left\langle \nabla \widetilde{u}_k, \widetilde{\psi}_j \right\rangle_{L^2_w} \left(1 + O(e^{-\frac{c}{h}})\right) = \varepsilon_{j,k} C_{j,k}\, h^{p_{j,k}} e^{-\frac{1}{h}(f(\mathbf{j}(x_k)) - f(x_k))}(1 + O(h)) & \text{if } z_j \in \mathbf{j}(x_k) \\ O\left(e^{-\frac{1}{h}(f(\mathbf{j}(x_k)) - f(x_k) + c)}\right) & \text{if } z_j \notin \mathbf{j}(x_k), \end{cases}$$

where we recall, from item 4 in Proposition C.21, $\varepsilon_{j,k} \in \{-1, 1\}$ and $C_{j,k} > 0$ and

$$p_{j,k} = \begin{cases} -\frac{1}{2} & \text{if } z_j \in \mathbf{j}(x_k) \cap \Omega \\ -\frac{3}{4} & \text{if } z_j \in \mathbf{j}(x_k) \cap \partial\Omega. \end{cases} \tag{C.143}$$

Moreover, when $k \in \left\{1, \dots, N_1\right\}$ and $j \in \left\{1, \dots, m_1^{\overline{\Omega}}\right\}$ such that $z_j \in \mathbf{j}(x_k)$, $C_{j,k}$ is defined in (C.129) *and if $z_j \in \mathbf{j}(x_k) \cap \partial\Omega$, $\varepsilon_{j,k} = -1$.*

To study the singular values of the matrix S, one defines the following matrices:

- let $\widetilde{S} = \left(\widetilde{S}_{j,k}\right)_{j,k}$ be the real value $m_1^{\overline{\Omega}} \times m_0^{\Omega}$ matrix defined by

$$\widetilde{S}_{j,k} := \begin{cases} S_{j,k} & \text{if } z_j \in \mathbf{j}(x_k) \\ 0 & \text{if } z_j \notin \mathbf{j}(x_k). \end{cases} \tag{C.144}$$

  Notice that from (C.144), Proposition C.23, (C.143) and (C.73), one has for all $k \in \{1, ..., N_0\}$, in the limit $h \to 0$:

$$\begin{cases} \sum_{j=1}^{k_1^{\partial\Omega}} \widetilde{S}_{j,k}^2 = h^{-\frac{3}{2}} \left(\sum_{j : z_j \in \mathbf{j}(x_k) \cap \partial\Omega} C_{j,k}^2 \right) e^{-\frac{2}{h}(f(z_1) - f(x_1))}(1 + O(h)) \\ \sum_{j=k_1^{\overline{\Omega}}+1}^{m_1^{\overline{\Omega}}} \widetilde{S}_{j,k}^2 = h^{-1} \left(\sum_{j : z_j \in \mathbf{j}(x_k) \cap \Omega} C_{j,k}^2 \right) e^{-\frac{2}{h}(f(z_1) - f(x_1))}(1 + O(h)) \end{cases}, \tag{C.145}$$

  where the constants $C_{j,k}$'s are defined in (C.129) and where all the remainder terms $O(h)$ admits a full expansion in h (see Remark C.10).

- let D be the diagonal $m_0^{\Omega} \times m_0^{\Omega}$ matrix defined by

$$\forall k \in \{1, \dots, m_0^{\Omega}\},\ D_{k,k} := h^{q_k} e^{-\frac{1}{h}(f(\mathbf{j}(x_k)) - f(x_k))} \quad \text{where} \quad q_k := \min_j \{p_{j,k}\}, \tag{C.146}$$

  and where $p_{j,k}$ is defined in (C.143). Notice that from the definition of N_1 introduced in Definition C.2, the labeling introduced in Definition C.8, the construction of the map $\mathbf{j}$ in Section C.2.3.3 and (C.143), it holds for all $k \in \{1, ..., m_0^{\Omega}\}$

$$q_k = \begin{cases} -\frac{3}{4} & \text{iff } k \in \{1, ..., N_1\} \\ -\frac{1}{2} & \text{otherwise.} \end{cases} \tag{C.147}$$

  In addition, from (C.146), (C.74) and (C.147), there exists $c > 0$ such that for all $\forall (k, l) \in \left\{1, \dots, N_0\right\} \times \left\{N_0 + 1, \dots, m_0^{\Omega}\right\}$, one has in the limit $h \to 0$:

$$D_{k,k} = h^{-\frac{3}{4}} e^{-\frac{1}{h}(f(z_1) - f(x_1))} \tag{C.148}$$

$$= O\big(e^{-\frac{c}{h}} D_{l,l}\big). \tag{C.149}$$

- let $\widetilde{C}$ be the real value $m_1^{\overline{\Omega}} \times m_0^{\Omega}$ matrix defined by

$$\widetilde{C} := \widetilde{S}\, D^{-1}. \tag{C.150}$$

The matrix $\widetilde{C}$ is the $m_1^{\overline{\Omega}} \times m_0^{\Omega}$ matrix whose coefficients are given by:

$$\widetilde{C}_{j,k} = \frac{\widetilde{S}_{j,k}}{D_{k,k}},$$

for all $(j,k) \in \{1, \dots, m_1^{\overline{\Omega}}\} \times \{1, \dots, m_0^{\Omega}\}$ and which satisfies, according to Proposition C.23, in the limit $h \to 0$:

$$\widetilde{C}_{j,k} = \begin{cases} \varepsilon_{j,k} C_{j,k}\, h^{p_{j,k}-q_k} \big(1 + O(h)\big) & \text{if } z_j \in \mathbf{j}(x_k) \\ 0 & \text{if } z_j \notin \mathbf{j}(x_k), \end{cases} \tag{C.151}$$

where $p_{j,k}$ is defined by (C.143), $\varepsilon_{j,k} \in \{-1, 1\}$ and $C_{j,k} > 0$. Notice that since the set $\big(\mathbf{j}(x_k) \cap \partial\Omega\big)_{k \in \{1,\dots,N_1\}}$ are two by two disjoint (where N_1 is defined in (C.263)) and since

$$\begin{cases} \cup_{k \in \{1,\dots,N_1\}} \mathbf{j}(x_k) \cap \partial\Omega = \{z_1, ..., z_{k_1^{\partial\Omega}}\} \text{ (see (C.17) and (C.75))}, \\ \forall k \in \{N_1 + 1, ..., m_0^{\Omega}\},\ \mathbf{j}(x_k) \cap \{z_1, ..., z_{k_1^{\partial\Omega}}\} = \emptyset \text{ (see (C.76))}, \end{cases}$$

one obtains that, from (C.151), for all $j \in \{1, ..., k_1^{\partial\Omega}\}$

$$\forall k \in \{1, ..., N_1\},\quad \widetilde{C}_{j,k} \neq 0 \Rightarrow\ \widetilde{C}_{j,l} = 0\ \ \forall l \in \{1, ..., m_0^{\Omega}\} \setminus \{k\}. \tag{C.152}$$

Finally, from (C.151), one has when $h \to 0$, $\widetilde{C} = O(1)$ which means that there exist $M > 0$ and $h_0 > 0$ such that for all $h \in (0, h_0)$:

$$\sup_{(j,k) \in \{1,\dots,m_1^{\overline{\Omega}}\} \times \{1,\dots,m_0^{\Omega}\}} |\widetilde{C}_{j,k}| \leq M. \tag{C.153}$$

By definition of the matrices S, $\widetilde{S}$, D and $\widetilde{C}$ (see Definition (C.10), (C.144), (C.146), (C.150)), there exists $c > 0$ such that the matrix $\big(S - \widetilde{S}\big)D^{-1}$ satisfies in the limit $h \to 0$:

$$\big(S - \widetilde{S}\big)D^{-1} = O(e^{-\frac{c}{h}}). \tag{C.154}$$

The following Lemma will be needed in the sequel.

Lemma C.24. *Let us assume that the assumptions* ***[H-Morse]*** *and* ***[H-Boundary]*** *hold. Let $\widetilde{C}$ be the matrix defined in* (C.150)*. Then, $\widetilde{C}$ is injective and there exist $c > 0$ and $h_0 > 0$ such that for all $h \in (0, h_0)$:*

$$\forall x \in \mathbb{R}^{m_0^{\Omega}},\ \big\|\widetilde{C}x\big\|_2 \geq c\big\|x\big\|_2, \tag{C.155}$$

where $\|.\|_2$ denotes the usual Euclidean norm on $\mathbb{R}^K$, $K \in \mathbb{N}^*$.

Proof. According to (C.150), (C.146) and (C.144), $\widetilde{C}$ has the form, up to reordering the z_i for $i \in \{1, \dots, m_1^{\overline{\Omega}}\}$:

$$\widetilde{C} = \begin{pmatrix} 0 & 0 \\ [\widetilde{C}]_a & 0 \\ [\widetilde{C}]_b & 0 \\ 0 & \widetilde{[\widetilde{C}]_c} \end{pmatrix},$$

where:

- the matrix $(0,0)$ corresponds to the rows of $\widetilde{C}$ associated with $j \in \{1, ..., m_1^{\overline{\Omega}}\}$ such that $z_j \notin \cup_{k=1}^{m_0^{\Omega}} \mathbf{j}(x_k)$.

- $[\widetilde{C}]_a$ is a matrix of size $k_1^{\partial\Omega} \times N_1$ (where N_1 is defined in (C.263) and $k_1^{\partial\Omega}$ is defined in (C.17)). The coefficients $([\widetilde{C}]_a)_{j,k} = \widetilde{C}_{j,k}$ are associated with 0-forms $\widetilde{u}_k$, for $k \in \{1, \dots, N_1\}$ (see Definition C.9 and (C.80)) and with 1-forms $\widetilde{\psi}_j$ for $j \in \{1, ..., k_1^{\partial\Omega}\}$ (or equivalently j such that $z_j \in \cup_{k=1}^{N_1} \mathbf{j}(x_k) \cap \partial\Omega$ since $\cup_{k=1}^{N_1} \mathbf{j}(x_k) \cap \partial\Omega = \{z_1, ..., z_{k_1^{\partial\Omega}}\}$, see (C.75)).

- $[\widetilde{C}]_b$ is a matrix of size $\mathrm{Card}\big(\cup_{k=1}^{N_1} \mathbf{j}(x_k) \cap \Omega\big) \times N_1$. The coefficients $\widetilde{B}_{j,k} = \widetilde{C}_{j,k}$ are associated with 0-forms $\widetilde{u}_k$, for $k \in \{1, \dots, N_1\}$ (see Definition C.9 and (C.80)) and with 1-forms $\widetilde{\psi}_j$ for $j \in \{1, ..., m_0^{\overline{\Omega}}\}$ such that $z_j \in \cup_{k=1}^{N_1} \mathbf{j}(x_k) \cap \Omega$.

- $[\widetilde{C}]_c$ is a matrix of size $\mathrm{Card}\big(\cup_{k=N_1+1}^{m_0^{\Omega}} \mathbf{j}(x_k)\big) \times (m_0^{\Omega} - N_1)$ which has the following block diagonal form:

$$[\widetilde{C}]_c = \begin{pmatrix} [\widetilde{C}]_{c,1} & 0 & \dots & 0 \\ 0 & [\widetilde{C}]_{c,2} & \dots & 0 \\ \vdots & \vdots & \ddots & \vdots \\ 0 & 0 & \dots & [\widetilde{C}]_{c,N_1} \end{pmatrix},$$

  where for $l \in \big\{1, ..., N_1\big\}$, $[\widetilde{C}]_{c,l}$ is a matrix of size

$$\mathrm{Card}\left(\bigcup_{k,\, \mathbf{j}(x_k) \subset C_l} \mathbf{j}(x_k) \right) \times \Big(\mathrm{Card}\big(\arg\min_{\overline{C_\ell}} f \big) \ - 1 \Big),,$$

  with the convention that $[\widetilde{C}]_{c,l}$ does not exist if $\arg\min_{\overline{C_l}} f = \{x_l\}$. Let us recall that for $l \in \big\{1, ..., N_1\big\}$, C_l is introduced in Definition C.2. For all $l \in \{1, ..., N_1\}$, $[\widetilde{C}]_{c,l}$ contains the non zero terms of $\widetilde{C}$ associated with 0-forms $\widetilde{u}_k$ and 1-forms $\widetilde{\psi}_j$ with:

  1. $\widetilde{u}_k$ such that $\mathrm{supp}(\widetilde{u}_k) \subset \{\widetilde{\chi}_l = 1\}$ (according to (C.88))
  2. for those $\widetilde{u}_k$, j is such that $z_j \in \mathbf{j}(x_k) \subset C_l$.

  This explains in particular the block structure of $[\widetilde{C}]_c$ since by construction $\widetilde{S}_{j,k} = 0$ if $z_j \notin \mathbf{j}(x_k)$ (see (C.150) and (C.144)).

Using (C.152), for all $j \in \{1, ..., k_1^{\partial\Omega}\}$, the j-th line of $[\widetilde{C}]_a$ contains only one non zero term which is $([\widetilde{C}]_a)_{j,k}$ where $k \in \{1, ..., N_1\}$ is the unique integer such that $j \in \mathbf{j}(x_k) \cap \partial\Omega$. Moreover, in the limit $h \to 0$, it holds for all $k \in \{1, ..., N_1\}$ and $j \in \{1, ..., k_1^{\partial\Omega}\}$ such that $j \in \mathbf{j}(x_k) \cap \partial\Omega$ (see (C.151), (C.147) and (C.143)),

$$([\widetilde{C}]_a)_{j,k} = \widetilde{C}_{j,k} = \varepsilon_{j,k} C_{j,k}(1 + O(h)),$$

where $\varepsilon_{j,k} \in \{-1, 1\}$ and $C_{j,k} > 0$. Thus, one obtains that there exist $c > 0$ and $h_0 > 0$ such that for all $h \in (0, h_0)$ and for all $y \in \mathbb{R}^{N_1}$

$$\big\|[\widetilde{C}]_a y\big\|_2 \geq c\big\|y\big\|_2. \tag{C.156}$$

Moreover, from [17, Sections 7.1 and 7.2], for all $\ell \in \big\{1, ..., N_1\big\}$ there exist $c_\ell > 0$ and $h_0 > 0$ such that for all $h \in (0, h_0)$ and for all $z \in \mathbb{R}^{\mathrm{Card}\left(\arg\min_{\overline{C_\ell}} f\right) -1}$,

$$\big\|[\widetilde{C}]_{c,\ell} z\big\|_2 \geq c_\ell \|z\|_2. \tag{C.157}$$

Therefore, the inequality (C.155) follows from (C.156), (C.157) together with the fact that for any $x = {}^t(y, z) \in \mathbb{R}^{m_0^\Omega}$ ($y \in \mathbb{R}^{N_1}$ and $z \in \mathbb{R}^{m_0^\Omega - N_1}$), it holds $\big\|\widetilde{C}x\big\|_2^2 \geq \big\|[\widetilde{C}]_a y\big\|_2^2 + \big\|[\widetilde{C}]_c z\big\|_2^2$. This concludes the proof of Lemma C.24. ∎

As a consequence of (C.155), the rectangular matrix $\widetilde{C}$ admits an a left inverse $\widetilde{C}^{-1}$ which satisfies

$$\sup_{(j,k) \in \{1,...,m_1^{\overline{\Omega}}\} \times \{1,...,m_0^\Omega\}} |(\widetilde{C}^{-1})_{j,k}| \leq M. \tag{C.158}$$

for some $M > 0$ independent of h. This implies that, using (C.154) and (C.150):

$$S = \big(I + R\big)\, \widetilde{S} \quad \text{where} \quad R = O(e^{-\frac{c}{h}}). \tag{C.159}$$

We are now in position to prove the following theorem on the smallest eigenvalues of $-L_{f,h}^{D,(0)}$ and which implies Theorem C.1.

Theorem C.4. *Let us assume that the hypotheses **[H-Morse]** and **[H-Boundary]** hold. Let N_0 be the integer introduced in Definition C.2. Let us reorder, for any small $h > 0$, the set $\{x_1, ..., x_{N_0}\}$, such that*

$$\sum_{j=1}^{k_1^{\partial\Omega}} \widetilde{S}_{j,1}^2 \leq \sum_{j=1}^{k_1^{\partial\Omega}} \widetilde{S}_{j,2}^2 \leq \cdots \leq \sum_{j=1}^{k_1^{\partial\Omega}} \widetilde{S}_{j,N_0}^2, \tag{C.160}$$

where the $m_1^{\overline{\Omega}} \times m_0^\Omega$ matrix $\widetilde{S} = (\widetilde{S}_{j,k})_{j,k}$ has been defined in (C.144) *and $k_1^{\partial\Omega}$ is defined in* (C.17)*. Let $\mathbf{j}$ be the map constructed in Section C.2.3.3. Let us reorder the set $\{x_{N_0+1}, ..., x_{m_0^\Omega}\}$ such that the sequence*

$$\big(\mathcal{S}_k\big)_{k \in \{1,...,m_0^\Omega\}} := \big(f(\mathbf{j}(x_k)) - f(x_k)\big)_{k \in \{1,...,m_0^\Omega\}} \tag{C.161}$$

is decreasing, with, on any $\mathcal{I} \subset \{1, \ldots, m_0^\Omega\}$ such that $\big(\mathcal{S}_k\big)_{k \in \mathcal{I}}$ is constant, the sequence $(q_k)_{k \in \mathcal{I}}$ is decreasing (where the q_k's satisfy (C.147)*). Finally let us denote by $\lambda_{k,h}$, for $k \in \mathbb{N}^*$, the k-th eigenvalue of $-L_{f,h}^{D,(0)}$ counted with multiplicity (with these notations, $\lambda_{1,h} = \lambda_h$, see* (C.5)*). Then:*

1) There exist $C > 0$ and $h_0 > 0$ such that for all $k \in \{1, \dots, m_0^\Omega\}$ and for all $h \in (0, h_0)$,

$$C^{-1}\, h^{1+2q_k}\, e^{-\frac{2}{h}\mathcal{S}_k} \leq \lambda_{k,h} \leq C\, h^{1+2q_k}\, e^{-\frac{2}{h}\mathcal{S}_k}\,.$$

In particular, using the fact that from (C.74) *and Definition C.8, $\forall k \in \{1, ..., N_0\}$ and $\forall l \in \{N_0 + 1, ..., m_0^\Omega\}$,*

$$\mathcal{S}_l = f(\mathbf{j}(x_l)) - f(x_l) < \mathcal{S}_1 = f(\mathbf{j}(x_k)) - f(x_k) = f(z_1) - f(x_{1,1}),$$

one obtains that there exists $c > 0$ such that in the limit $h \to 0$:

$$\lambda_{N_0,h} = \lambda_{N_0+1,h}\, O(e^{-\frac{c}{h}}). \tag{C.162}$$

2) It holds more precisely for all $k \in \{1, \dots, N_0\}$, in the limit $h \to 0$:

$$\lambda_{k,h} = \frac{h}{2} \sum_{j=1}^{k_1^{\partial\Omega}} \widetilde{S}_{j,k}^2\, (1 + O(\sqrt{h})) = \frac{1}{2\sqrt{h}} \left(\sum_{j : z_j \in \mathbf{j}(x_k) \cap \partial\Omega} C_{j,k}^2 \right) e^{-\frac{2}{h}(f(z_1) - f(x_1))}\, (1 + O(\sqrt{h}))$$

where the constants $C_{j,k}$ are defined by (C.129)*.*

3) Let us assume that there exists $K \in \{1, ..., N_0\}$ such that for all $k \in \{1, ..., K\}$, $\mathbf{j}(x_k) \cap \Omega = \emptyset$. Then, for all $k \in \{1, ..., K\}$, in the limit $h \to 0$:

$$\lambda_{k,h} = \frac{h}{2} \sum_{j=1}^{k_1^{\partial\Omega}} \widetilde{S}_{j,k}^2\, \big(1 + O(e^{-\frac{c}{h}})\big) = \frac{1}{2\sqrt{h}} \left(\sum_{j : z_j \in \mathbf{j}(x_k)} C_{j,k}^2 \right) e^{-\frac{2}{h}(f(z_1) - f(x_1))}\, (1 + O(h))$$

where the constants $C_{j,k}$'s are defined by (C.129) *and where the remainder term$O(h)$ admits a full asymptotic expansion in h.*

Theorem C.1 is a consequence of Theorem C.4. Indeed, when [**H-connexity**] holds, one has

$$\arg\min_{\Omega} f \subset C_1.$$

Thus, [**H-connexity**] is equivalent to $N_0 = 1$ and in that case (see (C.69))

$$\mathbf{j}(x_1) \cap \partial\Omega = \big\{ z_1, \dots, z_{k_1^{\partial C_1}} \big\}.$$

Thus, item 2 of Theorem C.4 implies the result stated in Theorem C.1 under the assumption [**H-connexity**]. Moreover, under [**H-Connexity**], $K = 1$ is equivalent to [**H-Connexity+**]. In particular, item 3 of Theorem C.4 implies the result stated in Theorem C.1 under the assumption [**H-connexity+**].

Remark C.11. *One of the interest of Theorem C.4 is to show, see indeed items 2 and 3 in Theorem C.4, that the N_0 smallest eigenvalues of $L_{f,h}^{D,(0)}$ can have exactly the same asymptotic estimate in the limit $h \to 0$ (choosing for instance f such that all the constant $C_{j,k}$'s, defined by* (C.129)*, are equal) making them hard to distinguish in the small temperature regime.*

Remark C.12. *Theorem C.1 is stated with the assumption* ***[H-connexity]*** *instead of the assumption* (C.160)*. The reason is that the assumption* (C.160) *is difficult to express simply since it requires to define the matrix* $\widetilde{S}$*, the map* $\mathbf{j}$ *and the quasi-modes of* $-L_{f,h}^{D,(0)}$*.*

Remark C.13. *Notice that if there are equalities between the first* M *terms in* (C.160)*, i.e if:*

$$\sum_{j=1}^{k_1^{\partial\Omega}} \widetilde{S}_{j,1}^2 = ... = \sum_{j=1}^{k_1^{\partial\Omega}} \widetilde{S}_{j,M}^2 < \sum_{j=1}^{k_1^{\partial\Omega}} \widetilde{S}_{j,M+1}^2 \leq ... \leq \sum_{j=1}^{k_1^{\partial\Omega}} \widetilde{S}_{j,N_0}^2$$

and if K $x_i's$ *among these* M *terms are such that* $\mathbf{j}(x_i) \cap \Omega = \emptyset$*, then, one can reorder these* M *terms such that the first ones satisfy* $\mathbf{j}(x_j) \cap \Omega = \emptyset$ *for all* $j \in \{1, ..., K\}$*. Thanks to item 3 in Theorem C.4, this thus yields a relative error term of order* $O(h)$ *(rather than* $O(\sqrt{h})$*) on the estimates of the* K *smallest eigenvalues.*

Remark C.14. *Notice that if there exists* $k \in \{1, ..., N_0 - 1\}$ *such that the* k*-th and the* $(k+1)$*-th inequalities in* (C.160) *are strict, (with the convention that the* 1*-st and the* N_0*-th inequality are always strict) then it follows from* (C.162) *and item 2 in Theorem C.4, that* $\lambda_{k+1,h}$ *is non degenerate.*

Remark C.15. *In some specific geometric cases, we are able to prove that remainder term* $O(\sqrt{h})$ *in item 2 in Theorem C.4 is exactly of the order* $\sqrt{h}$ *and admits a full asymptotic expansion in* $\sqrt{h}$*. This is the purpose of Proposition C.40 in Section C.4.*

Before starting the proof of Theorem C.4, let us give two consequences of the Fan inequalities which will be used in the proof of Theorem C.4 and which are stated in Lemmata C.26 and C.27. Let us first recall the Fan inequalities (see for instance [30, Theorem 1.6] or [21]).

Lemma C.25. *Let* $A \in M_{m,m}(\mathbb{C})$*,* $B \in M_{m,n}(\mathbb{C})$ *and* $C \in M_{n,n}(\mathbb{C})$*. Then, it holds*

$$\forall i \in \{1, ..., \max(n, m)\},\ \eta_i(A\,B\,C) \leq \big\|A\big\|\,\big\|C\big\|\,\eta_i(B),$$

where $\|T\| = \eta_1(T) \geq \cdots \geq \eta_{\max(n,m)}(T)$ *denote the singular values of the matrix* $T \in M_{m,n}(\mathbb{C})$ *and where* $\big\|T\big\| := \sqrt{\max \sigma({}^tTT)}$ *is the spectral norm of* T*.*

Let us recall that from Corollary C.22, there exists $h_0 > 0$ such that for all $h \in (0, h_0)$,

$$\operatorname{Ran} \pi_h^{(0)} = \operatorname{Span}\big(\pi_h^{(0)} \widetilde{u}_k,\ k = 1, \ldots, m_0^{\Omega}\big)$$

and

$$\operatorname{Ran} \pi_h^{(1)} = \operatorname{Span}\big(\pi_h^{(1)} \widetilde{\psi}_i,\ i = 1, \ldots, m_1^{\overline{\Omega}}\big)$$

where the projectors $\pi_h^{(0)}$ and $\pi_h^{(1)}$ are defined in (C.39). Let us define $\widetilde{\mathcal{U}} := \big(\pi_h^{(0)} \widetilde{u}_k\big)_{1 \leq k \leq m_0^{\Omega}}$ and $\widetilde{\Psi} := \big(\pi_h^{(1)} \widetilde{\psi}_j\big)_{1 \leq j \leq m_1^{\overline{\Omega}}}$. For $i \in \{0, 1\}$, let $\mathcal{B}_i$ be an orthonormal basis of $\operatorname{Ran} \pi_h^{(i)}$ and let us define the matrices

$$C_0 := \operatorname{Mat}_{\widetilde{\mathcal{U}}} \mathcal{B}_0 \ \text{ and } \ C_1 := \operatorname{Mat}_{\widetilde{\Psi}} \mathcal{B}_1. \tag{C.163}$$

Notice that from item 1 in Corollary C.22, there exist $M > 0$ and $h_0 > 0$ such that for all $h \in (0, h_0)$:

$$\sup_{(l,k)\in\{1,\dots,m_0^\Omega\}^2} |(C_0)_{l,k}| \leq M \tag{C.164}$$

and

$$\sup_{(l,k)\in\{1,\dots,m_0^\Omega\}^2} |(C_0^{-1})_{l,k}| \leq M. \tag{C.165}$$

A direct consequence of the Fan inequalities is the following.

Lemma C.26. *Let us assume that the hypotheses **[H-Morse]** and **[H-Boundary]** hold. Let us denote by $\lambda_{k,h}$, for $k \in \mathbb{N}^*$, the k-th eigenvalue of $-L_{f,h}^{D,(0)}$ counted with multiplicity and let $\tilde{S}$ be the matrix defined in* (C.144)*. Then, there exists $c > 0$ such that for all $k \in \{1, ..., m_0^\Omega\}$, one has in the limit $h \to 0$:*

$$\lambda_{k,h} = \frac{h}{2}\, \eta^2_{m_0^\Omega+1-k}\big(\widetilde{S}C_0\big)\big(1 + O(e^{-\frac{c}{h}})\big), \tag{C.166}$$

where $\|\widetilde{S}C_0\| = \eta_1(\widetilde{S}C_0) \geq \cdots \geq \eta_{m_0^\Omega}(\widetilde{S}C_0)$ denote the singular values of $\widetilde{S}C_0$.

Proof. The m_0^Ω smallest eigenvalues of $-L_{f,h}^{D,(0)}$ are the eigenvalues of

$$-L_{f,h}^{D,(0)}\big|_{\operatorname{Ran}\pi_h^{(0)}} = \frac{h}{2}\, d^*_{\frac{2f}{h},1}\big|_{\operatorname{Ran}\pi_h^{(1)}}\, d\big|_{\operatorname{Ran}\pi_h^{(0)}}.$$

Moreover, since the L^2_w-adjoint of $d\big|_{\operatorname{Ran}\pi_h^{(0)}} : \operatorname{Ran}\pi_h^{(0)} \to \operatorname{Ran}\pi_h^{(1)}$ is $d^*_{\frac{2f}{h},1}\big|_{\operatorname{Ran}\pi_h^{(1)}} : \operatorname{Ran}\pi_h^{(1)} \to \operatorname{Ran}\pi_h^{(0)}$, one has that the m_0^Ω smallest eigenvalues of $-L_{f,h}^{D,(0)}$ are given by $\frac{h}{2}$ times the squares of the singular values of $d\big|_{\operatorname{Ran}\pi_h^{(0)}} : \operatorname{Ran}\pi_h^{(0)} \to \operatorname{Ran}\pi_h^{(1)}$. Thus, the eigenvalues of $-L_{f,h}^{D,(0)}\big|_{\operatorname{Ran}\pi_h^{(0)}}$ are given by $\frac{h}{2}$ times the squares of the singular values of the matrix Q defined by

$$Q := \operatorname{Mat}_{\mathcal{B}_0,\mathcal{B}_1}\big(d\big|_{\operatorname{Ran}\pi_h^{(0)}}\big).$$

In addition, by definition of the matrices C_0 and C_1 (see (C.163)), one has

$$Q = {}^tC_1\, S\, C_0.$$

By (C.159), it holds

$$Q = {}^tC_1\, \big(I + R\big)\, \widetilde{S}\, C_0.$$

Furthermore, from (C.159), there exists $c > 0$ such that one has in the limit $h \to 0$

$$\|1 + R\| = 1 + O(e^{-\frac{c}{h}}),\ \|(1 + R)^{-1}\| = 1 + O(e^{-\frac{c}{h}}),$$

and from item 3 in Proposition C.21,

$$\|\,{}^tC_1\| = 1 + O(e^{-\frac{c}{h}}),\ \|({}^tC_1)^{-1}\| = 1 + O(e^{-\frac{c}{h}}),$$

where we recall $\big\|T\big\| := \sqrt{\max\sigma({}^tTT)}$ is the spectral norm of a matrix T. Therefore, it follows from the Fan inequalities (see Lemma C.25) that the singular values of Q are, up to multiplication by $1 + O(e^{-\frac{c}{h}})$, the singular values of $\widetilde{S}\, C_0$. This concludes the proof of Lemma C.26. ∎

Notice that in general, the spectral norm of the matrix C_0 defined in (C.163) does not equal $1 + O(e^{-\frac{c}{h}})$ when $h \to 0$.

Remark C.16. *For instance, in the case when f is a one dimensional symmetric double-well potential with the saddle point lower than $\min_{\partial\Omega} f$, it can be checked that the Gramian matrix of the functions $\widetilde{u}_1$ and $\widetilde{u}_2$ introduced in Definition C.9 converges when $h \to 0$ towards the matrix*

$$\begin{pmatrix} 1 & c_1 \\ c_1 & 1 \end{pmatrix},$$

where $0 < c_1 < 1$.

Actually, it is possible to replace in the Fan inequalities (C.166) the matrix C_0 by another matrix which has a simpler form than C_0. This is the purpose of Lemma C.27 which will be used to prove items 2 and 3 in Theorem C.4. Before stating Lemma C.27, let us choose a particular orthonormal basis $\mathcal{B}_0$ of $\operatorname{Ran} \pi_h^{(0)}$ to define C_0 in (C.163). Let $(e_1, \dots, e_{N_1})$ be the resulting functions of a Gram-Schmidt orthonormalization of the family $(\pi_h^{(0)} \widetilde{u}_1, \dots, \pi_h^{(0)} \widetilde{u}_{N_1})$. According to item 3 in Proposition C.21, there exists $c > 0$ such that $\forall (k,l) \in \{1, \dots, N_1\}^2$, it holds in the limit $h \to 0$:

$$e_k = \big(1 + O(e^{-\frac{c}{h}})\big)\, \pi_h^{(0)} \widetilde{u}_k + \sum_{q=1}^{k-1} O(e^{-\frac{c}{h}})\, \pi_h^{(0)} \widetilde{u}_q \quad \text{and} \quad \langle e_k, e_l \rangle_{L^2_w} = \delta_{k,l}.$$

Then, let us choose $\{e_{N_1+1}, \dots, e_{m_0^\Omega}\}$ such that

$$\mathcal{B}_0 := \{e_1, e_2, \dots, e_{m_0^\Omega}\} \tag{C.167}$$

is an orthonormal basis of $\operatorname{Ran} \pi_h^{(0)}$. In that case, the matrix C_0 defined in (C.163), satisfies in the limit $h \to 0$:

$$\forall (k,l) \in \{1, \dots, m_0^\Omega\} \times \{1, \dots, N_1\}, \quad (C_0)_{k,l} = \begin{cases} \delta_{k,l} + O(e^{-\frac{c}{h}}) & \text{if } k \le l \\ 0 & \text{if } k > l \end{cases}. \tag{C.168}$$

Let us now define the $m_0^\Omega \times m_0^\Omega$ matrix $\widetilde{C}_0$ by:

$$\forall (k,l) \in \{1, \dots, m_0^\Omega\} \times \{1, \dots, N_1\}, \quad (\widetilde{C}_0)_{k,l} := \begin{cases} \delta_{k,l} & \text{if } k \le l \\ 0 & \text{if } k > l \end{cases}, \tag{C.169}$$

and

$$\forall (k,l) \in \{1, \dots, m_0^\Omega\} \times \{N_1 + 1, ..., m_0^\Omega\}, \quad (\widetilde{C}_0)_{k,l} := (C_0)_{k,l}. \tag{C.170}$$

Lemma C.27. *Let us assume that the hypotheses **[H-Morse]** and **[H-Boundary]** hold. Let us denote by $\lambda_{k,h}$, for $k \in \mathbb{N}^*$, the k-th eigenvalue of $-L_{f,h}^{D,(0)}$ counted with multiplicity and let $\tilde{S}$ be the matrix defined in* (C.144)*. Then, there exists $c > 0$ such that in the limit $h \to 0$:*

$$\lambda_{k,h} = \frac{h}{2}\, \eta^2_{m_0^\Omega + 1 - k}\big(\widetilde{S}\, \widetilde{C}_0\big)\big(1 + O(e^{-\frac{c}{h}})\big),$$

where $\|\widetilde{S}\widetilde{C}_0\| = \eta_1(\widetilde{S}C_0) \ge \cdots \ge \eta_{m_0^\Omega}(\widetilde{S}\widetilde{C}_0)$ denote the singular values of $\widetilde{S}\widetilde{C}_0$.

Proof. Let us prove that there exists $c > 0$ such that in the limit $h \to 0$,

$$\|(\widetilde{C}_0)^{-1} C_0\| = 1 + O(e^{-\frac{c}{h}}) \text{ and } \|C_0^{-1}\widetilde{C}_0\| = 1 + O(e^{-\frac{c}{h}}), \tag{C.171}$$

From (C.168), the $m_0^\Omega \times m_0^\Omega$ matrix C_0 has the form

$$C_0 = \begin{pmatrix} [C_0]_1 & [C_0]_4 \\ 0 & [C_0]_2 \end{pmatrix},$$

where $[C_0]_1$ is matrix of size $N_1 \times N_1$ which satisfies, according to (C.168), $[C_0]_1 = \mathrm{Id}_{N_1} + O(e^{-\frac{c}{h}})$ for some $c > 0$. Moreover, according to (C.169) and (C.170), the $m_0^\Omega \times m_0^\Omega$ matrix $\widetilde{C}_0$ has the form

$$\widetilde{C}_0 = \begin{pmatrix} \mathrm{Id}_{N_1} & [C_0]_4 \\ 0 & [C_0]_2 \end{pmatrix}.$$

Let us recall that by definition of C_0 (see (C.163)) and from item 1 in Corollary C.22, C_0 is invertible and thus $[C_0]_1$ and $[C_0]_2$ are invertible. Therefore, one has

$$\widetilde{C}_0^{-1} = \begin{pmatrix} \mathrm{Id}_{N_1} & -[C_0]_4\,[C_0]_2^{-1} \\ 0 & [C_0]_2^{-1} \end{pmatrix}$$

and thus,

$$\widetilde{C}_0^{-1} C_0 = \begin{pmatrix} [C_0]_1 & 0 \\ 0 & I_{m_0^\Omega - N_1} \end{pmatrix}.$$

This proves (C.171) since $[C_0]_1 = \mathrm{Id}_{N_1} + O(e^{-\frac{c}{h}})$ and $[C_0]_1^{-1} = \mathrm{Id}_{N_1} + O(e^{-\frac{c}{h}})$. Lemma C.27 is a consequence (C.171) together with Lemma C.26 and Lemma C.25. ∎

We are now in position to prove Theorem C.4.

Proof. The proof is divided into two steps: we first prove item 1 in Theorem C.4 and then we prove items 2 and 3 in Theorem C.4.

<u>Proof of item 1 in Theorem C.4.</u>

Item 1 in Theorem C.4, is equivalent, according Lemma C.26, to the existence of $C > 0$ and $h_0 > 0$ such that for all $k \in \{1, \dots, m_0^\Omega\}$ and for all $h \in (0, h_0)$

$$C^{-1} h^{q_k} e^{-\frac{s_k}{h}} \le \eta_{m_0^\Omega + 1 - k}(\widetilde{S} C_0) \le C h^{q_k} e^{-\frac{s_k}{h}}. \tag{C.172}$$

Let us prove (C.172). According to (C.146) and to the ordering of $k \in \{1, \dots, m_0^\Omega\}$ introduced in the statement of Theorem C.4, the singular values of D satisfy for h small enough (see (C.146) and (C.161)):

$$\forall k \in \{1, \dots, m_0^\Omega\},\ \eta_{m_0^\Omega + 1 - k}(D) = D_{k,k} = h^{q_k} e^{-\frac{s_k}{h}}, \tag{C.173}$$

Using the fact that $\widetilde{S} C_0 = \widetilde{C} D C_0$ (see (C.150)) together with (C.153), (C.164) and Lemma C.25, one obtains that for all $k \in \{1, \dots, m_0^\Omega\}$

$$\eta_{m_0^\Omega + 1 - k}(\widetilde{S} C_0) \le \|\widetilde{C}\|\,\|C_0\|\,\eta_{m_0^\Omega + 1 - k}(D) = O\big(D_{k,k}\big), \tag{C.174}$$

which provide the required upper bound in (C.172). To obtain a lower bound on the singular values of $\widetilde{S}C_0$, we write

$$D = \widetilde{C}^{-1}\,\widetilde{S}\,C_0\,C_0^{-1}.$$

Using (C.158), (C.165) and Lemma C.25, one has for all $k \in \{1, \dots, m_0^\Omega\}$

$$\eta_{m_0^\Omega+1-k}(D) \leq \big\|\widetilde{C}^{-1}\big\|\,\big\|C_0^{-1}\big\|\,\eta_{m_0^\Omega+1-k}(\widetilde{S}\,C_0) = O\big(\eta_{m_0^\Omega+1-k}\big). \tag{C.175}$$

Then, (C.172) follows from (C.173), (C.175) and (C.174). This concludes the proof of item 1 in Theorem C.4.

<u>Proofs of items 2 and 3 in Theorem C.4.</u>

The proofs of items 2 and 3 in Theorem C.4 is divided into two steps. First, one proves, for $k = 1$, item 2 and item 3. Then, one proves, for $k \in \{2, ..., N_0\}$, item 2 and item 3.

<u>Proofs for $k = 1$ of item 2 and item 3 in Theorem C.4.</u>

Our proof is partly inspired by the analysis led in [17, Section 7.4]. According to Lemma C.27, there exists $c > 0$ such that in the limit $h \to 0$:

$$\lambda_{1,h} = \frac{h}{2}\eta^2_{m_0^\Omega}(\widetilde{S}\widetilde{C}_0)\big(1 + O(e^{-\frac{c}{h}})\big), \tag{C.176}$$

where $\widetilde{C}_0$ is defined in (C.169) and (C.170). Therefore, the analysis of the estimate of λ_h is then reduced to precisely computing $\eta_{m_0^\Omega}(\widetilde{S}\widetilde{C}_0)$. One has:

$$\eta_{m_0^\Omega}(\widetilde{S}\widetilde{C}_0) = \min_{y \in \mathbb{R}^{m_0^\Omega}\,;\,\|y\|_2=1} \big\|\widetilde{S}\,C_0\,y\big\|_2. \tag{C.177}$$

Let us first obtain an upper bound on $\eta_{m_0^\Omega}(\widetilde{S}\widetilde{C}_0)$. Let us denote by $y_0 =^t (1, 0, \dots, 0)$. Then, it holds from (C.177),

$$\eta^2_{m_0^\Omega} \leq \big\|\widetilde{S}\,C_0\,y_0\big\|_2^2.$$

Using in addition the fact from (C.169), one has $\widetilde{C}_0 y_0 = y_0$, one obtains

$$\eta^2_{m_0^\Omega} \leq \big\|\widetilde{S}y_0\big\|_2^2 = \sum_{j=1}^{m_1^{\overline{\Omega}}} \widetilde{S}^2_{j,1}. \tag{C.178}$$

This provides the required upper bound. Notice that (C.178) and (C.145) imply that in the limit $h \to 0$

$$\eta_{m_0^\Omega}(\widetilde{S}\widetilde{C}_0) = O\big(h^{-\frac{3}{4}}e^{-\frac{1}{h}(f(z_1)-f(x_1))}\big). \tag{C.179}$$

Let us now give a lower bound on $\eta^2_{m_0^\Omega}$. To this end let us consider $y^* \in \mathbb{R}^{m_0^\Omega}$ with $\|y^*\|_2 = 1$, realizing the minimum in (C.177). Let us write $y^* =^t (y^*_\alpha, y^*_\beta)$, where $y^*_\alpha \in \mathbb{R}^{N_0}$ and $y^*_\beta \in \mathbb{R}^{m_0^\Omega - N_0}$. We claim that there exists $\mu > 0$ such that for h small enough,

$$\|y^*_\beta\|_2 = O(e^{-\frac{\mu}{h}}). \tag{C.180}$$

Let us prove (C.180). By definition of y^* and according to (C.150), one has

$$\eta_{m_0^\Omega} = \big\|\widetilde{S}\widetilde{C}_0 y^*\big\|_2 = \big\|\widetilde{C}D\widetilde{C}_0 y^*\big\|_2.$$

To prove (C.180), we use the block structure of the matrices $\widetilde{C}$, $\widetilde{C}_0$ and D. Let us define

$$n_1 = \mathrm{Card}\big(\cup_{k=1}^{N_0} \mathbf{j}(x_k) \cap \partial\Omega\big). \tag{C.181}$$

According to (C.150), (C.146) and (C.144), the $m_1^{\overline{\Omega}} \times m_0^\Omega$ matrix $\widetilde{C}$ has the form, up to reordering the z_i, $i \in \{1, \dots, m_1^{\overline{\Omega}}\}$,

$$\widetilde{C} = \begin{pmatrix} [\widetilde{C}]_1 & 0 \\ [\widetilde{C}]_3 & [\widetilde{C}]_2 \end{pmatrix}, \tag{C.182}$$

where:

- $[\widetilde{C}]_1$ is a matrix of size $n_1 \times N_0$ (where N_0 is introduced in Definition C.2 and n_1 is defined in (C.181)). The coefficients $([\widetilde{C}]_1)_{j,k} = \widetilde{C}_{j,k}$ are associated with 0-forms $\widetilde{u}_k$, for $k \in \{1, \dots, N_0\}$ (see Definition C.9 and (C.80)) and with 1-forms $\widetilde{\psi}_j$ for $j \in \{1, ..., m_1^{\overline{\Omega}}\}$ such that $z_j \in \mathbf{j}(x_k) \cap \partial\Omega$.
- $[\widetilde{C}]_3$ is a matrix of size $\big(m_1^{\overline{\Omega}} - n_1\big) \times N_0$. The coefficients $([\widetilde{C}]_3)_{j,k} = \widetilde{C}_{j,k}$ are associated with 0-forms $\widetilde{u}_k$, for $k \in \{1, \dots, N_0\}$ and with 1-forms $\widetilde{\psi}_j$ for $j \in \{1, ..., m_1^{\overline{\Omega}}\}$ such that $z_j \notin \cup_{k=1}^{N_0} \mathbf{j}(x_k) \cap \partial\Omega$.
- $[\widetilde{C}]_2$ is a matrix of size $\big(m_1^{\overline{\Omega}} - n_1\big) \times \big(m_0^\Omega - N_0\big)$. The coefficients $([\widetilde{C}]_2)_{j,k} = \widetilde{C}_{j,k}$ are associated with 0-forms $\widetilde{u}_k$, for $k \in \{N_0 + 1, ..., m_0^\Omega\}$ and with 1-forms $\widetilde{\psi}_j$ for $j \in \{1, ..., m_1^{\overline{\Omega}}\}$ such that $z_j \notin \cup_{k=1}^{N_0} \mathbf{j}(x_k) \cap \partial\Omega$.

From (C.152) the columns of $[\widetilde{C}]_1$ are two by two orthogonal,

$$\forall k \in \{1, \dots, k_1^{\partial\Omega}\},\ \forall j \neq j' \in \{1, \dots, N_0\},\ \widetilde{C}_{k,j} \neq 0 \ \Rightarrow\ \widetilde{C}_{k,j'} = 0. \tag{C.183}$$

Moreover, (C.155) and (C.182) imply that $[\widetilde{C}]_2$ is injective and satisfies, for some constant $c > 0$ and for all $h > 0$ small enough,

$$\forall x \in \mathbb{R}^{m_0^\Omega - N_0},\quad \big\|[\widetilde{C}]_2 x\big\|_2 \geq c\big\|x\big\|_2. \tag{C.184}$$

Let us now decompose the square matrices D and $\widetilde{C}_0$ in blocks which are compatible with the decomposition of $\widetilde{C}$ made in (C.182). According to (C.146), (C.169) and (C.170) together with the fact that $N_0 \leq N_1$ (see Definition C.2), one has

$$\widetilde{D} = \begin{pmatrix} [\widetilde{D}]_\alpha & 0 \\ 0 & [\widetilde{D}]_\beta \end{pmatrix} \ \text{ and } \widetilde{C}_0 = \begin{pmatrix} \mathrm{Id}_{N_0} & [\widetilde{C}_0]_\gamma \\ 0 & [\widetilde{C}_0]_\beta \end{pmatrix}, \tag{C.185}$$

where for a square matrix U of size m_0^Ω:

$$[U]_\alpha = (U_{i,j})_{1 \leq i,j \leq N_0},\ [U]_\beta = (U_{i,j})_{N_0+1 \leq i,j \leq m_0^\Omega},\ \text{and } [U]_\gamma = (U_{i,j})_{1 \leq i \leq N_0, N_0+1 \leq j \leq m_0^\Omega}.$$

Notice that from (C.148), it holds

$$[D]_\alpha = h^{-\frac{3}{4}} e^{-\frac{1}{h}(f(z_1)-f(x_1))} I_{N_0}, \tag{C.186}$$

and from (C.165), there exists $M > 0$ such that when $h > 0$

$$\|[\widetilde{C}_0]_\beta^{-1}\| \leq M \tag{C.187}$$

We are now in position to prove (C.180). Le us recall that by definition of y^* , one has

$$\eta_{m_0^\Omega} = \big\|\widetilde{S}\,\widetilde{C}_0\,{}^t(y^*_\alpha, y^*_\beta)\big\|_2 \geq \big\|\widetilde{S}\,\widetilde{C}_0\,{}^t(0, y^*_\beta)\big\|_2 - \big\|\widetilde{S}\,\widetilde{C}_0\,{}^t(y^*_\alpha, 0)\big\|_2.$$

Therefore, since $\widetilde{C}_0\,{}^t(y^*_\alpha, 0) = {}^t(y^*_\alpha, 0)$ (see (C.169)) and $\widetilde{S} = \widetilde{C}D$ (see (C.150)), one has using (C.182) and (C.186) together with the fact that $\big\|y^*_\alpha\big\|_2 \leq 1$ and $[\widetilde{C}]_1 = O(1)$ (see (C.182) and (C.153)),

$$\|\widetilde{S}\,\widetilde{C}_0\,{}^t(0, y^*_\beta)\|_2 \leq \eta_{m_0^\Omega} + \big\|\widetilde{C}D\,{}^t(y^*_\alpha, 0)\big\|_2 \leq \eta_{m_0^\Omega} + \big\|[\widetilde{C}]_1[D]_\alpha y^*_\alpha\big\|_2 = O\big(h^{-\frac{3}{4}} e^{-\frac{1}{h}(f(z_1)-f(x_1))}\big). \tag{C.188}$$

Moreover, using (C.186) and since $[\widetilde{C}]_3 = O(1)$ (see (C.182) and (C.153)) and $[\widetilde{C}_0]_\gamma = O(1)$ (since $\widetilde{C}_0 = C_0 + O(e^{-\frac{c}{h}})$ and $C_0 = O(1)$ see (C.169), (C.170) and (C.164)), one has

$$\begin{aligned}
\big\|\widetilde{S}\,C_0\,{}^t(0, y^*_\beta)\big\|_2 &= \Big(\big\|[\widetilde{C}]_1\,[D]_\alpha\,[\widetilde{C}_0]_\gamma\,y^*_\beta\big\|_2^2 + \big\|[\widetilde{C}]_3\,[D]_\alpha\,[\widetilde{C}_0]_\gamma\,y^*_\beta + [\widetilde{C}]_2\,[D]_\beta\,[\widetilde{C}_0]_\beta\,y^*_\beta\big\|_2^2\Big)^{\frac{1}{2}} \\
&\geq \big\|[\widetilde{C}]_2\,[D]_\beta\,[\widetilde{C}_0]_\beta\,y^*_\beta\big\|_2 - \big\|[\widetilde{C}]_3\,[D]_\alpha\,[\widetilde{C}_0]_\gamma\,y^*_\beta\big\|_2 \\
&= \big\|[\widetilde{C}]_2\,[D]_\beta\,[\widetilde{C}_0]_\beta\,y^*_\beta\big\|_2 + O\big(h^{-\frac{3}{4}} e^{-\frac{1}{h}(f(z_1)-f(x_1))}\big).
\end{aligned}$$

Therefore, one deduces from the latter inequality and from (C.188) and (C.184) that

$$\big\|[D]_\beta\,[\widetilde{C}_0]_\beta\,y^*_\beta\big\|_2 = O\Big(\|[\widetilde{C}]_2[D]_\beta\,[C_0]_\beta\,y^*_\beta\|_2\Big) = O\big(h^{-\frac{3}{4}} e^{-\frac{1}{h}(f(z_1)-f(x_1))}\big), \tag{C.189}$$

In addition, since $[\widetilde{C}_0]_\beta^{-1} = O(1)$ (which follows from $\widetilde{C}_0 = C_0 + O(e^{-\frac{c}{h}})$, see indeed (C.169), (C.170), (C.165) and (C.185)) and since there exists $c > 0$ such that it holds:

$$[D]_\beta^{-1} = O\big(e^{\frac{1}{h}(f(z_1)-f(x_1)-c)}\big),$$

which follows from (C.146) and (C.149), one obtains from (C.189) that there exists $\mu > 0$ such that for h small enough,

$$\|y^*_\beta\|_2 = O(e^{-\frac{\mu}{h}}).$$

This ends the proof of (C.180). We are now in position to give a lower bound on $\eta_{m_0^\Omega}(\widetilde{S}\widetilde{C}_0)$. Notice that from (C.180) together with the fact that $\|y^*\|_2 = 1$, one has

$$\|y^*_\alpha\|_2 = 1 + O(e^{-\frac{\mu}{h}}). \tag{C.190}$$

Using (C.182), (C.185), and since $\widetilde{C}_0 = O(1)$, there exists $c > 0$ such that

$$\eta^2_{m_0^\Omega}(\widetilde{S}\widetilde{C}_0) \geq \sum_{j=1}^{n_1} (\widetilde{C}\,D\,\widetilde{C}_0\,y^*)_j^2 = \sum_{j=1}^{n_1} \left(\sum_{k=1}^{N_0} \widetilde{C}_{j,k} D_{k,k} \left(y^*_k + \sum_{\ell=N_0+1}^{m_0^\Omega} (C_0)_{k,\ell}\,y^*_\ell\right)\right)^2,$$

where we recall n_1 is defined in (C.181). Using in addition (C.180) and (C.183), there exists $c > 0$ such that in the limit $h \to 0$:

$$\eta^2_{m_0^\Omega}(\widetilde{S}\widetilde{C}_0) \geq \sum_{j=1}^{n_1}\sum_{k=1}^{N_0} \widetilde{C}^2_{j,k} D^2_{k,k}\big(y^*_k + O(e^{-\frac{c}{h}})\big)^2.$$

Since for all $k \in \{1, ..., N_0\}$, $\widetilde{C}_{j,k} = 0$ for all $j \in \{1, ..., k_1^{\partial\Omega}\} \setminus \mathbf{j}(x_k) \cap \partial\Omega$, it holds by definition of n_1 (see (C.181)):

$$\sum_{j=1}^{n_1}\sum_{k=1}^{N_0} \widetilde{C}^2_{j,k} D^2_{k,k}\big(y^*_k+O(e^{-\frac{c}{h}})\big)^2 = \sum_{j=1}^{k_1^{\partial\Omega}}\sum_{k=1}^{N_0} \widetilde{C}^2_{j,k} D^2_{k,k}\big(y^*_k+O(e^{-\frac{c}{h}})\big)^2 \geq \sum_{j=1}^{k_1^{\partial\Omega}} \widetilde{S}^2_{j,1}\big(1+O(e^{-\frac{c}{h}})\big),$$

where the inequality follows from (C.150), (C.160) and (C.190). Thus, one obtains the following lower bound:

$$\eta^2_{m_0^\Omega}(\widetilde{S}\widetilde{C}_0) \geq \sum_{j=1}^{k_1^{\partial\Omega}} \widetilde{S}^2_{j,1}\big(1 + O(e^{-\frac{c}{h}})\big). \tag{C.191}$$

In conclusion, from (C.178) and (C.191), one has for some $c > 0$, in the limit $h \to 0$:

$$\sum_{j=1}^{k_1^{\partial\Omega}} \widetilde{S}^2_{j,1}\left(1 + O(e^{-\frac{c}{h}})\right) \leq \eta^2_{m_0^\Omega}(\widetilde{S}\widetilde{C}_0) \leq \sum_{j=1}^{m_1^{\overline{\Omega}}} \widetilde{S}^2_{j,1}. \tag{C.192}$$

Using (C.145), one gets

$$\sum_{j=1}^{m_1^{\overline{\Omega}}} \widetilde{S}^2_{j,1} = \begin{cases} \sum_{j=1}^{k_1^{\partial\Omega}} \widetilde{S}^2_{j,1} & \text{if } \mathbf{j}(x_1) \cap \Omega = \emptyset \\ \sum_{j=1}^{k_1^{\partial\Omega}} \widetilde{S}^2_{j,1}\big(1 + O(\sqrt{h})\big) & \text{if } \mathbf{j}(x_1) \cap \Omega \neq \emptyset \end{cases},$$

and thus, from (C.192), it holds int the limit $h \to 0$:

$$\eta^2_{m_0^\Omega}(\widetilde{S}\,\widetilde{C}_0) = \begin{cases} \sum_{j=1}^{k_1^{\partial\Omega}} \widetilde{S}^2_{j,1}\big(1 + O(e^{-\frac{c}{h}})\big) & \text{if } \mathbf{j}(x_1) \cap \Omega = \emptyset \\ \sum_{j=1}^{k_1^{\partial\Omega}} \widetilde{S}^2_{j,1}\big(1 + O(\sqrt{h})\big) & \text{if } \mathbf{j}(x_1) \cap \Omega \neq \emptyset \end{cases}.$$

This last estimate together with (C.176) and (C.145) imply, when $k = 1$, item 2 and item 3 (since $K \geq 1$ if and only if $\mathbf{j}(x_1) \cap \Omega = \emptyset$).

<u>Proofs, for $k \in \{2, ..., N_0\}$, of item 2 and item 3 in Theorem C.4.</u>

The estimates stated in item 2 and item 3 in Theorem C.4 for $k \in \{2, ..., N_0\}$ are obtained with a similar analysis than the one made above for $k = 1$ together with the Max-Min principle. From Lemma C.27, for all $k \in \{2, ..., N_0\}$, there exists $c > 0$ such that in the limit $h \to 0$:

$$\lambda_{k,h} = \frac{h}{2}\eta^2_{m_0^\Omega+1-k}(\widetilde{S}\widetilde{C}_0)\big(1 + O(e^{-\frac{c}{h}})\big), \tag{C.193}$$

where $\widetilde{C}_0$ is defined in (C.169) and (C.170). Let us prove item 2 and item 3 for $k=2$ (the estimates of $\lambda_{k,h}$ for $k\geq 3$ are obtained similarly). By the Max-Min principle,

$$\eta_{m_0^\Omega-1}(\widetilde{S}\,\widetilde{C}_0) = \max_{Y\in\mathbb{R}^{m_0^\Omega}}\ \min_{y\perp Y\,;\,\|y\|_2=1} \big\|\widetilde{S}\,\widetilde{C}_0\,y\big\|_2 \tag{C.194}$$

$$= \min_{E\subset\mathbb{R}^{m_0^\Omega},\,\dim E=2}\ \max_{y\in E\,;\,\|y\|_2=1} \big\|\widetilde{S}\,\widetilde{C}_0\,y\big\|_2. \tag{C.195}$$

From (C.145), (C.152) together with the fact that $\widetilde{S}=\widetilde{C}D$ (see (C.150))), one has in the limit $h\to 0$

$$\frac{\big\langle \widetilde{S}^{\,t}(1,0,\dots,0),\widetilde{S}^{\,t}(0,1,\dots,0)\big\rangle_2}{\big\|\widetilde{S}^{\,t}(1,0,\dots,0)\big\|_2\big\|\widetilde{S}^{\,t}(0,1,\dots,0)\big\|_2} = \begin{cases} 0 & \text{if } \mathbf{j}(x_1)\cap\mathbf{j}(x_2)=\emptyset \\ O(\sqrt{h}) & \text{if } \mathbf{j}(x_1)\cap\mathbf{j}(x_2)\neq\emptyset \end{cases}. \tag{C.196}$$

Moreover, for all $y={}^t(y_1,y_2,0,\dots,0)\}$, since $\widetilde{C}_0\,y=y$ (see (C.169)), one has:

$$\big\|\widetilde{S}\,\widetilde{C}_0\,y\big\|_2^2 = \big\|\widetilde{S}\,y\big\|_2^2 = y_1^2\sum_{j=1}^{m_1^{\overline{\Omega}}}\widetilde{S}_{j,1}^2 + y_2^2\sum_{j=1}^{m_1^{\overline{\Omega}}}\widetilde{S}_{j,2}^2 + 2y_1y_2\big\langle\widetilde{S}^{\,t}(1,0,\dots,0),\widetilde{S}^{\,t}(0,1,\dots,0)\big\rangle_2, \tag{C.197}$$

Therefore, since one has $\sum_{j=1}^{k_1^{\partial\Omega}}\widetilde{S}_{j,1}^2\leq\sum_{j=1}^{k_1^{\partial\Omega}}\widetilde{S}_{j,2}^2$ (see (C.160)), it holds according to (C.195), (C.196), (C.197) and (C.145):

$$\eta_{m_0^\Omega-1}^2(\widetilde{S}\,\widetilde{C}_0) \leq \begin{cases} \sum_{j=1}^{k_1^{\partial\Omega}}\widetilde{S}_{j,2}^2 & \text{if } (\mathbf{j}(x_1)\cup\mathbf{j}(x_2))\cap\Omega=\emptyset \\ \sum_{j=1}^{k_1^{\partial\Omega}}\widetilde{S}_{j,2}^2\big(1+O(\sqrt{h})\big) & \text{if } (\mathbf{j}(x_1)\cup\mathbf{j}(x_2))\cap\Omega\neq\emptyset \end{cases}. \tag{C.198}$$

This provides the required upper bound on $\eta_{m_0^\Omega-1}(\widetilde{S}\,\widetilde{C}_0)$. Let us now give a lower bound on $\eta_{m_0^\Omega-1}(\widetilde{S}\,\widetilde{C}_0)$. To this end, we use (C.194). Let $y^*\in\mathbb{R}^{m_0^\Omega}$ be such that $\|y^*\|_2=1$, $y^*\perp{}^t(1,0,\dots,0)$, and

$$\big\|\widetilde{S}\,\widetilde{C}_0\,y^*\big\|_2 = \min_{y\perp{}^t(1,0,\dots,0)\,;\,\|y\|_2=1}\big\|\widetilde{S}\,\widetilde{C}_0\,y\big\|_2.$$

According to (C.194), it holds:

$$\eta_{m_0^\Omega-1}(\widetilde{S}\,\widetilde{C}_0) \geq \big\|\widetilde{S}\,\widetilde{C}_0\,y^*\big\|_2. \tag{C.199}$$

Let us write $y^*={}^t(y_\alpha^*,y_\beta^*)$ where $y_\alpha^*\in\mathbb{R}^{N_0}$, $y_\beta^*\in\mathbb{R}^{m_0^\Omega-N_0}$. The same arguments as those used to prove (C.180) imply that there exists $\mu>0$ such that

$$\|y_\beta^*\|_2 = O(e^{-\frac{\mu}{h}}), \tag{C.200}$$

and thus since $\|y\|_2=1$ and $y^*\perp{}^t(1,0,\dots,0)$, one obtains

$$\|y_\alpha^*\|_2 = \|\,{}^t(0,y_2^*,\dots,y_{N_0}^*)\|_2 = 1+O(e^{-\frac{\mu}{h}}). \tag{C.201}$$

Therefore, one obtains from (C.199), (C.200), (C.150), (C.182), (C.183), (C.185)

$$\eta_{m_0^\Omega-1}^2(\widetilde{S}\,\widetilde{C}_0) \geq \sum_{j=1}^{n_1}(\widetilde{S}\widetilde{C}_0\,y^*)_j^2 = \sum_{j=1}^{n_1}\sum_{k=1}^{N_0}\widetilde{S}_{j,k}^2\big(y_k^*+O(e^{-\frac{c}{h}})\big)^2,$$

and thus using in addition (C.160), (C.201) and (C.145), it holds

$$\begin{aligned}\eta^2_{m_0^\Omega-1}(\widetilde{S}\,\widetilde{C}_0) &\geq \sum_{j=1}^{k_1^{\partial\Omega}} \widetilde{S}^2_{j,1}\, O(e^{-\frac{c}{h}}) + \sum_{j=1}^{k_1^{\partial\Omega}} \widetilde{S}^2_{j,2} \sum_{k=2}^{N_0} \big(y_k^* + O(e^{-\frac{c}{h}})\big)^2 \\ &= \sum_{j=1}^{k_1^{\partial\Omega}} \widetilde{S}^2_{j,2}\big(1+O(e^{-\frac{c}{h}})\big). \end{aligned} \tag{C.202}$$

In conclusion, one has from (C.198) and (C.202), in the limit $h \to 0$:

$$\eta^2_{m_0^\Omega-1}(\widetilde{S}\,\widetilde{C}_0) = \begin{cases} \sum_{j=1}^{k_1^{\partial\Omega}} \widetilde{S}^2_{j,2}\big(1+O(e^{-\frac{c}{h}})\big) & \text{if } (\mathbf{j}(x_1)\cup\mathbf{j}(x_2))\cap\Omega=\emptyset \\ \sum_{j=1}^{k_1^{\partial\Omega}} \widetilde{S}^2_{j,2}\big(1+O(\sqrt{h})\big) & \text{if } (\mathbf{j}(x_1)\cup\mathbf{j}(x_2))\cap\Omega\neq\emptyset \end{cases}.$$

This last estimate together with (C.145) and (C.193), imply the result stated for $k=2$ in item 2 and item 3 in Theorem C.4. This concludes the proof of Theorem C.4. ∎

C.3.1.3 Proof of Proposition C.5

This section is dedicated to Proposition C.29. Proposition C.5 is a consequence of Proposition C.29. Let us first give a corollary of Theorem C.4.

Corollary C.28. *Let us assume that **[H-Morse]** and **[H-Boundary]** hold. Then, there exists $\beta_0>0$ such that for all $\beta\in(0,\beta_0)$, there exists $h_0>0$ such that for all $h\in(0,h_0)$, the orthogonal projector*

$$\widetilde{\pi}_h^{(0)} := \pi_{[0,e^{-\frac{2}{h}(f(z_1)-f(x_1)-\beta)})}(-L^{D,(0)}_{f,h}),$$

has rank N_0. Moreover for all $h\in(0,h_0)$, it holds

$$\operatorname{Ran}\widetilde{\pi}_h^{(0)} = \operatorname{Span}\big\{\widetilde{\pi}_h^{(0)}\widetilde{u}_k,\, k=1,...,N_0\big\}, \tag{C.203}$$

where the functions $(\widetilde{u}_k)_{k=1,...,N_0}$ are introduced in Definition C.9.

Proof. The fact that $\dim\operatorname{Ran}\widetilde{\pi}_h^{(0)} = N_0$ is direct consequence of (C.162). Let us now prove (C.203). Using Lemma C.8, Proposition C.2 and using the second estimate in item 2.a) of Proposition C.21, one has for any fixed $\delta>0$, fixing the parameter ε appearing in (C.80) and in (C.85) small enough, and for all $k\in\{1,\dots,N_0\}$ and $h>0$ small enough,

$$\begin{aligned}\big\|(1-\widetilde{\pi}_h^{(0)})\widetilde{u}_k\big\|^2_{L^2_w} &\leq e^{\frac{2}{h}(f(z_1)-f(x_1)-\beta)}\,\frac{h}{2}\big\|\nabla\widetilde{u}_k\big\|^2_{L^2_w} \\ &\leq e^{\frac{2}{h}(f(z_1)-f(x_1)-\beta)}\, e^{-\frac{2}{h}(f(z_1)-f(x_1)-\delta)} \\ &\leq e^{-\frac{2}{h}(\beta-\delta)}. \end{aligned} \tag{C.204}$$

Therefore, fixing $\delta>0$ and thus $\varepsilon>0$ small enough, there exists $c>0$ such that for all $(k,l)\in\{1,\dots,N_0\}$ and h small enough,

$$\langle\widetilde{\pi}_h^{(0)}\widetilde{u}_k,\widetilde{\pi}_h^{(0)}\widetilde{u}_l\rangle_{L^2_w} = \langle\widetilde{u}_k,\widetilde{u}_l\rangle_{L^2_w} - \langle(\widetilde{\pi}_h^{(0)}-1)\widetilde{u}_k,(\widetilde{\pi}_h^{(0)}-1)\widetilde{u}_l\rangle_{L^2_w} = \delta_{k,l}+O(e^{-\frac{c}{h}}). \tag{C.205}$$

Therefore, for h small enough, the space spanned by the N_0 first eigenfunctions of $-L_{f,h}^{D,(0)}$ is then spanned by the L^2_w-normalized functions $\frac{\widetilde{\pi}_h^{(0)}\widetilde{u}_k}{\|\widetilde{\pi}_h^{(0)}\widetilde{u}_k\|_{L^2_w}}$, $k \in \{1,\dots,N_0\}$. This concludes the proof of (C.203) and thus the proof of Corollary C.28. ∎

Let us recall that u_h is the eigenfunction associated with the smallest eigenvalue λ_h of $-L_{f,h}^{D,(0)}$ (see (C.5)) which satisfies (C.6). As a direct consequence of Corollary C.28, there exist N_0 unique real numbers $a_1,\dots,a_{N_0}$ which depend on h such that

$$u_h = \sum_{k=1}^{N_0} a_k \frac{\widetilde{\pi}_h^{(0)}\widetilde{u}_k}{\|\widetilde{\pi}_h^{(0)}\widetilde{u}_k\|_{L^2_w}}. \tag{C.206}$$

Using (C.206) and (C.205), for all $k \in \{1,\dots,N_0\}$, one has when $\to 0$

$$a_k = \langle u_h, \widetilde{u}_k\rangle_{L^2_w} + O(e^{-\frac{c}{h}}). \tag{C.207}$$

Moreover, for all $k \in \{1,\dots,N_0\}$, one has $\langle u_h, \widetilde{u}_k\rangle_{L^2_w} \in (0,1]$ which is a consequence of the positivity of u_h and the non negativity of $\widetilde{u}_k$ (see Definition C.9 and (C.80)). Therefore, one obtains using in addition (C.207), for all $k \in \{1,\dots,N_0\}$

$$a_k \le 0 \text{ for all } h \text{ small enough } \Rightarrow a_k = O(e^{-\frac{c}{h}}). \tag{C.208}$$

Using (C.206) and (C.205) and since $\|u_h\|_{L^2_w} = 1$, it holds

$$\sum_{k=1}^{N_0} a_k^2 = 1 + O(e^{-\frac{c}{h}}). \tag{C.209}$$

In addition, from (C.207) together wit the fact that for all $k \in \{1,\dots,N_0\}$, $\langle u_h, \widetilde{u}_k\rangle_{L^2_w} \in (0,1]$, it holds when $h \to 0$

$$a_k^2 + O(e^{-\frac{c}{h}}) = \langle u_h, \widetilde{\pi}_h^{(0)}\widetilde{u}_k\rangle^2_{L^2_w} = \langle u_h, \widetilde{u}_k\rangle^2_{L^2_w} \le \langle u_h, \widetilde{u}_k\rangle_{L^2_w} = \langle u_h, \widetilde{\pi}_h^{(0)}\widetilde{u}_k\rangle_{L^2_w} = a_k + O(e^{-\frac{c}{h}}).$$

which leads, using also (C.209) and (C.208), to

$$1 + O(e^{-\frac{c}{h}}) \le \sum_{k=1,\, a_k \ge 0}^{N_0} a_k. \tag{C.210}$$

Let us now prove the following proposition which implies Proposition C.5.

Proposition C.29. *Assume **[H-Morse]** and **[H-Boundary]**. Let us consider u_h the eigenfunction associated with the smallest eigenvalue λ_h of $-L_{f,h}^{D,(0)}$ (see* (C.5)*) which satisfies* (C.6)*. Then, there exists $c > 0$ such that in the limit $h \to 0$:*

$$\int_\Omega u_h\ e^{-\frac{2}{h}f} = (h\pi)^{\frac{d}{4}} e^{-\frac{1}{h}f(x_1)} \sum_{k=1, a_k \ge 0}^{N_0} a_k \Big(\sum_{x \in \arg\min_{C_k} f} \big(\det \operatorname{Hess} f(x)\big)^{-\frac{1}{2}} \Big)^{\frac{1}{2}} \big(1 + O(h)\big),$$

where the family $(a_k)_{k\in\{1,\dots,N_0\}}$ is defined by (C.206)*.*

Proposition C.29 implies Proposition C.5 since under [**H-Connexity**], it holds $N_0 = 1$ and hence $a_1 = 1$.

Remark C.17. *We have stated Proposition C.29 without assuming **[H-Connexity]** (i.e without assuming $N_0 = 1$) because we think it could be possible to identify the wells C_k's ($k \in \{1, \dots, N_0\}$, where the C_k's are introduced in Definition C.2) for which $\lim_{h\to 0} a_k \in (0,1)$. This is a tricky problem except in some very specific settings in dimension one. The reason why we assumed **[H-Connexity]** in Theorem C.2 and Proposition C.5 is that under this assumption, when $h \to 0$, the L^2_w-norm of u_h is non zero only in C_1 (since $u_h = \frac{\widetilde{\pi}_h^{(0)}\widetilde{u}_1}{\|\widetilde{\pi}_h^{(0)}\widetilde{u}_1\|_{L^2_w}}$ under **[H-Connexity]** and $\operatorname{supp}\widetilde{u}_1 \subset \Omega \cap (C_1 + B(0, 3\varepsilon_1))$, see Definition C.9,* (C.80) *and* (C.81)*) which permits also to obtain the asymptotic behaviour of its normal derivative (see Theorem C.2 and Proposition C.5).*

Proof. Using (C.206), we have in the limit $h \to 0$:

$$\begin{aligned}\int_\Omega u_h\, e^{-\frac{2}{h}f} &= \sum_{i=1}^{N_0} a_i \int_\Omega \frac{\widetilde{\pi}_h^{(0)}\widetilde{u}_i}{\|\widetilde{\pi}_h^{(0)}\widetilde{u}_i\|_{L^2_w}} e^{-\frac{2}{h}f} \\ &= \sum_{i=1}^{N_0} a_i \int_\Omega \frac{\widetilde{u}_i}{\|\widetilde{\pi}_h^{(0)}\widetilde{u}_i\|_{L^2_w}} e^{-\frac{2}{h}f} + a_i \int_\Omega \frac{(\widetilde{\pi}_h^{(0)} - 1)\widetilde{u}_i}{\|\widetilde{\pi}_h^{(0)}\widetilde{u}_i\|_{L^2_w}} e^{-\frac{2}{h}f}. \end{aligned} \tag{C.211}$$

Thanks to the Cauchy-Schwarz inequality, to (C.205) and (C.204), there exists $c > 0$ such that for all $i \in \{1, \dots, N_0\}$ and h small enough,

$$\int_\Omega \frac{(\widetilde{\pi}_h^{(0)} - 1)\widetilde{u}_i}{\|\widetilde{\pi}_h^{(0)}\widetilde{u}_i\|_{L^2_w}} e^{-\frac{2}{h}f} = O\big(e^{-\frac{1}{h}(f(x_1)+c)}\big). \tag{C.212}$$

Let us moreover recall that for $i \in \{1, ..., N_0\}$, $\widetilde{u}_i = \frac{1}{\|\chi_i^{\varepsilon,\varepsilon_1}\|_{L^2_w}} \chi_i^{\varepsilon,\varepsilon_1}$ (see Definition C.9 and (C.80)) and that, from the definition of $\chi_i^{\varepsilon,\varepsilon_1}$ (see (C.80) and the lines below) and Laplace's method (see indeed (C.134) stated for $i = 1$), one has in the limit $h \to 0$,

$$\text{for } (\chi_i^{\varepsilon,\varepsilon_1})^2 : \int_\Omega (\chi_i^{\varepsilon,\varepsilon_1})^2\, e^{-\frac{2}{h}f} = (h\pi)^{\frac{d}{2}} e^{-\frac{2}{h}f(x_1)} \sum_{x \in \arg\min_{C_i} f} \big(\det \operatorname{Hess} f(x)\big)^{-\frac{1}{2}} \, (1 + O(h)) \tag{C.213}$$

and

$$\text{for } \chi_i^{\varepsilon,\varepsilon_1} : \int_\Omega \chi_i^{\varepsilon,\varepsilon_1}\, e^{-\frac{2}{h}f} = (h\pi)^{\frac{d}{2}} e^{-\frac{2}{h}f(x_1)} \sum_{x \in \arg\min_{C_i} f} \big(\det \operatorname{Hess} f(x)\big)^{-\frac{1}{2}} \, (1 + O(h)). \tag{C.214}$$

The statement of Proposition C.29 then follows from (C.211)–(C.214) together with (C.208). ∎

C.3.2 Proof of Theorem C.2

This section is devoted to the proof of the following result which implies Theorem C.2.

Proposition C.30. *Let us assume that the assumptions **[H-Morse]** and **[H-Connexity]** hold. Let u_h be the eigenfunction associated with the smallest eigenvalue λ_h of $-L_{f,h}^{D,(0)}$ (see* (C.5)*) which satisfies* (C.6)*. Let $F \in L^\infty(\partial\Omega, \mathbb{R})$ and Σ be an open subset of $\partial\Omega$.*

i) When $\overline{\Sigma} \cap \{z_1, \dots, z_{k_1^{\partial\Omega}}\} = \emptyset$, one has in the limit $h \to 0$:

$$\int_\Sigma F\, \partial_n u_h\, e^{-\frac{2}{h}f} = O\big(e^{-\frac{1}{h}(2f(z_1)-f(x_1)+c)}\big),$$

where $c > 0$ is independent of h.

ii) When $\overline{\Sigma} \cap \{z_1, \dots, z_{k_1^{\partial C_1}}\} = \emptyset$, one has in the limit $h \to 0$:

$$\int_\Sigma F\, \partial_n u_h\, e^{-\frac{2}{h}f} = O\big(h^{\frac{d-6}{4}} e^{-\frac{1}{h}(2f(z_1)-f(x_1))} \sqrt{\varepsilon_h}\big),$$

where, for some $c > 0$ independent of h,

$$\varepsilon_h = \begin{cases} \sqrt{h} & \text{under } \textbf{[H-Connexity]} \\ e^{-\frac{c}{h}} & \text{under } \textbf{[H-Connexity+]} \end{cases}. \tag{C.215}$$

iii) When, for some $i \in \{1, \dots, k_1^{\partial C_1}\}$, $\overline{\Sigma} \cap \{z_1, \dots, z_{k_1^{\partial C_1}}\} = \{z_i\}$, $z_i \in \Sigma$, and F is C^∞ in a neighborhood of z_i, it holds in the limit $h \to 0$:

$$\int_\Sigma F\, \partial_n u_h\, e^{-\frac{2}{h}f} = \big(F(z_i) + O(\sqrt{\varepsilon_h}) + O(h)\big) C_{i,1} B_i\; h^{\frac{d-6}{4}}\; e^{-\frac{1}{h}(2f(z_1)-f(x_1))},$$

where ε_h satisfies (C.215) *and the constants B_i and $C_{i,1}$ are defined in* (C.129)–(C.120)*.*

Let us briefly explain the strategy for the proof of Proposition C.30 before entering into the technical details below. The basic idea is to notice that, since ∇u_h belongs to $\operatorname{Ran} \pi_h^{(1)}$ (according to (C.40)), one has for any open set Σ of $\partial\Omega$ and for any L^2_w-orthonormal basis $(\psi_1, \dots, \psi_{m_1^{\overline{\Omega}}})$ of $\operatorname{Ran} \pi_h^{(1)}$,

$$\int_\Sigma F\, \partial_n u_h\; e^{-\frac{2}{h}f} = \sum_{i=1}^{m_1^{\overline{\Omega}}} \langle \nabla u_h, \psi_i \rangle_{L^2_w} \int_\Sigma F\, \psi_i \cdot n\; e^{-\frac{2}{h}f}. \tag{C.216}$$

Notice that, this decomposition of ∇u_h is valid on $\partial\Omega$ since for all $i \in \{1, ..., m_1^{\overline{\Omega}}\}$, $\psi_i \in \Lambda^1 C^\infty(\overline{\Omega})$ (due to the fact that that the eigenforms of $L_{f,h}^{D,(1)}$ belongs to $C^\infty(\overline{\Omega})$ and $\pi_h^{(1)}$ is a projector onto a finite number of eigenforms of $-L_{f,h}^{D,(1)}$) and thus ψ_i is C^∞ on $\partial\Omega$. In the rest of this section, one first introduces such a family $(\psi_1, \dots, \psi_{m_1^{\overline{\Omega}}})$ using a Gram–Schmidt orthonormalization of the family $(\pi_h^{(1)}\widetilde{\psi}_1, \dots, \pi_h^{(1)}\widetilde{\psi}_{m_1^{\overline{\Omega}}})$. Then, on gives the estimate of the terms $\langle \nabla u_h, \psi_i \rangle_{L^2_w}$ appearing in (C.216). Finally, one concludes the proof of Proposition C.30 in Section C.3.2.3, with estimations of the boundary terms $\int_\Sigma F\, \psi_i \cdot n\; e^{-\frac{2}{h}f}$.

C.3.2.1 Gram-Schmidt orthonormalization

Let us assume that the hypotheses [**H-Morse**] and [**H-Boundary**] hold, and assume $h > 0$ small enough such that the family $\left\{\pi_h^{(1)}\widetilde{\psi}_i, i = 1, \dots, m_1^{\overline{\Omega}}\right\}$ is independent (which is guaranteed for small h by Corollary C.22). Using a Gram-Schmidt procedure, there exists, for all $j \in \left\{1, \dots, m_1^{\overline{\Omega}}\right\}$, a family $(\kappa_{ji})_{i=1,\dots,j-1} \subset \mathbb{R}^{j-1}$ such that the 1-forms

$$f_j := \pi_h^{(1)}\Big[\widetilde{\psi}_j + \sum_{i=1}^{j-1} \kappa_{ji}\widetilde{\psi}_i\ \Big] \tag{C.217}$$

satisfy:

i) for all $k \in \{1, \dots, m_1^{\overline{\Omega}}\}$, $\mathrm{Span}\big(\{f_i, i = 1, \dots, k\}\big) = \mathrm{Span}\big(\{\pi_h^{(1)}\widetilde{\psi}_i, i = 1, \dots, k\}\big)$,

ii) for all $i \neq j$, $\langle f_i, f_j\rangle_{L^2_w} = 0$.

One defines moreover, for $j \in \left\{1, \dots, m_1^{\overline{\Omega}}\right\}$,

$$Z_j := \|f_j\|_{L^2_w} \text{ and } \psi_j := \frac{1}{Z_j} f_j, \tag{C.218}$$

so that $(\psi_j)_{j\in\left\{1,\dots,m_1^{\overline{\Omega}}\right\}}$ is a L^2_w-orthonormal basis of $\mathrm{Ran}\,\pi_h^{(1)}$. By reasoning by induction, item 3 in Proposition C.21, easily leads, to the following estimates showing in particular that the family $(\pi_h^{(1)}\widetilde{\psi}_i)_{i\in\{1,\dots,m_1^{\overline{\Omega}}\}}$ is close to the family $(\psi_i)_{i\in\{1,\dots,m_1^{\overline{\Omega}}\}}$.

Lemma C.31. *Let us assume that the assumptions **[H-Morse]** and **[H-Boundary]** hold. Then, there exists $c > 0$ such that for all $j \in \left\{1, \dots, m_1^{\overline{\Omega}}\right\}$, $i \in \{1, \dots, j-1\}$ and $h > 0$ small enough,*

$$Z_j = 1 + O(e^{-\frac{c}{h}}) \text{ and } \kappa_{ji} = O(e^{-\frac{c}{h}}).$$

C.3.2.2 Estimates of the interaction terms $\big(\langle\nabla u_h, \psi_j\rangle_{L^2_w}\big)_{j\in\{1,\dots,m_1^{\overline{\Omega}}\}}$

Let us begin with the estimates of the terms $\langle\nabla\pi_h^{(0)}\widetilde{u}_1, \psi_j\rangle_{L^2_w}$, where $j \in \left\{1, \dots, m_1^{\overline{\Omega}}\right\}$.

Lemma C.32. *Let us assume that the assumptions **[H-Morse]** and **[H-Boundary]** hold. Then:*

i) For all $j \in \left\{1, \dots, m_1^{\overline{\Omega}}\right\}$ such that $z_j \in \mathbf{j}(x_1)$, one has when $h \to 0$:

$$\begin{aligned}\langle\nabla\pi_h^{(0)}\widetilde{u}_1, \psi_j\rangle_{L^2_w} &= \langle\nabla\widetilde{u}_1, \widetilde{\psi}_j\rangle_{L^2_w}\ \big(1 + O(e^{-\frac{c}{h}})\big)\\ &= \varepsilon_{j,1}C_{j,1}\ h^{p_{j,1}}e^{-\frac{1}{h}(f(z_1)-f(x_1))}\ \big(1 + O(h)\big)\end{aligned}$$

where $\varepsilon_{j,1} \in \{-1, 1\}$ and $\varepsilon_{j,1} = -1$ when $z_j \in \mathbf{j}(x_1) \cap \partial\Omega$, the constants $C_{j,1}$ are defined in (C.129)*, and*

$$p_{j,1} = \begin{cases} -\frac{1}{2} & \text{if } z_j \in \mathbf{j}(x_1) \cap \Omega \\ -\frac{3}{4} & \text{if } z_j \in \mathbf{j}(x_1) \cap \partial\Omega. \end{cases}$$

ii) For all $j \in \left\{1, \dots, m_1^{\overline{\Omega}}\right\}$ such that $z_j \notin \mathbf{j}(x_1)$, one has when $h \to 0$:

$$\langle \nabla \pi_h^{(0)} \widetilde{u}_1, \psi_j \rangle_{L^2_w} = O\big(e^{-\frac{1}{h}(f(z_1)-f(x_1)+c)}\big),$$

for some $c > 0$ independent of h.

Proof. Using (C.217), (C.218), and Lemma C.31, one has for some $c > 0$ and for all $j \in \left\{1, \dots, m_1^{\overline{\Omega}}\right\}$ and $h > 0$ small enough,

$$\begin{aligned}\langle \nabla \pi_h^{(0)} \widetilde{u}_1, \psi_j \rangle_{L^2_w} &= Z_j^{-1} \left[\langle \nabla \pi_h^{(0)} \widetilde{u}_1, \pi_h^{(1)} \widetilde{\psi}_j \rangle_{L^2_w} + \sum_{i=1}^{j-1} \kappa_{ji} \langle \nabla \pi_h^{(0)} \widetilde{u}_1, \pi_h^{(1)} \widetilde{\psi}_i \rangle_{L^2_w} \right] \\ &= \big(1 + O(e^{-\frac{c}{h}})\big) \left[\langle \nabla \pi_h^{(0)} \widetilde{u}_1, \pi_h^{(1)} \widetilde{\psi}_j \rangle_{L^2_w} + \sum_{i=1}^{j-1} O(e^{-\frac{c}{h}}) \langle \nabla \pi_h^{(0)} \widetilde{u}_1, \pi_h^{(1)} \widetilde{\psi}_i \rangle_{L^2_w} \right].\end{aligned}$$

Applying now Proposition C.23, one has moreover for all $j \in \left\{1, \dots, m_1^{\overline{\Omega}}\right\}$ and $h > 0$ small enough, taking maybe c smaller,

$$\langle \nabla \pi_h^{(0)} \widetilde{u}_1, \pi_h^{(1)} \widetilde{\psi}_j \rangle_{L^2_w} = \begin{cases} \langle \nabla \widetilde{u}_1, \widetilde{\psi}_j \rangle_{L^2_w} \big(1 + O(e^{-\frac{c}{h}})\big) & \text{if } z_j \in \mathbf{j}(x_1) \\ O\left(e^{-\frac{1}{h}(f(z_1)-f(x_1)+c)}\right) & \text{if } z_j \notin \mathbf{j}(x_1), \end{cases}$$

with, when $z_j \in \mathbf{j}(x_1)$,

$$\langle \nabla \widetilde{u}_1, \widetilde{\psi}_j \rangle_{L^2_w} = \varepsilon_{j,1} C_{j,1}\, h^{p_{j,1}} e^{-\frac{1}{h}(f(z_1)-f(x_1))} \big(1 + O(h)\big).$$

The statement of Lemma C.32 follows immediately. ∎

Let us now prove that when assuming in addition **[H-Connexity]**, a similar result still holds if one replaces $\pi_h^{(0)} \widetilde{u}_1$ by u_h (where u_h is the eigenfunction associated with λ_h and satisfying (C.6)). This requires in particular to show that $\pi_h^{(0)} \widetilde{u}_1$ is an accurate approximation of u_h in $H^1_w(\Omega)$.

Before, let us recall that under **[H-Connexity]** (since in that case $N_0 = 1$), Corollary C.28 implies that there exists $\beta_0 > 0$ such that for all $\beta \in (0, \beta_0)$, there exists $h_0 > 0$ such that for all $h \in (0, h_0)$, the orthogonal projector

$$\widetilde{\pi}_h^{(0)} = \pi_{[0, e^{-\frac{2}{h}(f(z_1)-f(x_1)-\beta)})}(-L_{f,h}^{D,(0)}),$$

has rank 1. Therefore, under **[H-Connexity]**, $\widetilde{\pi}_h^{(0)}$ is the orthogonal projector onto $\operatorname{Span} u_h$. The following lemma then shows that $\widetilde{u}_1$ (and hence $\pi_h^{(0)} \widetilde{u}_1$) is an accurate approximation of $\widetilde{\pi}_h^{(0)} \widetilde{u}_1$ in $L^2_w(\Omega)$.

Lemma C.33. *Let us assume that the assumptions **[H-Morse]** and **[H-Connexity]** hold. There exists $c > 0$ such that for all $h > 0$ small enough,*

$$\left\| (\pi_h^{(0)} - \widetilde{\pi}_h^{(0)}) \widetilde{u}_1 \right\|_{L^2_w} \leq \left\| (1 - \widetilde{\pi}_h^{(0)}) \widetilde{u}_1 \right\|_{L^2_w} = O(e^{-\frac{c}{h}}).$$

Proof. The first inequality is an immediate consequence of $\|\pi_h^{(0)}\| \leq 1$ and $\pi_h^{(0)}\widetilde{\pi}_h^{(0)} = \widetilde{\pi}_h^{(0)}$. Moreover, from Lemma C.8 and item 2 of Proposition C.21, one has for any fixed $\delta > 0$, fixing the parameter ε appearing in (C.80) and in (C.85) small enough, and for all $h > 0$ small enough,

$$\begin{aligned}\left\|(1-\widetilde{\pi}_h^{(0)})\widetilde{u}_1\right\|_{L^2_w}^2 &\leq e^{\frac{2}{h}(f(z_1)-f(x_1)-\beta)}\,\frac{h}{2}\|\nabla\widetilde{u}_1\|_{L^2_w}^2\\ &\leq e^{\frac{2}{h}(f(z_1)-f(x_1)-\beta)}\,e^{-\frac{2}{h}(f(z_1)-f(x_1)-\delta)}\\ &\leq\ e^{-\frac{2}{h}(\beta-\delta)}.\end{aligned}$$

Fixing $\delta < \beta$, one gets the statement of Lemma C.33. ∎

Lemma C.33 obviously implies that for all $h > 0$ small enough, $\left\|\widetilde{\pi}_h^{(0)}\widetilde{u}_1\right\|_{L^2_w} = 1 + O(e^{-\frac{c}{h}}) > 0$, and since the functions u_h and $\widetilde{u}_1$ are non negative, one gets the following relation in the limit $h \to 0$:

$$u_h = \frac{\widetilde{\pi}_h^{(0)}\widetilde{u}_1}{\left\|\widetilde{\pi}_h^{(0)}\widetilde{u}_1\right\|_{L^2_w}} = \widetilde{\pi}_h^{(0)}\widetilde{u}_1\left(1+O(e^{-\frac{c}{h}})\right). \tag{C.219}$$

Therefore, Lemma C.33 implies in particular that $\pi_h^{(0)}\widetilde{u}_1$ is an accurate approximation of u_h in $L^2_w(\Omega)$. The following result extends this result in $H^1_w(\Omega)$.

Lemma C.34. *Assume **[H-Morse]** and **[H-Connexity]**. Then, it holds in the limit $h \to 0$:*

$$\left\|\nabla\pi_h^{(0)}\widetilde{u}_1\right\|_{L^2_w}^2 = \frac{2}{h}\lambda_h\left(1+O(\varepsilon_h)\right)$$

and

$$\left\|\nabla(\pi_h^{(0)}-\widetilde{\pi}_h^{(0)})\widetilde{u}_1\right\|_{L^2_w}^2 = \frac{2}{h}\lambda_h\,O(\varepsilon_h) = O\big(h^{-\frac{3}{2}}\,e^{-\frac{2}{h}(f(z_1)-f(x_1))}\,\varepsilon_h\big),$$

where in the limit $h \to 0$, ε_h satisfies (C.215).

Proof. First, applying the Parseval identity to $\nabla\pi_h^{(0)}\widetilde{u}_1 \in \operatorname{Ran}\pi_h^{(1)}$ (see (C.38)), one gets

$$\left\|\nabla\pi_h^{(0)}\widetilde{u}_1\right\|_{L^2_w}^2 = \sum_{j=1}^{m_1^{\overline{\Omega}}}\langle\nabla\pi_h^{(0)}\widetilde{u}_1,\psi_j\rangle_{L^2_w}^2.$$

Using Lemma C.32, there exists consequently $c > 0$ such that for all $h > 0$ small enough, (by definition of $\widetilde{S}$, see (C.144))

$$\left\|\nabla\pi_h^{(0)}\widetilde{u}_1\right\|_{L^2_w}^2 = \sum_{j:\,z_j\in\mathbf{j}(x_1)}\left\langle\nabla\widetilde{u}_1,\widetilde{\psi}_j\right\rangle_{L^2_w}^2(1+O(e^{-\frac{c}{h}})) = \sum_{j:\,z_j\in\mathbf{j}(x_1)}\widetilde{S}_{j,1}^2\,(1+O(e^{-\frac{c}{h}})).$$

Using in addition items 2 and 3 in Theorem C.4 (in the case where $N_0 = 1$), one then obtains the first part of Lemma C.34:

$$\left\|\nabla\pi_h^{(0)}\widetilde{u}_1\right\|_{L^2_w}^2 = \frac{2}{h}\lambda_h\big(1+O(\varepsilon_h)\big), \tag{C.220}$$

where, in the limit $h \to 0$, ε_h satisfies (C.215).

Now, since the projectors $\pi_h^{(0)}$ and $\widetilde{\pi}_h^{(0)}$ commute with $L_{f,h}^{D,(0)}$, and $\widetilde{\pi}_h^{(0)}\pi_h^{(0)} = \widetilde{\pi}_h^{(0)}$, one has

$$\begin{aligned}
\frac{h}{2}\big\|\nabla(\pi_h^{(0)} - \widetilde{\pi}_h^{(0)})\widetilde{u}_1\big\|_{L^2_w}^2 &= \big\langle(\pi_h^{(0)} - \widetilde{\pi}_h^{(0)})\widetilde{u}_1, -L_{f,h}^{D,(0)}\,(\pi_h^{(0)} - \widetilde{\pi}_h^{(0)})\widetilde{u}_1\big\rangle_{L^2_w} \\
&= \big\langle\pi_h^{(0)}\widetilde{u}_1, -L_{f,h}^{D,(0)}\,(\pi_h^{(0)} - \widetilde{\pi}_h^{(0)})\widetilde{u}_1\big\rangle_{L^2_w} \\
&= \big\langle\pi_h^{(0)}\widetilde{u}_1, -L_{f,h}^{D,(0)}\pi_h^{(0)}\widetilde{u}_1\big\rangle_{L^2_w} - \big\langle\widetilde{\pi}_h^{(0)}\widetilde{u}_1, -L_{f,h}^{D,(0)}\widetilde{\pi}_h^{(0)}\widetilde{u}_1\big\rangle_{L^2_w} \\
&= \frac{h}{2}\big\|\nabla\pi_h^{(0)}\widetilde{u}_1\big\|_{L^2_w}^2 - \lambda_h\big(1 + O(e^{-\frac{c}{h}})\big),
\end{aligned}$$

where the last line follows from (C.219). Using in addition (C.220), one obtains in the limit $h \to 0$:

$$\frac{h}{2}\big\|\nabla(\pi_h^{(0)} - \widetilde{\pi}_h^{(0)})\widetilde{u}_1\big\|_{L^2_w}^2 = \lambda_h\big(1 + O(\varepsilon_h)\big) - \lambda_h\big(1 + O(e^{-\frac{c}{h}})\big) = \lambda_h\, O(\varepsilon_h),$$

which proves Lemma C.34, using also the expression of λ_h written in item 2 in Theorem C.4 in the case $N_0 = 1$. ∎

We are now in position to estimate the interaction terms $\big(\langle\nabla u_h, \psi_j\rangle_{L^2_w}\big)_{j\in\{1,\dots,m_1^{\overline{\Omega}}\}}$.

Corollary C.35. *Let us assume that the hypotheses **[H-Morse]** and **[H-Connexity]** hold. Let u_h the eigenfunction associated with the smallest eigenvalue λ_h of $-L_{f,h}^{D,(0)}$ (see* (C.5)*) which satisfies* (C.6)*. Then, one has in the limit $h \to 0$:*

i) for all $j \in \Big\{1, \dots, m_1^{\overline{\Omega}}\Big\}$ such that $z_j \in \mathbf{j}(x_1) \cap \partial\Omega$ (i.e. for all $j \in \big\{1, \dots, k_1^{\partial C_1}\big\}$),

$$\begin{aligned}
\big\langle\nabla u_h, \psi_j\big\rangle_{L^2_w} &= \big\langle\nabla\widetilde{u}_1, \widetilde{\psi}_j\big\rangle_{L^2_w}\,\big(1 + O(\sqrt{\varepsilon_h})\big) \\
&= -C_{j,1}\; h^{-\frac{3}{4}} e^{-\frac{1}{h}(f(z_1)-f(x_1))}\,\big(1 + O(\sqrt{\varepsilon_h}) + O(h)\big),
\end{aligned}$$

ii) for all $j \in \big\{1, \dots, m_1^{\overline{\Omega}}\big\}$ such that $z_j \in \mathbf{j}(x_1) \cap \Omega$,

$$\begin{aligned}
\big\langle\nabla u_h, \psi_j\big\rangle_{L^2_w} &= \big\langle\nabla\widetilde{u}_1, \widetilde{\psi}_j\big\rangle_{L^2_w}\,\big(1 + O(h^{-\frac{1}{4}}\sqrt{\varepsilon_h})\big) \\
&= O\big(h^{-\frac{1}{2}} e^{-\frac{1}{h}(f(z_1)-f(x_1))}\big),
\end{aligned}$$

iii) and for all $j \in \big\{1, \dots, m_1^{\overline{\Omega}}\big\}$ such that $z_j \notin \mathbf{j}(x_1)$,

$$\big\langle\nabla u_h, \psi_j\big\rangle_{L^2_w} = O\big(h^{-\frac{3}{4}} e^{-\frac{1}{h}(f(z_1)-f(x_1))}\,\sqrt{\varepsilon_h}\big),$$

where in the limit $h \to 0$, ε_h satisfies (C.215)*.*

Proof. Using (C.219), there exists $c > 0$ such that for all $j \in \Big\{1, \dots, m_1^{\overline{\Omega}}\Big\}$, one has in the limit $h \to 0$:

$$\big\langle\nabla u_h, \psi_j\big\rangle_{L^2_w} = \big\langle\nabla\widetilde{\pi}_h^{(0)}\widetilde{u}_1, \psi_j\big\rangle_{L^2_w}\,\big(1 + O(e^{-\frac{c}{h}})\big). \tag{C.221}$$

In addition, using the Cauchy-Schwarz inequality and Lemma C.34, it holds for all $j \in \left\{1, \dots, m_1^{\overline{\Omega}}\right\}$, in the limit $h \to 0$:

$$\begin{aligned}\left\langle \nabla \widetilde{\pi}_h^{(0)} \widetilde{u}_1, \psi_j \right\rangle_{L^2_w} &= \left\langle \nabla \pi_h^{(0)} \widetilde{u}_1, \psi_j \right\rangle_{L^2_w} + \left\langle \nabla (\widetilde{\pi}_h^{(0)} - \pi_h^{(0)}) \widetilde{u}_1, \psi_j \right\rangle_{L^2_w} \\ &= \left\langle \nabla \pi_h^{(0)} \widetilde{u}_1, \psi_j \right\rangle_{L^2_w} + O\big(h^{-\frac{3}{4}}\, e^{-\frac{1}{h}(f(z_1)-f(x_1))} \sqrt{\varepsilon_h}\big), \end{aligned} \tag{C.222}$$

where ε_h is of the order given by (C.215). Then, the statement of Corollary C.35 follows by injecting (C.222) into (C.221) and by using the estimates of the terms $\left\langle \nabla \pi_h^{(0)} \widetilde{u}_1, \psi_j \right\rangle_{L^2_w}$, $j \in \{1, \dots, m_1^{\overline{\Omega}}\}$ given in Lemma C.32. ∎

C.3.2.3 Estimates of the boundary terms $\left(\int_\Sigma F\, \psi_j \cdot n\, e^{-\frac{2}{h} f}\right)_{j \in \{1, \dots, m_1^{\overline{\Omega}}\}}$

Proposition C.36. *Assume **[H-Morse]** and **[H-Boundary]**, and let us consider $i \in \{1, \dots, m_1^{\overline{\Omega}}\}$, an open set Σ of $\partial\Omega$, and $F \in L^\infty(\partial\Omega, \mathbb{R})$. Then, one has in the limit $h \to 0$:*

$$\int_\Sigma F\, \psi_i \cdot n\; e^{-\frac{2}{h} f} = \begin{cases} O\big(e^{-\frac{1}{h}(f(z_1)+c)}\big) & \text{if } i \in \left\{k_1^{\partial\Omega}+1, \dots, m_1^{\overline{\Omega}}\right\} \\ O\big(e^{-\frac{1}{h}(f(z_1)+c)}\big) & \text{if } i \in \left\{1, \dots, k_1^{\partial\Omega}\right\} \text{ and } z_i \notin \overline{\Sigma} \\ O\big(h^{\frac{d-3}{4}} e^{-\frac{1}{h} f(z_1)}\big) & \text{if } i \in \left\{1, \dots, k_1^{\partial\Omega}\right\} \text{ and } z_i \in \overline{\Sigma}, \end{cases}$$

where the constant $c > 0$ is independent of h. Moreover, when $i \in \left\{1, \dots, k_1^{\partial\Omega}\right\}$, $z_i \in \Sigma$, and F is C^∞ in a neighborhood of z_i, it holds in the limit $h \to 0$:

$$\int_\Sigma F\, \psi_i \cdot n\; e^{-\frac{2}{h} f} = B_i\; h^{\frac{d-3}{4}}\; e^{-\frac{1}{h} f(z_1)}\; \big(F(z_i) + O(h)\big),$$

where the constant B_i is defined in (C.120).

Proof. Let $F \in L^\infty(\partial\Omega, \mathbb{R})$. Using (C.217), (C.218), the trace theorem, and the Cauchy-Schwarz inequality, one has for any $j \in \{1, \dots, m_1^{\overline{\Omega}}\}$,

$$\begin{aligned} Z_j \int_\Sigma F\, \psi_j \cdot n\, e^{-\frac{2}{h} f} &= \left[\int_\Sigma F\, \widetilde{\psi}_j \cdot n\, e^{-\frac{2}{h} f} + \int_\Sigma F\, \big((\pi_h^{(1)} - 1)\widetilde{\psi}_j\big) \cdot n\, e^{-\frac{2}{h} f}\right] \\ &\quad + \sum_{i=1}^{j-1} \kappa_{ji}\; \left[\int_\Sigma F\, \widetilde{\psi}_i \cdot n\, e^{-\frac{2}{h} f} + \int_\Sigma F\, \big((\pi_h^{(1)} - 1)\widetilde{\psi}_i\big) \cdot n\, e^{-\frac{2}{h} f}\right] \\ &= \left[\int_\Sigma F\, \widetilde{\psi}_j \cdot n\, e^{-\frac{2}{h} f} + \|(1 - \pi_h^{(1)})\widetilde{\psi}_j\|_{H^1_w} O\big(h^{-1}\, e^{-\frac{f(z_1)}{h}}\big)\right] \\ &\quad + \sum_{i=1}^{j-1} \kappa_{ji}\; \left[\int_\Sigma F\, \widetilde{\psi}_i \cdot n\, e^{-\frac{2}{h} f} + \|(1 - \pi_h^{(1)})\widetilde{\psi}_i\|_{H^1_w} O\big(h^{-1}\, e^{-\frac{f(z_1)}{h}}\big)\right] \end{aligned}$$

From Lemma C.31 and Proposition C.21, there exists $c > 0$ such that for all $j \in \left\{1, \dots, m_1^{\overline{\Omega}}\right\}$, $i \in \{1, \dots, j-1\}$, one has in the limit $h \to 0$:

$$Z_j = 1 + O(e^{-\frac{c}{h}}),\; \kappa_{ji} = O(e^{-\frac{c}{h}}),\; \text{and } \left\|(1 - \pi_h^{(1)})\widetilde{\psi}_j\right\|_{H^1_w} = O(e^{-\frac{c}{h}}).$$

The statement of Proposition C.36 is then a straightforward consequence of Proposition C.20. ∎

We are now in position to prove Proposition C.30.

Proof of Proposition C.30. Assume [**H-Morse**] and [**H-Connexity**]. Let $F \in L^\infty(\partial\Omega, \mathbb{R})$ and Σ be an open subset of $\partial\Omega$. First, since $\{\psi_j,\, j = 1, \dots, m_1^{\overline{\Omega}}\}$ is an orthonormal basis of $\operatorname{Ran} \pi_h^{(1)} \ni \nabla u_h$, one has the decomposition:

$$\int_\Sigma F\, \partial_n u_h\, e^{-\frac{2}{h}f} = \sum_{j=1}^{m_1^{\overline{\Omega}}} \langle \nabla u_h, \psi_j \rangle_{L^2_w} \int_\Sigma F\, \psi_j \cdot n\; e^{-\frac{2}{h}f}.$$

Using in addition Corollary C.35 and Proposition C.36, there exists $c > 0$ such that for all $h > 0$ small enough,

$$\begin{aligned}\int_\Sigma F \partial_n u_h\, e^{-\frac{2}{h}f} &= \sum_{j=1}^{k_1^{\partial\Omega}} \langle \nabla u_h, \psi_j \rangle_{L^2_w} \int_\Sigma F\, \psi_j \cdot n\; e^{-\frac{2}{h}f} \\ &\quad + \sum_{j=k_1^{\partial\Omega}+1}^{m_1^{\overline{\Omega}}} O\big(h^{-\frac{1}{2}} e^{-\frac{1}{h}(f(z_1)-f(x_1))}\big)\, O\big(e^{-\frac{1}{h}(f(z_1)+c)}\big). \qquad \text{(C.223)}\end{aligned}$$

Hence, when $\overline{\Sigma}$ does not contain any of the z_i, $i \in \{1, \dots, k_1^{\partial\Omega}\}$, one deduces from (C.223), Corollary C.35 and Proposition C.36 the following relation for some $c > 0$ independent of h and every $h > 0$ small enough:

$$\begin{aligned}\int_\Sigma F\, \partial_n u_h e^{-\frac{2}{h}f} &= \sum_{j=1}^{k_1^{\partial\Omega}} O\big(h^{-\frac{3}{4}} e^{-\frac{1}{h}(f(z_1)-f(x_1))}\big) O\big(e^{-\frac{1}{h}(f(z_1)+c)}\big) + O\big(e^{-\frac{1}{h}(2f(z_1)-f(x_1)+c)}\big) \\ &= O\big(e^{-\frac{1}{h}(2f(z_1)-f(x_1)+\frac{c}{2})}\big).\end{aligned}$$

This proves the first part of Proposition C.30.

Assume now that $\overline{\Sigma}$ does not contain any of the z_i, $i \in \{1, \dots, k_1^{\partial C_1}\}$. Then , one deduces from (C.223), Corollary C.35 and Proposition C.36 that in the limit $h \to 0$:

$$\begin{aligned}\int_\Sigma F\, \partial_n u_h\, e^{-\frac{2}{h}f} &= \sum_{j=1}^{k_1^{\partial C_1}} O\big(h^{-\frac{3}{4}} e^{-\frac{1}{h}(f(z_1)-f(x_1))}\big) O\big(e^{-\frac{1}{h}(f(z_1)+c)}\big) + O\big(e^{-\frac{1}{h}(2f(z_1)-f(x_1)+c)}\big) \\ &\quad + \sum_{j=k_1^{\partial C_1}+1}^{k_1^{\partial\Omega}} O\big(h^{-\frac{3}{4}} e^{-\frac{1}{h}(f(z_1)-f(x_1))}\, \sqrt{\varepsilon_h}\big)\; O\big(h^{\frac{d-3}{4}} e^{-\frac{1}{h}f(z_1)}\big) \\ &= O\big(e^{-\frac{1}{h}(2f(z_1)-f(x_1)+\frac{c}{2})}\big) + O\big(h^{\frac{d-6}{4}} e^{-\frac{1}{h}(2f(z_1)-f(x_1))}\, \sqrt{\varepsilon_h}\big),\end{aligned}$$

where the constant $c > 0$ is independent of h and ε_h satisfies (C.215). This proves the second part of Proposition C.30.

Assume lastly that $\overline{\Sigma} \cap \{z_1, \dots, z_{k_1^{\partial C_1}}\} = \{z_i\}$, that F is C^∞ in a neighborhood of z_i, and that $z_i \in \Sigma$. One then deduces from (C.223), Corollary C.35, Proposition C.36 that in the limit $h \to 0$, it holds for some $c > 0$ and ε_h with the form above,

$$\begin{aligned}\int_\Sigma F\, \partial_n u_h\, e^{-\frac{2}{h}f} &= \langle \nabla u_h, \psi_i \rangle_{L^2_w} \int_\Sigma F\, \psi_i \cdot n\; e^{-\frac{2}{h}f} + O\big(h^{\frac{d-6}{4}} e^{-\frac{1}{h}(2f(z_1)-f(x_1))} \sqrt{\varepsilon_h}\big) \\ &= -B_i\, C_{i,1}\; h^{\frac{d-6}{4}}\; e^{-\frac{1}{h}(2f(z_1)-f(x_1))}\; \big(F(z_i) + O(\sqrt{\varepsilon_h}) + O(h)\big),\end{aligned}$$

where the constants B_i and $C_{i,1}$ are defined in (C.129)–(C.120). This concludes the proof of the third part of Proposition C.30 and then Proposition C.30 is proved. ∎

C.3.3 Proof of Theorem C.3

Theorem C.3 is an extension of Corollary C.6 to deterministic initial conditions $x \in C_1$. To prove Theorem C.3, one first proves that a sufficiently accurate leveling property (as introduced in [4]) holds in C_1 for $x \mapsto \mathbb{E}_x[F(X_{\tau_\Omega})]$, see Proposition C.37 in Section C.3.3.1. Then, combining Corollary C.6 with Proposition C.37, one proves Theorem C.3 in Section C.3.3.2.

C.3.3.1 Leveling results

The leveling property for $x \mapsto \mathbb{E}_x[F(X_{\tau_\Omega})]$ is defined as follows.

Definition C.11. *Let K be a compact subset of Ω and $F \in C^\infty(\partial\Omega, \mathbb{R})$. We say that $x \mapsto \mathbb{E}_x[F(X_{\tau_\Omega})]$ satisfies a leveling property on K if uniformly with respect to $(x, y) \in K \times K$,*

$$\big|\, \mathbb{E}^x\left[F\left(X_{\tau_\Omega}\right)\right] - \mathbb{E}^y\left[F\left(X_{\tau_\Omega}\right)\right] \,\big| = o_{K,F}(1). \tag{C.224}$$

The leveling property (C.224) has been widely studied in the literature in various geometrical settings and we refer for example to [4,6,8,11,18,26]. In [6], the authors deal with the reversible case whereas [4,8,11,18,26] deal with the non reversible case. When there is only one attractor of the dynamics $\dot{x} = -\nabla f(x)$ in Ω one can refer to [4,18,26] and for a generalization with several attractors in Ω one can refer to [8]. We prove the following proposition which is a leveling property in our framework.

Proposition C.37. *Let us assume that the assumption **[H-Morse]** holds and let us assume that the set $\{f < \min_{\partial\Omega} f\}$ is not empty. Then, for any path-connected compact set $K \subset \{f < \min_{\partial\Omega} f\}$ and for any $F \in C^\infty(\partial\Omega, \mathbb{R})$, there exists $c > 0$, such that for all $(x, y) \in K \times K$,*

$$|\, \mathbb{E}^x\left[F\left(X_{\tau_\Omega}\right)\right] - \mathbb{E}^y\left[F\left(X_{\tau_\Omega}\right)\right] \,| \le C e^{-\frac{c}{h}}.$$

Proof. The proof is inspired from techniques used in [6]. The proof of Proposition C.37 is divided into two steps. Before starting the proof, let us recall the following elliptic regularity estimate which will be used several times in the proof of Proposition C.37. For $g \in L^2(\Omega)$, let $u \in H^1(\Omega)$ be the weak solution of the elliptic boundary value problem

$$\begin{cases} \Delta u = g \text{ on } \Omega \\ \quad u = 0 \text{ on } \partial\Omega. \end{cases}$$

Let $m \geq 0$ and assume that $g \in H^m(\Omega)$, then $u \in H^{m+2}(\Omega)$ and there exists $C > 0$ which depends only on Ω and m such that

$$\|u\|_{H^{m+2}(\Omega)} \leq C\|g\|_{H^m(\Omega)}. \tag{C.225}$$

The proof of (C.225) can be found for instance in [9, Theorem 5, Section 6.3]. In the following $C > 0$ is a constant which can change from one occurrence to another and which does not depend on h.

Step 1. Let $F \in C^\infty(\partial\Omega, \mathbb{R})$. Let us denote by $v_h \in H^1(\Omega)$ the unique weak solution to the elliptic boundary value problem

$$\begin{cases} \dfrac{h}{2}\,\Delta v_h - \nabla f \cdot \nabla v_h = 0 \text{ on } \Omega \\ \qquad\qquad\qquad\qquad v_h = F \text{ on } \partial\Omega. \end{cases} \tag{C.226}$$

Then, v_h belongs to $C^\infty(\overline{\Omega}, \mathbb{R})$ and for all $k \in \mathbb{N}$, there exist $C > 0$, $n \in \mathbb{N}$ and $h_0 > 0$ such that for all $h \in (0, h_0)$, it holds

$$\|v_h\|_{H^{k+2}(\Omega)} \leq \frac{C}{h^n}\left(\|\nabla v_h\|_{L^2(\Omega)} + 1\right). \tag{C.227}$$

Moreover, the Dynkin's formula implies that

$$\forall x \in \overline{\Omega},\ v_h(x) = \mathbb{E}^x\left[F\left(X_{\tau_\Omega}\right)\right]. \tag{C.228}$$

Let us prove that v_h belongs to $C^\infty(\overline{\Omega}, \mathbb{R})$ and (C.227). Since F is C^∞, for all $k \geq 1$, the exists $\widetilde{F} \in H^k(\Omega)$ such that $\widetilde{F} = F$ on $\partial\Omega$ and $\|\widetilde{F}\|_{H^k} \leq C\|F\|_{H^{k-\frac{1}{2}}(\partial\Omega)}$. From (C.226), the function $\widetilde{v}_h = v_h - \widetilde{F} \in H^1(\Omega)$ and the weak solution to

$$\begin{cases} \Delta\widetilde{v}_h = \dfrac{2}{h}\nabla f \cdot \nabla v_h - \Delta\widetilde{F} \text{ on } \Omega \\ \quad \widetilde{v}_h = 0 \text{ on } \partial\Omega. \end{cases} \tag{C.229}$$

Thus, using (C.225), $\widetilde{v}_h \in H^2(\Omega)$ (and thus $v_h \in H^2(\Omega)$) and there exist $C > 0$ and $h_0 > 0$ such that for all $h \in (0, h_0)$

$$\|\widetilde{v}_h\|_{H^2(\Omega)} \leq C\left(\frac{1}{h}\|\nabla v_h\|_{L^2(\Omega)} + \|\widetilde{F}\|_{H^2(\Omega)}\right) \leq \frac{C}{h}\Big(\|\nabla v_h\|_{L^2(\Omega)} + \|F\|_{H^{\frac{3}{2}}(\partial\Omega)}\Big),$$

and thus

$$\|v_h\|_{H^2(\Omega)} \leq \frac{C}{h}\left(\|\nabla v_h\|_{L^2(\Omega)} + 1\right). \tag{C.230}$$

This proves (C.227) for $k = 2$. Let us prove (C.227) for $k = 3$ (the fact that v_h belongs to $C^\infty(\overline{\Omega}, \mathbb{R})$ and the inequality (C.227) are then obtained by a bootstrap argument). Since $\nabla v_h \in H^1(\Omega)$, using (C.229) and (C.225), the function $\widetilde{v}_h \in H^3(\Omega)$ (and thus $v_h \in H^3(\Omega)$) and there exist $C > 0$ and $h_0 > 0$ such that for all $h \in (0, h_0)$

$$\|\widetilde{v}_h\|_{H^3(\Omega)} \leq C\left(\frac{1}{h}\|\nabla v_h\|_{H^1(\Omega)} + \|\widetilde{F}\|_{H^3(\Omega)}\right) \leq \frac{C}{h}\Big(\|v_h\|_{H^2(\Omega)} + \|F\|_{H^{\frac{5}{2}}(\partial\Omega)}\Big),$$

and thus, using (C.230), it holds

$$\|v_h\|_{H^3(\Omega)} \leq \frac{C}{h^2}\left(\|\nabla v_h\|_{L^2(\Omega)} + 1\right).$$

Let us now prove that there exist $\alpha > 0$ and $C > 0$ such that

$$\|v_h\|_{L^\infty(\Omega)} + \|\nabla v_h\|_{L^\infty(\Omega)} \leq C h^{-\alpha}. \tag{C.231}$$

Notice that from (C.228), one has that for all $h > 0$, $\|v_h\|_{L^\infty(\Omega)} \leq \|F\|_{L^\infty(\partial\Omega)}$. From (C.226) and (C.227) there exists $C > 0$ such that for any $\varepsilon > 0$ and $\varepsilon' > 0$,

$$\begin{aligned}
h\int_\Omega |\nabla v_h|^2 &\leq C\left(h\int_{\partial\Omega} |F\,\partial_n v_h|\,d\sigma + \int_\Omega |\nabla f\cdot\nabla v_h|\right)\\
&\leq C\left(h\frac{\|F\|^2_{L^2(\partial\Omega)}}{4\varepsilon} + h\,\varepsilon\,\|v_h\|^2_{H^2(\Omega)} + \frac{\|\nabla f\|^2_{L^2(\Omega)}}{4\varepsilon'} + \varepsilon'\,\|\nabla v_h\|^2_{L^2(\Omega)}\right)\\
&\leq C\left(h\frac{\|F\|^2_{L^2(\partial\Omega)}}{4\varepsilon} + h\,\varepsilon\,C_1\left(h^{-2}\|\nabla v_h\|^2_{L^2(\Omega)} + 1\right) + \frac{\|\nabla f\|^2_{L^2(\Omega)}}{4\varepsilon'} + \varepsilon'\,\|\nabla v_h\|^2_{L^2(\Omega)}\right).
\end{aligned}$$

Choosing $\varepsilon = \frac{h^2}{4(CC_1+1)}$ and $\varepsilon' = \frac{h}{4(C+1)}$ we get

$$\|\nabla v_h\|_{L^2(\Omega)} \leq \frac{C}{h}.$$

Therefore, using (C.227), one obtains that for all $k \geq 0$, there exist $C > 0$, $n \in \mathbb{N}$ and $h_0 > 0$ such that for all $h \in (0, h_0)$

$$\|v_h\|_{H^k(\Omega)} \leq \frac{C}{h^n}.$$

Let $k \geq 0$ such that $k - \frac{d}{2} > 1$. Then, one obtains (C.231) from the continuous Sobolev injection $H^k(\Omega) \subset W^{1,\infty}(\Omega)$.

Step 2. Let us assume that the assumption **[H-Morse]** holds and let us assume in addition that $\{f < \min_{\partial\Omega} f\}$ is not empty. To prove Proposition C.37, we will prove that for any compact K of $\{f < \min_{\partial\Omega} f\}$, there exists $c_K > 0$ such that

$$\|\nabla v_h\|_{L^\infty(K)} \leq C\,e^{-\frac{c_K}{h}}. \tag{C.232}$$

Indeed, if in addition K is path-connected, one can make use of the following inequality

$$\forall (x,y) \in K\times K,\ |v_h(x) - v_h(y)| \leq C_K\|\nabla v_h\|_{L^\infty(K)},$$

where $C_K > 0$ depends on K. Let us now define the set O_r by

$$O_r = \{f < \min_{\partial\Omega} f - r\},$$

which is not empty (by assumption) and C^∞ for all $r \in (0, r_1)$, for some $r_1 > 0$. Indeed, the boundary of O_r is included in the set $\{f = \min_{\partial\Omega} f - r\}$ which contains no critical points of f for $r > 0$ small enough (since they are in finite number under the assumption

[**H-Morse**]). We are going to prove that for all $r_0 \in (0, r_1)$ there exists $\alpha_0 > 0$ such that

$$\|\nabla v_h\|_{L^\infty(O_{r_0})} \leq e^{-\frac{\alpha_0}{h}}. \tag{C.233}$$

Let r such that $2^n r = r_0$ where $n \in \mathbb{N}$ will be fixed later (since $r < r_0$, $r \in (0, r_1)$ and thus O_r is nonempty). Equation (C.226) rewrites

$$\begin{cases} \operatorname{div}\left(e^{-\frac{2}{h}f}\nabla v_h\right) = 0 \text{ on } \Omega \\ \qquad\qquad\qquad v_h = F \text{ on } \partial\Omega. \end{cases}$$

Using (C.231), there exist $C > 0$ and $\gamma > 0$ such that,

$$\left| \int_{O_{r/2}} |\nabla v_h|^2 \, e^{-\frac{2}{h}f} \right| = \left| \int_{\partial O_{r/2}} e^{-\frac{2}{h}f} v_h \, \partial_n v_h \, d\sigma \right| \leq \frac{C}{h^\gamma} \, e^{-\frac{2}{h}(\min_{\partial\Omega} f - \frac{r}{2})},$$

where we used the Green formula (valid since O_r is C^∞) and the equality $\partial O_{r/2} = \{f = \min_{\partial\Omega} f - \frac{r}{2}\}$. In addition, since $O_r \subset O_{r/2}$ it holds,

$$e^{-\frac{2}{h}(\min_{\partial\Omega} f - r)} \int_{O_r} |\nabla v_h|^2 \leq \int_{O_r} |\nabla v_h|^2 \, e^{-\frac{2}{h}f} \leq \int_{O_{r/2}} |\nabla v_h|^2 \, e^{-\frac{2}{h}f} \leq \frac{C}{h^\gamma} \, e^{-\frac{2}{h}(\min_{\partial\Omega} f - \frac{r}{2})}.$$

Therefore there exists $\beta > 0$ such that for h small enough,

$$\int_{O_r} |\nabla v_h|^2 \leq \frac{C}{h^\gamma} \, e^{-\frac{r}{h}} \leq C \, e^{-\frac{\beta}{h}},$$

and from (C.226), we have $\|\Delta v_h\|_{L^2(O_r)} \leq C \, e^{-\frac{\beta}{h}}$ for some constant $\beta > 0$ have been reduced. In the following, $\beta > 0$ is a constant which may change from one occurrence to another and does not depend on h. Let $\chi_1 \in C_c^\infty(O_r)$ be such that $\chi_1 \equiv 1$ on O_{2r}. Since $\Delta(\chi_1 v_h) = \chi_1 \, \Delta v_h + v_h \, \Delta\chi_1 + 2\nabla\chi_1 \cdot \nabla v_h$, there exists C, such that $\|\Delta(\chi_1 v_h)\|_{L^2(O_r)} \leq C$ for h small enough. By elliptic regularity (see (C.225) for $k = 2$ there) it comes

$$\|v_h\|_{H^2(O_{2r})} \leq C.$$

Let $\alpha \in (0, 1)$ and take $p_1 = \frac{2d}{d-2\alpha}$. From the Gagliardo-Nirenberg interpolation inequality (see [25, Lecture II]), the following inequality holds

$$\|\nabla v_h\|_{L^{p_1}(O_{2r})} \leq C \|v_h\|^\alpha_{H^2(O_{2r})} \|\nabla v_h\|^{1-\alpha}_{L^2(O_{2r})} \leq C \, e^{-\frac{\beta}{h}}.$$

Then it comes from (C.226), $\|\Delta v_h\|_{L^{p_1}(O_{2r})} \leq C \, e^{-\frac{\beta}{h}}$. Using a cutoff function $\chi_2 \in C_c^\infty(O_{2r})$ such that $\chi_2 \equiv 1$ on O_{4r}, we get, as previously, from the elliptic regularity $\|v_h\|_{W^{2,p_1}(O_{4r})} \leq C$. Let $p_2 = \frac{2d}{d-4\alpha}$ (i.e. $1/p_2 = 1/p_1 - \alpha/d$), from the Gagliardo-Nirenberg interpolation inequality (see [25, Lecture II]), we get

$$\|\nabla v_h\|_{L^{p_2}(O_{4r})} \leq C \|v_h\|^\alpha_{W^{2,p_1}(O_{4r})} \|\nabla v_h\|^{1-\alpha}_{L^{p_1}(O_{2r})} \leq C \, e^{-\frac{\beta}{h}}.$$

We repeat this procedure n times such that $d - 2n\alpha \leq 0$, the Galgliardo-Nirenberg interpolation inequality implies that $\|\nabla v_h\|_{L^\infty(O_{2^n r})} \leq C \, e^{-\frac{\beta}{h}}$ which ends the proof of (C.233). Since for any compact K of $\{f < \min_{\partial\Omega} f\}$, there exists $r_0 \in (0, r_1)$ such that $K \subset \{f < \min_{\partial\Omega} f - r_0\}$, the inequality (C.232) is proved. This concludes the proof of Proposition C.37. ∎

C.3.3.2 Proof of Theorem C.3

To prove Theorem C.3, the following lemma will be needed.

Lemma C.38. *Assume that **[H-Connexity]** and **[H-Morse]** hold. Let us recall that according to Definition C.2, C_1 is the connected component of $\{f < \min_{\partial\Omega} f\}$ which contains all the global minima of f in Ω. For $\alpha > 0$, let $C_1(\alpha)$ be as defined in item 3 in Lemma C.9 (see* (C.44)*): $C_1(\alpha) = C_1 \cap \{f < \min_{\partial\Omega} f - \alpha\} \subset C_1$. Let $F \in C^\infty(\partial\Omega, \mathbb{R})$. Then, $\exists \alpha_0 > 0$, $\forall \alpha \in (0, \alpha_0)$, $\exists c > 0$, $\forall y \in \overline{C_1(\alpha)}$:*

$$\mathbb{E}^{\nu_h}\left[F\left(X_{\tau_\Omega}\right)\right] = \mathbb{E}^{y}\left[F\left(X_{\tau_\Omega}\right)\right] + O\left(e^{-\frac{c}{h}}\right)$$

in the limit $h \to 0$ and uniformly in $y \in \overline{C_1(\alpha)}$.

Proof. Let us define for $x \in \overline{\Omega}$:

$$g_h(x) := \mathbb{E}^{x}\left[F\left(X_{\tau_\Omega}\right)\right].$$

From (C.8), one has:

$$\begin{aligned}\mathbb{E}^{\nu_h}\left[F\left(X_{\tau_\Omega}\right)\right] &= \left(\int_\Omega u_h\, e^{-\frac{2}{h}f}\right)^{-1} \int_\Omega g_h\, u_h\, e^{-\frac{2}{h}f} \\ &= \frac{1}{Z_h(\Omega)} \int_{\Omega\setminus\{f\le \min_{\partial\Omega} f-\alpha\}} g_h\, u_h\, e^{-\frac{2}{h}f} + \frac{1}{Z_h(\Omega)} \int_{\{f\le \min_{\partial\Omega} f-\alpha\}} g_h\, u_h\, e^{-\frac{2}{h}f},\end{aligned} \tag{C.234}$$

where $Z_h(\Omega) := \int_\Omega u_h\ e^{-\frac{2}{h}f}$ and u_h is the eigenfunction associated with the smallest eigenvalue λ_h of $-L_{f,h}^{D,(0)}$ (see (C.5)) which satisfies (C.6). Let us assume that hypothesis **[H-Connexity]** and **[H-Morse]** hold. Let us first deal with the first term of (C.234). From (C.25), there exists $C > 0$ such that for small h, one has:

$$Z_h(\Omega)^{-1} \le C h^{-\frac{d}{4}} e^{\frac{1}{h}\min\limits_{\Omega} f}.$$

Since $\|g_h\|_{L^\infty(\overline{\Omega})} \le \|F\|_{L^\infty(\partial\Omega)}$, from the Cauchy-Schwarz inequality, for any $\alpha > 0$ one has for h small enough:

$$\begin{aligned}\frac{1}{Z_h(\Omega)}\left|\int_{\Omega\setminus\{f\le \min_{\partial\Omega} f-\alpha\}} g_h\, u_h\, e^{-\frac{2}{h}f}\right| &\le C\, h^{-\frac{d}{4}} e^{-\frac{1}{h}(\min_{\Omega\setminus\{f\le \min_{\partial\Omega} f-\alpha\}} f - \min\limits_{\Omega} f)} \\ &\le C\, h^{-\frac{d}{4}} e^{-\frac{1}{h}(\min_{\partial\Omega} f - \min_{\Omega} f - \alpha)}\end{aligned}$$

Since $\min_{\partial\Omega} f - \min\limits_{\Omega} f > 0$, $\exists c > 0$, $\exists \alpha_0 > 0$, $\forall \alpha \in (0, \alpha_0)$,

$$\frac{1}{Z_h(\Omega)}\left|\int_{\Omega\setminus\{f\le \min_{\partial\Omega} f-\alpha\}} g_h\, u_h\, e^{-\frac{2}{h}f}\right| \le C\, e^{-\frac{c}{h}} \tag{C.235}$$

for all h small enough. Let us now deal with the second term of (C.234). For $k \in \{2, ...N_1\}$ and $\alpha > 0$ small enough, let $C_k(\alpha)$ be as defined in (C.44):

$$C_j(\alpha) = C_j \cap \{f < \min_{\partial\Omega} f - \alpha\}.$$

Using the second equality in (C.45) together with the fact that the sets $(\overline{C_k(\alpha)})_{k=1,\dots,N_1}$ are disjoint, one has:

$$\frac{1}{Z_h(\Omega)}\int_{\{f\le \min_{\partial\Omega} f-\alpha\}} g_h\, u_h\, e^{-\frac{2}{h}f} = \frac{1}{Z_h(\Omega)}\int_{\overline{C_1(\alpha)}} g_h\, u_h\, e^{-\frac{2}{h}f} + \sum_{k=2}^{N_1}\frac{1}{Z_h(\Omega)}\int_{\overline{C_k(\alpha)}} g_h\, u_h\, e^{-\frac{2}{h}f}. \tag{C.236}$$

Let us recall that under hypothesis [**H-Connexity**], it holds for $k\in\{2,...,N_1\}$, $\inf_{C_k} f > \min_\Omega f$. Therefore, for $k\in\{2,...,N_1\}$, since $\overline{C_k(\alpha)}\subset C_k$, one has for h small enough:

$$\frac{1}{Z_h(\Omega)}\Big|\int_{\overline{C_k(\alpha)}} g_h\, u_h\, e^{-\frac{2}{h}f}\Big| \le C\, h^{-\frac{d}{4}} e^{-\frac{1}{h}(\inf_{C_k} f-\min_\Omega f)} \le Ce^{-\frac{c}{h}}, \tag{C.237}$$

for some $c>0$ independent of h. For $\alpha\in(0,\alpha_0)$ ($\alpha_0>0$ small enough), from item 3 in Lemma C.9, the compact set $\overline{C_1(\alpha)}$ is connected and $\overline{C_1(\alpha)}\subset C_1$. Therefore, from Proposition C.37 applied with $K=\overline{C_1(\alpha)}$ for $\alpha\in(0,\alpha_0)$: there exists $\delta_\alpha>0$ such that for all $y\in\overline{C_1(\alpha)}$,

$$\frac{1}{Z_h(\Omega)}\int_{\overline{C_1(\alpha)}} g_h\, u_h\, e^{-\frac{2}{h}f} = \frac{g_h(y)}{Z_h(\Omega)}\int_{\overline{C_1(\alpha)}} u_h\, e^{-\frac{2}{h}f} + \frac{O\big(e^{-\frac{\delta_\alpha}{h}}\big)}{Z_h(\Omega)}\int_{\overline{C_1(\alpha)}} u_h\, e^{-\frac{2}{h}f} \tag{C.238}$$

in the limit $h\to 0$ and uniformly in $y\in\overline{C_1(\alpha)}$. Moreover, there exist $c>0$, and $\alpha_0>0$ such that for any $\alpha\in(0,\alpha_0)$, in the limit $h\to 0$:

$$\frac{1}{Z_h(\Omega)}\int_{\overline{C_1(\alpha)}} u_h\, e^{-\frac{2}{h}f} = 1+O\left(e^{-\frac{c}{h}}\right). \tag{C.239}$$

Let us prove (C.239). One has:

$$\frac{1}{Z_h(\Omega)}\int_{\overline{C_1(\alpha)}} u_h\, e^{-\frac{2}{h}f} = 1-\frac{1}{Z_h(\Omega)}\int_{\Omega\setminus\overline{C_1(\alpha)}} u_h\, e^{-\frac{2}{h}f}.$$

In addition, there exists $C>0$ such that for any $\alpha>0$ small enough, and for h small enough:

$$\frac{1}{Z_h(\Omega)}\int_{\Omega\setminus\overline{C_1(\alpha)}} u_h\, e^{-\frac{2}{h}f} \le \frac{1}{Z_h(\Omega)}\int_{\Omega\setminus\overline{C_1(\alpha)}} e^{-\frac{2}{h}f} \le C\, h^{-\frac{d}{4}}\, e^{-\frac{1}{h}(\inf_{\Omega\setminus\overline{C_1(\alpha)}} f-\min_\Omega f)}$$

The set $\arg\min_{\overline{\Omega}} f$ is finite (since [**H-Morse**] holds) and is included in C_1 (since [**H-Connexity**] holds): it is thus included in $\overline{C_1(\alpha)}$ for any $\alpha>0$ small enough. This implies that there exists $\alpha_0>0$ such that for any $\alpha\in(0,\alpha_0)$ it holds $\inf_{\Omega\setminus\overline{C_1(\alpha)}} f > \min_\Omega f$. Therefore, $\exists c>0$, $\exists\alpha_0>0$, $\forall\alpha\in(0,\alpha_0)$, $\exists h_0>0$, $\forall h\in(0,h_0)$:

$$\frac{1}{Z_h(\Omega)}\int_{\Omega\setminus\overline{C_1(\alpha)}} u_h\, e^{-\frac{2}{h}f} = O\left(e^{-\frac{c}{h}}\right).$$

This concludes the proof of (C.239).
Let us now fix $\alpha\in(0,\alpha_0)$. Then, using (C.238) and (C.239), $\exists c>0$, $\exists\delta_\alpha>0$, $\forall y\in\overline{C_1(\alpha)}$:

$$\frac{1}{Z_h(\Omega)}\int_{\overline{C_1(\alpha)}} g_h\, u_h\, e^{-\frac{2}{h}f} = g_h(y)\left(1+O\left(e^{-\frac{c}{h}}\right)\right)+O\left(e^{-\frac{\delta_\alpha}{h}}\right) \tag{C.240}$$

in the limit $h \to 0$ and uniformly in $y \in \overline{C_1(\alpha)}$. Therefore, using (C.234)-(C.235)-(C.236)-(C.237)-(C.240), $\exists \alpha_0 > 0$, $\forall \alpha \in (0, \alpha_0)$, $\exists c > 0$, $\forall y \in \overline{C_1(\alpha)}$:

$$\mathbb{E}^{\nu_h}\left[F\left(X_{\tau_\Omega}\right)\right] = \mathbb{E}^{y}\left[F\left(X_{\tau_\Omega}\right)\right] + O\left(e^{-\frac{c}{h}}\right), \tag{C.241}$$

in the limit $h \to 0$ and uniformly in $y \in \overline{C_1(\alpha)}$. This concludes the proof of Lemma C.38. ∎

Let us now end the proof of Theorem C.3. Let us notice that it is sufficient to prove (C.30)-(C.31)-(C.32) when replacing in the statement the compact set $K \subset C_1$ by $\overline{C_1(\alpha)}$ for $\alpha > 0$. Indeed, for any compact set K of C_1 there exists $\alpha > 0$ such that $K \subset \overline{C_1(\alpha)}$. Let us notice that the proof is not a direct consequence of Lemma C.38 since in Theorem C.3, less regular test functions F are considered. The proof of Theorem C.3 is divided into two steps. In the following we assume that the hypothesises **[H-Connexity]** and **[H-Morse]** are satisfied.

Step 1. Proof of (C.30) and (C.31).

Let us first show that if $\Sigma \subset \partial\Omega$ is open and there exists $\beta > 0$ such that $\Sigma \cap \bigcup_{i=1}^{k_1^{\partial\Omega}} B^{\partial\Omega}(z_i, \beta) = \emptyset$ (where $B^{\partial\Omega}(z_i, \beta)$ is the open ball in $\partial\Omega$ of radius β centered at z_i), then, $\exists \alpha_0 > 0$, $\forall \alpha \in (0, \alpha_0)$, $\exists c > 0$, $\forall y \in \overline{C_1(\alpha)}$:

$$\mathbb{P}^{y}\left[X_{\tau_\Omega} \in \Sigma\right] = O\left(e^{-\frac{c}{h}}\right) \tag{C.242}$$

in the limit $h \to 0$ and uniformly in $y \in \overline{C_1(\alpha)}$. Indeed, let $\tilde{F} \in C^\infty(\partial\Omega, [0,1])$ be such that

$$\tilde{F} = 1 \text{ on } \Sigma \quad \text{and} \quad \tilde{F} = 0 \text{ on } \bigcup_{i=1}^{k_1^{\partial\Omega}} B^{\partial\Omega}(z_i, \frac{\beta}{2}).$$

Using Lemma C.38, $\exists \alpha_0 > 0$, $\forall \alpha \in (0, \alpha_0)$, $\exists c > 0$, $\forall y \in \overline{C_1(\alpha)}$:

$$\mathbb{P}^{y}\left[X_{\tau_\Omega} \in \Sigma\right] \leq \mathbb{E}^{y}\left[F(X_{\tau_\Omega})\right] \leq \mathbb{E}^{\nu_h}\left[F(X_{\tau_\Omega})\right] + O\left(e^{-\frac{c}{h}}\right)$$

in the limit $h \to 0$ and uniformly in $y \in \overline{C_1(\alpha)}$. Then, (C.242) follows from (C.26) applied with $\tilde{F}$ and the family of sets $\Sigma_i = B^{\partial\Omega}(z_i, \frac{\beta}{2})$ for $i \in \{1, ..., k_1^{\partial\Omega}\}$.

Let us now prove (C.30) and (C.31). Let $F \in L^\infty(\partial\Omega, \mathbb{R})$ and for all $i \in \{1, \ldots, k_1^{\partial\Omega}\}$, let $\Sigma_i \subset \partial\Omega$ be an open set which contains z_i. Let us assume in addition that $\Sigma_i \cap \Sigma_j = \emptyset$ if $i \neq j$. One has for any $y \in \overline{C_1(\alpha)}$:

$$\mathbb{E}^{y}\left[F(X_{\tau_\Omega})\right] = \sum_{i=1}^{k_1^{\partial\Omega}} \mathbb{E}^{y}\left[\mathbf{1}_{\Sigma_i} F\left(X_{\tau_\Omega}\right)\right] + \mathbb{E}^{y}\Big[\mathbf{1}_{\partial\Omega \setminus \bigcup_{i=1}^{k_1^{\partial\Omega}} \Sigma_i} F\left(X_{\tau_\Omega}\right)\Big].$$

Moreover, one has:

$$\Big|\mathbb{E}^{y}\Big[\mathbf{1}_{\partial\Omega \setminus \bigcup_{i=1}^{k_1^{\partial\Omega}} \Sigma_i} F\left(X_{\tau_\Omega}\right)\Big]\Big| \leq \|F\|_{L^\infty}\, \mathbb{P}^{y}\Big[X_{\tau_\Omega} \in \partial\Omega \setminus \bigcup_{i=1}^{k_1^{\partial\Omega}} \Sigma_i\Big].$$

Using (C.242) with $\Sigma = \partial\Omega \setminus \bigcup_{i=1}^{k_1^{\partial\Omega}} \Sigma_i$, one gets (C.30).

Let us now prove (C.31). Let $j \in \{k_1^{\partial C_1}+1, ..., k_1^{\partial\Omega}\}$. Let $\delta > 0$ be such that for any $k \in \{1, ..., k_1^{\partial\Omega}\}$ with $k \neq j$, the sets $\Sigma_k \cap B^{\partial\Omega}(z_k, \delta)$ and $\Sigma_j + B^{\partial\Omega}(z_j, \delta)$ are disjoint. Let $G \in C_c^\infty(\Sigma_j + B^{\partial\Omega}(z_j, \delta), [0,1])$ be such that $G = 1$ on Σ_j. Using Lemma C.38, $\exists \alpha_0 > 0$, $\forall \alpha \in (0, \alpha_0)$, $\exists c > 0$, $\forall y \in \overline{C_1(\alpha)}$:

$$\begin{aligned}|\mathbb{E}^y\left[\mathbf{1}_{\Sigma_j} F(X_{\tau_\Omega})\right]| \leq \|F\|_{L^\infty}\, \mathbb{P}^y[X_{\tau_\Omega} \in \Sigma_j] &\leq \|F\|_{L^\infty}\, \mathbb{E}^y\left[G(X_{\tau_\Omega})\right] \\ &= O(\mathbb{E}^{\nu_h}\left[G(X_{\tau_\Omega})\right]) + O(e^{-\frac{c}{h}})\end{aligned}$$

in the limit $h \to 0$ and uniformly in $y \in \overline{C_1(\alpha)}$. Then, using (C.27) with G, it holds when $h \to 0$: $\mathbb{E}^y\left[\mathbf{1}_{\Sigma_j} F(X_{\tau_\Omega})\right] = O(h^{\frac{1}{4}})$ and when **[H-Connexity+]** holds, one has when $h \to 0$:

$$\mathbb{E}^y\left[\mathbf{1}_{\Sigma_j} F(X_{\tau_\Omega})\right] = O(e^{-\frac{c}{h}}),$$

for some $c > 0$ depending on α. This concludes the proof of (C.31).

Step 2. Proof of (C.32).

For all $j \in \{1, \ldots, k_1^{\partial\Omega}\}$, let Σ_j be open subset of $\partial\Omega$ such that $z_j \in \Sigma_j$. Let us assume that $\Sigma_k \cap \Sigma_j = \emptyset$ if $k \neq j$. Let $F \in L^\infty(\partial\Omega, \mathbb{R})$ be C^∞ in a neighborhood of z_i for some $i \in \{1, \ldots, k_1^{\partial C_1}\}$. Let $\beta > 0$ be such that F is C^∞ on $B^{\partial\Omega}(z_i, 2\beta) \subset \Sigma_i$ and let $\chi_i \in C^\infty(\partial\Omega, [0,1])$ be such that $\operatorname{supp}\chi_i \subset B^{\partial\Omega}(z_i, \beta)$, $\chi_i = 1$ on $B^{\partial\Omega}(z_i, \frac{\beta}{2})$. One has:

$$\mathbb{E}^y\left[\mathbf{1}_{\Sigma_i} F(X_{\tau_\Omega})\right] = \mathbb{E}^y\left[\chi_i F(X_{\tau_\Omega})\right] + \mathbb{E}^y\left[(\mathbf{1}_{\Sigma_i} - \chi_i) F(X_{\tau_\Omega})\right].$$

Using Lemma C.38 with $\chi_i F$ and (C.26)-(C.28) with $F\chi_i$ and $\{\Sigma_j, j = 1, ..., k_1^{\partial\Omega}, j \neq i\} \cup \{B^{\partial\Omega}(z_i, \frac{\beta}{2})\}$, $\exists \alpha_0 > 0$, $\forall \alpha \in (0, \alpha_0)$, $\exists c > 0$, $\forall y \in \overline{C_1(\alpha)}$:

$$\begin{aligned}\mathbb{E}^y\left[\chi_i F(X_{\tau_\Omega})\right] &= \mathbb{E}^{\nu_h}\left[\chi_i F(X_{\tau_\Omega})\right] + O\left(e^{-\frac{c}{h}}\right) \\ &= \mathbb{E}^{\nu_h}\left[\mathbf{1}_{B^{\partial\Omega}(z_i, \frac{\beta}{2})} F(X_{\tau_\Omega})\right] + O\left(e^{-\frac{c}{h}}\right) = F(z_i)\, a_i + O(h^{\frac{1}{4}})\end{aligned}$$

in the limit $h \to 0$ and uniformly in $y \in \overline{C_1(\alpha)}$, and where a_i is defined in (C.29). In addition, using Corollary C.6, when **[H-Connexity+]** holds, one can replace $O(h^{\frac{1}{4}})$ in the last computation by $O(h)$. Moreover, using (C.242) with $\Sigma = \Sigma_i \setminus B^{\partial\Omega}(z_i, \frac{\beta}{2})$: $\exists \alpha_0 > 0$, $\forall \alpha \in (0, \alpha_0)$, $\exists c > 0$, $\forall y \in \overline{C_1(\alpha)}$:

$$|\mathbb{E}^y\left[(\mathbf{1}_{\Sigma_i} - \chi_i) F(X_{\tau_\Omega})\right]| \leq \|F\|_{L^\infty}\, \mathbb{P}^y\left[X_{\tau_\Omega} \in \Sigma_i \setminus B^{\partial\Omega}(z_i, \frac{\beta}{2})\right] = O\left(e^{-\frac{c}{h}}\right)$$

in the limit $h \to 0$ and uniformly in $y \in \overline{C_1(\alpha)}$. Thus, one has when $h \to 0$ and uniformly with respect to $y \in \overline{C_1(\alpha)}$:

$$\mathbb{E}^y\left[\mathbf{1}_{\Sigma_i} F(X_{\tau_\Omega})\right] = F(z_i)\, a_i + O(h^{\frac{1}{4}})$$

and when **[H-Connexity+]** holds, one has:

$$\mathbb{E}^y\left[\mathbf{1}_{\Sigma_i} F(X_{\tau_\Omega})\right] = F(z_i)\, a_i + O(h).$$

This concludes the proof of Theorem C.3.

C.4 Optimality of the remainder terms and generalization of the results of Section C.1.4

This section is organized as follows. In Section C.4.1, the assumption [**H-Boundary**] is discussed and we show that the metastability of Ω depends on the initial distribution of the process (C.1). Then, in Section C.4.2, we discuss the optimality of the remainder terms appearing in Theorem C.1, Theorem C.2, Corollary C.6 and Theorem C.3 under the assumption [**H-connexity**]. Finally, in Section C.4.3, we generalized the results stated in Section C.1.4.

C.4.1 Assumption [H-Boundary] and Metastability

C.4.1.1 On the assumption [H-Boundary]

In this section we would like to discuss the necessity of the assumption [**H-Boundary**] in the results of Section C.1.4. More precisely, in the statement of Theorems C.1, C.2, C.3, and of Corollary C.6, it is assumed that the closure of each connected component of $\{f < \min_{\partial\Omega} f\}$ intersects $\partial\Omega$. We would like to exhibit a case for which this assumption does not hold and for which the results of Section C.1.4 are no longer valid. To this end, let us consider a one dimensional example in which there exists a connected component C of $\{f < \min_{\partial\Omega} f\}$ such that $\partial C \cap \partial\Omega = \emptyset$ (see Figure C.9). Let $z_1 < z_2$ and $f\colon [z_1, z_2] \to \mathbb{R}$ be a C^∞ Morse function. Let us assume that $\{x \in [z_1, z_2], f'(x) = 0\} = \{x_2, c, x_1, d\}$ with $z_1 < x_2 < c < x_1 < d < z_2$ and $f(x_1) < f(x_2) < f(z_1) < f(z_2) < f(d) < f(c)$ (see Figure C.9). From [15, Theorem 1], one has in the limit $h \to 0$:

$$\lambda_h = \frac{2}{\pi}\sqrt{\frac{f''(x_1)}{|f''(d)|}}\, e^{-\frac{2}{h}(f(d)-f(x_1))}(1 + O(h)). \tag{C.243}$$

This implies that the results of Theorem C.1 is no longer valid in the one dimensional example represented in Figure C.9.
Moreover, the Dynkin's formula (see (C.226) and (C.228)) implies that the function $x \in [z_1, z_2] \mapsto \mathbb{P}^x\big[X_{\tau_{(z_1,z_2)}} = z_2\big]$ satisfies the elliptic boundary value problem:

$$\frac{h}{2}g'' - g'f' = 0 \text{ and } g(z_1) = 0,\ g(z_2) = 1.$$

Then, one obtains that for any $x \in [z_1, z_2]$:

$$\mathbb{P}^x[X_{\tau_{(z_1,z_2)}} = z_2] = \frac{\displaystyle\int_{z_1}^{x} e^{\frac{2}{h}f}}{\displaystyle\int_{z_1}^{z_2} e^{\frac{2}{h}f}},$$

and thus, one has for any $x \in [z_1, z_2]$:

$$\mathbb{P}^x[X_{\tau_{(z_1,z_2)}} = z_1] = \frac{\displaystyle\int_{x}^{z_2} e^{\frac{2}{h}f}}{\displaystyle\int_{z_1}^{z_2} e^{\frac{2}{h}f}}. \tag{C.244}$$

Using (C.244) and Laplace's method, for all $x \in (c, z_2]$ there exists $c > 0$ such that one has in the limit $h \to 0$:

$$\mathbb{P}^x[X_{\tau_{(z_1,z_2)}} = z_1] = O(e^{-\frac{c}{h}}) \text{ and thus } \mathbb{P}^x[X_{\tau_{(z_1,z_2)}} = z_2] = 1 + O(e^{-\frac{c}{h}}).$$

In addition, the same results holds starting from ν_h: there exists $c > 0$ such that in the limit $h \to 0$:

$$\mathbb{P}^{\nu_h}[X_{\tau_{(z_1,z_2)}} = z_1] = O(e^{-\frac{c}{h}}) \text{ and thus } \mathbb{P}^{\nu_h}[X_{\tau_{(z_1,z_2)}} = z_2] = 1 + O(e^{-\frac{c}{h}}). \tag{C.245}$$

Let us explain briefly how to get (C.245). One can show that there exits $\chi \in C_c^\infty((c,d),[0,1])$ such that $\chi = 1$ on a neighborhood of x_1 and:

$$u_h = \frac{\chi}{\|\chi\|_{L^2_w}}\big(1 + O(e^{-\frac{c}{h}})\big) + r, \tag{C.246}$$

where $r \in L^2_w(z_1, z_2)$ satisfies $\|r\|_{L^2_w} = O(e^{-\frac{c}{h}})$ and $c > 0$ is independent of h. This implies in particular that in the limit $h \to 0$:

$$\int_{z_1}^{z_2} u_h\, e^{-\frac{2}{h}f} = f''(x_1)^{-\frac{1}{4}}(\pi h)^{\frac{1}{4}} e^{-\frac{1}{h}f(x_1)}(1 + O(h)).$$

Moreover, if we denote by $g(x) = \mathbb{P}^x[X_{\tau_{(z_1,z_2)}} = z_1]$ for $x \in [z_1, z_2]$, since $\chi \in C_c^\infty((c,d),[0,1])$ and $\|g\|_{L^\infty} \leq 1$, one has in the limit $h \to 0$ (using (C.244) in the third equality and (C.246)):

$$\begin{aligned}
\mathbb{P}^{\nu_h}[X_{\tau_{(z_1,z_2)}} = z_1] &= \frac{1}{\displaystyle\int_{z_1}^{z_2} u_h\, e^{-\frac{2}{h}f}}\left[\int_{z_1}^{c} u_h g e^{-\frac{2}{h}f} + \int_{c}^{d} u_h g e^{-\frac{2}{h}f} + \int_{d}^{z_2} u_h g e^{-\frac{2}{h}f}\right] \\
&= \frac{1}{\displaystyle\int_{z_1}^{z_2} u_h\, e^{-\frac{2}{h}f}}\left[\int_{z_1}^{c} r g e^{-\frac{2}{h}f} + \int_{c}^{d} \frac{\chi g e^{-\frac{2}{h}f}}{\|\chi\|_{L^2_w}} + \int_{c}^{d} r g e^{-\frac{2}{h}f} + \int_{d}^{z_2} r g e^{-\frac{2}{h}f}\right] \\
&= \frac{1}{\displaystyle\int_{z_1}^{z_2} u_h\, e^{-\frac{2}{h}f}}\left[\frac{\displaystyle\int_{c}^{d} \chi(x) \int_{x}^{z_2} e^{\frac{2}{h}(f(y)-f(x))} dy dx}{\|\chi\|_{L^2_w} \displaystyle\int_{z_1}^{z_2} e^{\frac{2}{h}f}} + O(e^{-\frac{1}{h}(f(x_1)+c)})\right] \\
&= \frac{1}{\displaystyle\int_{z_1}^{z_2} u_h\, e^{-\frac{2}{h}f}}\left[\frac{O(e^{\frac{2}{h}(f(d)-f(x_1))})}{\|\chi\|_{L^2_w} \displaystyle\int_{z_1}^{z_2} e^{\frac{2}{h}f}} + O(e^{-\frac{1}{h}(f(x_1)+c)})\right] = O(e^{-\frac{c}{h}}).
\end{aligned}$$

This proves (C.245). Therefore, in the small temperature regime and starting from $x \in (c, z_2)$ or from the quasi stationary distribution, the process (C.1) leaves $\Omega = (z_1, z_2)$ through z_2 when $h \to 0$. Notice that z_2 is not the global minimum of $f_{|\partial\Omega}$ and is even not a generalized critical point of order 1. Therefore, the results of Corollary C.6 and Theorem C.3 do not hold in the one dimensional example represented in Figure C.9.

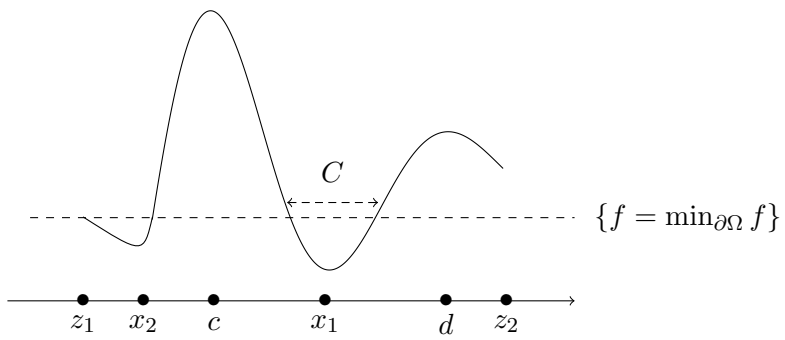

Figure C.9: A one dimensional example when there exists a connected component C of $\{f < \min_{\partial\Omega} f\}$ such that $\overline{C} \cap \partial\Omega = \emptyset$.

C.4.1.2 Metastability depends on the initial distribution

Let us recall (see Section C.1.2) that a domain Ω is metastable for the process (C.1) if the convergence to the quasi stationary distribution ν_h (see (C.3)) is much quicker than the exit from Ω. In this section, we would like to show that there exist probability distributions in Ω such that this separation of timescales does not hold when the process (C.1) starts from these distributions. To this end, let us show that for $k \in \{2, ..., N_1\}$ (where N_1 is introduced in Definition C.2), in the limit $h \to 0$, the law of X_{τ_Ω} concentrates on $\partial C_k \cap \partial\Omega$ when $X_0 = x \in C_k$ whereas the law of X_{τ_Ω} concentrates on $\partial C_1 \cap \partial\Omega$ when $X_0 \sim \nu_h$.
We will need the following assumption

- **[H-C]** The assumptions **[H-Morse]** and **[H-Connexity]** hold. In addition, for all $(\ell, k) \in \{1, ..., N_1\}^2$, $\ell \neq k$, $\overline{C_\ell} \cap \overline{C_k} = \emptyset$. Finally, for all $k \in \{2, ..., N_1\}$, there exist $\varepsilon > 0$ and a C^∞ open connected subset of Ω denoted by Ω_k^ε such that

  1. $C_k \subset \Omega_k^\varepsilon$,
  2. for all $\ell \in \{1, ..., N_1\} \setminus \{k\}$, $\overline{\Omega_k^\varepsilon} \cap \overline{C_\ell} = \emptyset$,
  3. $\partial\Omega_k^\varepsilon \cap \partial C_k = \partial\Omega \cap \partial C_k$,
  4. $\overline{B^{\partial\Omega}(z, \varepsilon)} \cap \overline{B^{\partial\Omega}(y, \varepsilon)} = \emptyset$ for all $y \neq z \in \partial\Omega \cap \partial C_k$ and
  $$\overline{\Omega_k^\varepsilon} \cap \partial\Omega = \bigcup_{z \in \partial\Omega \cap \partial C_k} \overline{B^{\partial\Omega}(z, \varepsilon)}.$$
  5. $f_{|\partial\Omega_k^\varepsilon}$ is a Morse function.

Let us recall that for $z \in \partial\Omega$, $B^{\partial\Omega}(z, \varepsilon)$ is the ball in$\partial\Omega$ centred in z and of radius ε. Moreover recall that $\partial C_k \cap \partial\Omega \subset \arg\min_{\partial\Omega} f \cap \{y \in \partial\Omega,\ \partial_n f(y) > 0\}$. In Figure C.10 is represented Ω_2^ε when $N_1 = 2$. Under **[H-Morse]** and **[H-Connexity]** and if for all $(\ell, k) \in \{1, ..., N_1\}^2$, $\ell \neq k$, $\overline{C_\ell} \cap \overline{C_k} = \emptyset$, we expect that for all $k \in \{2, ..., N_1\}$ there always exist $\varepsilon > 0$ and a C^∞ open connected subset Ω_k^ε of Ω satisfying items 1, 2, 3, 4 and 5 in **[H-C]**. For instance, this is the case in dimension 1 (see for instance Figure C.11).

For $k \in \{2, ..., N_1\}$, the following result shows that the law of X_{τ_Ω} in the limit $h \to 0$ concentrates on $\partial\Omega \cap \partial C_k$ when $X_0 = x \in C_k$.

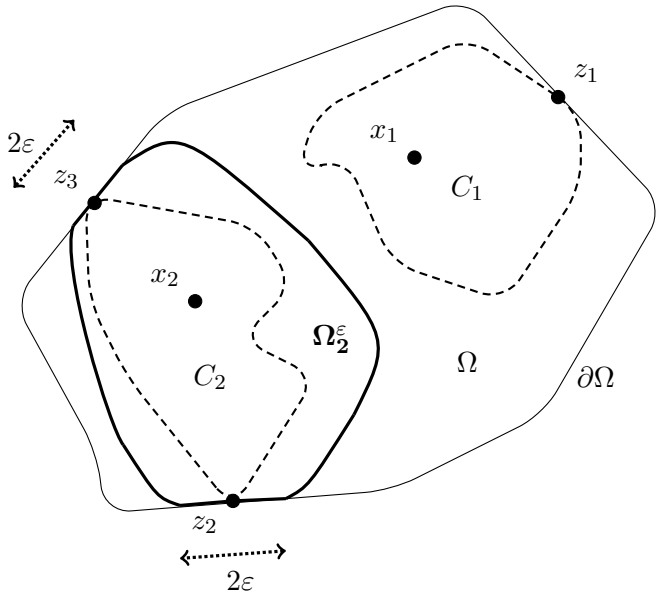

Figure C.10: Schematic representation of Ω_2^ε when $N_1 = 2$ and **[H-C]** holds. In the figure, one has $\partial C_2 \cap \partial\Omega = \{z_2, z_3\}$.

Proposition C.39. *Let us assume that the assumption **[H-C]** holds and let ε be as in **[H-C]**. Let $k \in \{2, ..., N_1\}$ and K be a compact subset of C_k. Then, for any $z \in \partial\Omega \cap \partial C_k$ and $\alpha \in (0, \varepsilon]$,*

$$\mathbb{P}^x\big[X_{\tau_\Omega} \in B^{\partial\Omega}(z, \alpha)\big] = a_z + O(h)$$

in the limit $h \to 0$ and uniformly in $x \in K$, where

$$a_z = \frac{\partial_n f(z)}{\sqrt{\det \text{ Hess} f\big|_{\partial\Omega}(z)}} \left(\sum_{y \in \partial\Omega \cap \partial C_k} \frac{\partial_n f(y)}{\sqrt{\det \text{ Hess} f\big|_{\partial\Omega}(y)}} \right)^{-1}. \tag{C.247}$$

Proof. Let us assume that the assumption **[H-C]** holds. Let $k \in \{2, ..., N_1\}$ and let us introduce

$$\tau_{\Omega_k^\varepsilon} = \inf\{t \geq 0 | X_t \notin \Omega_k^\varepsilon\}.$$

Then, from item 1 in **[H-C]** and since $\Omega_k^\varepsilon \subset \Omega$, it holds almost surely when $X_0 = x \in C_k$,

$$\tau_{\Omega_k^\varepsilon} \leq \tau_\Omega.$$

Let K be a compact subset of C_k, $z \in \partial\Omega \cap \partial C_k$ and $\alpha \in (0, \varepsilon]$. Then, for any $x \in C_k$, one has

$$\begin{aligned}
\mathbb{P}^x\big[X_{\tau_\Omega} \in B^{\partial\Omega}(z, \alpha)\big] &= \mathbb{P}^x\big[X_{\tau_\Omega} \in B^{\partial\Omega}(z, \alpha), \tau_{\Omega_k^\varepsilon} = \tau_\Omega\big] \\
&\quad + \mathbb{P}^x\big[X_{\tau_\Omega} \in B^{\partial\Omega}(z, \alpha), \tau_{\Omega_k^\varepsilon} < \tau_\Omega\big] \\
&= \mathbb{P}^x\big[X_{\tau_{\Omega_k^\varepsilon}} \in B^{\partial\Omega}(z, \alpha), \tau_{\Omega_k^\varepsilon} = \tau_\Omega\big] \\
&\quad + \mathbb{P}^x\big[X_{\tau_\Omega} \in B^{\partial\Omega}(z, \alpha), \tau_{\Omega_k^\varepsilon} < \tau_\Omega\big].
\end{aligned} \tag{C.248}$$

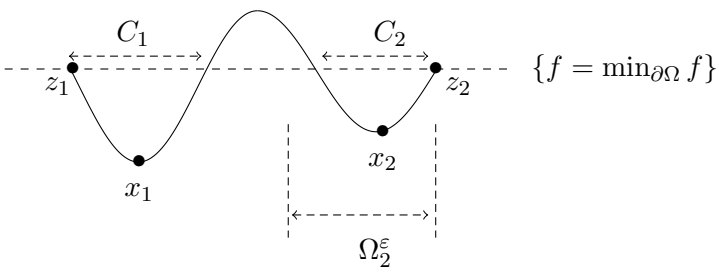

Figure C.11: A one dimensional example when **[H-C]** holds.

From item 4 in **[H-C]**, it holds

$$\tau_{\Omega_k^\varepsilon} < \tau_\Omega \Rightarrow X_{\tau_{\Omega_k^\varepsilon}} \in \partial\Omega_k^\varepsilon \setminus \partial\Omega = \partial\Omega_k^\varepsilon \setminus \bigcup_{y \in \partial\Omega \cap \partial C_k} B^{\partial\Omega}(y, \varepsilon). \tag{C.249}$$

Moreover, from items 1, 2 and 3 in **[H-C]**, one has

$$\arg\min_{\partial\Omega_k^\varepsilon} f = \partial C_k \cap \partial\Omega,$$

and then, using (C.249), item 5 in **[H-C]** and Theorem C.3 with Ω_k^ε instead of Ω (notice that from items 1, 2, 3 and 4 in **[H-C]**, $\{x \in \Omega_k^\varepsilon, f(x) < \min_{\partial\Omega_k^\varepsilon} f\} = C_k$ and thus **[H-Connexity+]** holds for Ω_k^ε), there exists $c > 0$ such that

$$\begin{aligned}\mathbb{P}^x\big[X_{\tau_\Omega} \in B^{\partial\Omega}(z, \alpha), \tau_{\Omega_k^\varepsilon} < \tau_\Omega\big] &\leq \mathbb{P}^x\Big[X_{\tau_{\Omega_k^\varepsilon}} \in \partial\Omega_k^\varepsilon \setminus \partial\Omega\Big] \\ &= O(e^{-\frac{c}{h}}),\end{aligned}$$

and

$$\mathbb{P}^x\big[X_{\tau_{\Omega_k^\varepsilon}} \in B^{\partial\Omega}(z, \alpha)\big] = a_z + O(h),$$

in the limit $h \to 0$ and uniformly in $x \in K$, where a_z is defined by (C.247). Using (C.248), one finally obtains that

$$\mathbb{P}^x\big[X_{\tau_\Omega} \in B^{\partial\Omega}(z, \alpha)\big] = a_z + O(h),$$

in the limit $h \to 0$ and uniformly in $x \in K$. This concludes the proof of Proposition C.39. ∎

In conclusion, for $k \in \{2, ..., N_1\}$, the law of X_{τ_Ω} concentrates on $\partial C_k \cap \partial\Omega$ in the limit $h \to 0$ when $X_0 = x \in C_k$ whereas the law of X_{τ_Ω} concentrates on $\partial C_1 \cap \partial\Omega$ when $X_0 \sim \nu_h$. Therefore, one deduces that the exit event from Ω is not the same starting from the quasi stationary distribution ν_h or starting from deterministic initial conditions in C_k. This also shows that the process (C.1) starting from $x \in C_k$ leaves Ω before reaching the quasi stationary distribution ν_h in the small temperature regime. The domain Ω is metastable for deterministic initial conditions in C_1 but not for deterministic initial conditions in C_k for $k \neq 1$.

C.4.2 On the optimality of the remainder terms in Theorem C.1, C.2 and C.3, and Corollary C.6 under [H-connexity]

C.4.2.1 On the optimality of the remainder term $O(\sqrt{h})$ in (C.20)

This section is dedicated to the following proposition which aims at giving a framework in which one can show that, in (C.20), λ_h (see (C.5)) admits a full asymptotic expansion in power of $\sqrt{h}$. This shows in particular the optimality of the remainder term $O(\sqrt{h})$ in (C.20) under [**H-Connexity**].

Proposition C.40. *Assume that **[H-Morse]** and **[H-Connexity]** hold. Let us denote by $(C_j)_{j\in\{1,...,N_1\}}$ the connected components of $\{f < \min_{\partial\Omega} f\}$ (see Definition C.2). Let us assume that $N_1 \geq 2$, $\overline{C}_1 \cap \overline{C}_2 \neq \emptyset$ and for all $i \in \{1,2\}$ and all $j \in \{3,...,N_1\}$, $\overline{C}_i \cap \overline{C}_j = \emptyset$. Let us recall that $\overline{C}_1 \cap \overline{C}_2 \subset \mathcal{U}_1^{ssp} \cap \Omega$ (see Definition C.3 and* (C.70)*). Then, the following holds*

1. *There exists a sequence $(a_k)_{k\geq 0} \in \mathbb{R}^{\mathbb{N}}$ such that for any $N \in \mathbb{N}$, it holds in the limit $h \to 0$:*

$$\lambda_h = \frac{1}{\sqrt{h}}\Big(\sum_{k=0}^{N} a_k h^{\frac{k}{2}} + O(h^{\frac{N+1}{2}})\Big)\, e^{-\frac{2}{h}(f(z_1)-f(x_1))}, \tag{C.250}$$

with

$$a_0 = \frac{\sum\limits_{j=1}^{k_1^{\partial C_1}} \partial_n f(z_j)\big(\det \mathrm{Hess} f\big|_{\partial\Omega}(z_j)\big)^{-\frac{1}{2}}}{\sqrt{\pi\, h}\sum\limits_{k=1}^{k_0^{\Omega}}\big(\det \mathrm{Hess} f(x_k)\big)^{-\frac{1}{2}}},\ a_1 = \frac{\sum\limits_{z\in\overline{C}_1\cap\overline{C}_2} |\lambda_-(z)|\big(|\det \mathrm{Hess} f(z)|\big)^{-\frac{1}{2}}}{2\pi\sum\limits_{k=1}^{k_0^{\Omega}}\big(\det \mathrm{Hess} f(x_k)\big)^{-\frac{1}{2}}},$$

where $\lambda_-(z)$ is the negative eigenvalue of $\mathrm{Hess} f(z)$ *for $z \in \overline{C}_1 \cap \overline{C}_2$.*

2. *The remainder term $O(h^{\frac{d-5}{4}} e^{-\frac{1}{h}(2f(z_1)-f(x_1))})$ in* (C.22) *is actually of the order $O(h^{\frac{d-4}{4}} e^{-\frac{1}{h}(2f(z_1)-f(x_1))})$ and the remainder term $O(h^{\frac{1}{4}})$ in* (C.23) *is is actually of the order $O(\sqrt{h})$.*

3. *The remainder terms $O(h^{\frac{1}{4}})$ in* (C.27), (C.28), (C.31) *and* (C.32) *are of the order $O(\sqrt{h})$.*

Item 1 in Proposition C.40 shows that the remainder term $O(\sqrt{h})$ in (C.20) is optimal. Notice that in Proposition C.40, the assumption [**H-Connexity+**] does not hold: this is consistent with the fact that, from Theorem C.1, we know that λ_h admits a full asymptotic expansion in h under [**H-Connexity+**].

The example of Section C.4.2.2 shows that all the remainder terms given in items 2 and 3 of Proposition C.40 are optimal.

Proof. Let us use the notations used in the proof of Theorem C.4 and let us first prove (C.250). Let us recall that [**H-Connexity**] is equivalent to $N_0 = 1$. According to Lemma C.27, there exists $c > 0$ such that in the limit $h \to 0$:

$$\lambda_{1,h} = \frac{h}{2}\eta^2_{m_0^{\Omega}}(\widetilde{S}\widetilde{C}_0)\big(1 + O(e^{-\frac{c}{h}})\big), \tag{C.251}$$

where $\widetilde{S}$ is defined in (C.144) and $\widetilde{C}_0$ is defined in (C.169) and (C.170). Moreover, it holds

$$\eta_{m_0^\Omega}(\widetilde{S}\widetilde{C}_0) = \min_{y\in\mathbb{R}^{m_0^\Omega}\,;\,\|y\|_2=1} \big\|\widetilde{S}\,\widetilde{C}_0\,y\big\|_2 \tag{C.252}$$

According to (C.144), the matrix $\widetilde{S}$ has the form, up to reordering the z_i, $i\in\{1,\dots,m_1^{\overline{\Omega}}\}$

$$\widetilde{S} = \begin{pmatrix} [\widetilde{S}]_1 & 0 \\ 0 & [\widetilde{S}]_2 \end{pmatrix}, \tag{C.253}$$

where

- $[\widetilde{S}]_1$ is a matrix of size $\mathrm{Card}\big(\cup_{k=1}^2 \mathbf{j}(x_k)\big)\times 2$. The coefficients $([\widetilde{S}]_1)_{j,k} = \widetilde{S}_{j,k}$ are associated with the 0-forms $\widetilde{u}_k$, for $k\in\{1,2\}$ (see Definition C.9 and (C.80)) and with the 1-forms $\widetilde{\psi}_i$ for $i\in\{1,...,m_0^\Omega\}$ such that $z_i\in\mathbf{j}(x_k)$,
- $[\widetilde{S}]_2$ is a matrix of size $\Big(m_1^{\overline{\Omega}} - \mathrm{Card}\big(\cup_{k=1}^2 \mathbf{j}(x_k)\big)\Big)\times\big(m_0^\Omega-2\big)$. The coefficients $([\widetilde{S}]_2)_{j,k} = \widetilde{S}_{j,k}$ are associated with the 0-forms $\widetilde{u}_1$, 0-forms $\widetilde{u}_k$, for $k\in\{3,...,m_1^{\overline{\Omega}}\}$ and with the 1-forms $\widetilde{\psi}_i$ for $i\in\{1,...,m_1^{\overline{\Omega}}\}$ such that $z_i\in\mathbf{j}(x_k)$.

Then, the following holds:

$$\eta_2([\widetilde{S}]_1)\,(1+O(e^{-\frac{c}{h}})) \le \eta_{m_0^\Omega}(\widetilde{S}\widetilde{C}_0) \le \eta_2([\widetilde{S}]_1), \tag{C.254}$$

where $\eta_2[\widetilde{S}]_1$ is the smallest singular value of $[\widetilde{S}]_1$.

Remark C.18. *Notice that without the assumption that for all $i\in\{1,2\}$ and all $j\in\{3,...,N_1\}$, $\overline{C}_i\cap\overline{C}_j=\emptyset$, the matrix at the bottom left of* (C.253) *is not the zero matrix and in that case, we are not able to compare $\eta_{m_0^\Omega}(\widetilde{S}\widetilde{C}_0)$ with $\eta_2([\widetilde{S}]_1)$.*

Let us prove (C.254). For any $z\in\mathbb{R}^2$, one has $\widetilde{C}_0 z = z$ and thus $\widetilde{S}\,\widetilde{C}_0\,{}^t(z,0) = [\widetilde{S}]_1 z$. Therefore, it holds: $\eta_{m_0^\Omega}(\widetilde{S}\widetilde{C}_0)\le\eta_2([\widetilde{S}]_1)$. Let us now prove a reverse inequality. To this end, let us consider $y^* = {}^t(x^*,w^*)$, $x^*\in\mathbb{R}^2$, $w^*\in\mathbb{R}^{m_0^\Omega-2}$, $\|y^*\|_2=1$, realizing the minimum in (C.252). From (C.180) together with the fact that $N_0=1$ and since $\|y^*\|_2=1$, one obtains that there exists $\mu>0$ such that for h small enough, $x_1^* = 1+O(e^{-\frac{\mu}{h}})$, $x_2^* = O(e^{-\frac{\mu}{h}})$ and

$$\|w^*\|_2 = O(e^{-\frac{\mu}{h}}). \tag{C.255}$$

In particular, it holds

$$\|x^*\|_2 = 1+O(e^{-\frac{\mu}{h}}). \tag{C.256}$$

Let us recall that from (C.169) (since $2\le N_1$), the $m_0^\Omega\times m_0^\Omega$ matrix $\widetilde{C}_0$ has the form

$$\widetilde{C}_0 = \begin{pmatrix} \mathrm{Id}_2 & [\widetilde{C}_0]_4 \\ 0 & [\widetilde{C}_0]_2 \end{pmatrix}.$$

Since $\widetilde{C}_0 x^* = x^*$, using (C.255), (C.256) (C.253) and the fact that $[\widetilde{C}_0]_4 = O(1)$ (since $\widetilde{C}_0 = C_0 + O(e^{-\frac{c}{h}})$ and $C_0 = O(1)$ see (C.169), (C.170) and (C.164)), one obtains that there exists $c>0$ such that when $h\to 0$:

$$\big\|\widetilde{S}\widetilde{C}_0 y^*\big\|_2 \ge \big\|[\widetilde{S}]_1\big(x^* + [\widetilde{C}_0]_4 w^*\big)\big\|_2 \ge \eta_2([\widetilde{S}]_1)\big(1+O(e^{-\frac{c}{h}})\big).$$

This concludes the proof of (C.254). Let us now prove (C.250). To this end and in view of (C.254), let us estimate $\eta_2([\widetilde{S}]_1)^2$ which is, by definition, the smallest eigenvalue of the 2×2 matrix

$$A :=^t [\widetilde{S}]_1[\widetilde{S}]_1 = \begin{pmatrix} a_{1,1} & a_{1,2} \\ a_{1,2} & a_{2,2} \end{pmatrix}.$$

The smallest eigenvalue of A is given by

$$\eta_2([\widetilde{S}]_1)^2 = \frac{1}{2}\Big(a_{1,1}+a_{2,2}-\sqrt{(a_{1,1}-a_{2,2})^2+4a_{1,2}^2}\Big). \tag{C.257}$$

By definition of $\widetilde{S}$ (see (C.144)) and $[\widetilde{S}]_1$ (see C.253), one has

$$A = \begin{pmatrix} \sum_{j,\, z_j\in \mathbf{j}(x_1)} \widetilde{S}_{j,1}^2 & \sum_{j,\, z_j\in \mathbf{j}(x_1)\cap \mathbf{j}(x_2)} \widetilde{S}_{j,1}\widetilde{S}_{j,2} \\ \sum_{j,\, z_j\in \mathbf{j}(x_1)\cap \mathbf{j}(x_2)} \widetilde{S}_{j,1}\widetilde{S}_{j,2} & \sum_{j,\, z_j\in \mathbf{j}(x_2)} \widetilde{S}_{j,2}^2 \end{pmatrix}. \tag{C.258}$$

Let us recall that for $k\in\{1,...,N_1\}$, $f(x)=f(z_1)$ for all $x\in\mathbf{j}(x_k)$ (see (C.72)). Therefore, using in addition Proposition C.23, it follows that in the limit $h\to 0$:

$$\widetilde{S}_{j,1} = \begin{cases} -C_{j,1}\, h^{-\frac{3}{4}} e^{-\frac{1}{h}(f(z_1)-f(x_1))}(1+O(h)) & \text{if } j \text{ is s.t } z_j\in\mathbf{j}(x_1)\cap\partial\Omega \\ \varepsilon_{j,1}C_{j,1}\, h^{-\frac{1}{2}} e^{-\frac{1}{h}(f(z_1)-f(x_1))}(1+O(h)) & \text{if } j \text{ is s.t } z_j\in\mathbf{j}(x_1)\cap\mathbf{j}(x_2) \end{cases}, \tag{C.259}$$

and

$$\widetilde{S}_{j,2} = \begin{cases} -C_{j,2}\, h^{-\frac{3}{4}} e^{-\frac{1}{h}(f(z_1)-f(x_2))}(1+O(h)) & \text{if } j \text{ is s.t } z_j\in\mathbf{j}(x_2)\cap\partial\Omega \\ \varepsilon_{j,2}C_{j,2}\, h^{-\frac{1}{2}} e^{-\frac{1}{h}(f(z_1)-f(x_2))}(1+O(h)) & \text{if } j \text{ is s.t } z_j\in\mathbf{j}(x_1)\cap\mathbf{j}(x_2) \end{cases}. \tag{C.260}$$

where the constants $C_{j,k}$'s are defined in (C.129), $\varepsilon_{j,k}\in\{1,-1\}$ for all j and k and, in all the previous estimates, the remainder terms $O(h)$ admits a full expansion in h (see Remark C.10). By **[H-Connexity]**, it holds $f(z_1)-f(x_1)>f(z_1)-f(x_2)$ (see (C.74) together with the fact that $N_0=1$) and thus, using (C.258), (C.259) (C.260) and (C.257), there exists $c>0$ such that in the limit $h\to 0$:

$$\begin{aligned}
\eta_2([\widetilde{S}]_1)^2 &= \frac{1}{2}\left(a_{1,1}+a_{2,2}-a_{2,2}\sqrt{1+\Big(-2\frac{a_{1,1}}{a_{2,2}}+4\frac{a_{1,2}^2}{a_{2,2}^2}\Big)\big(1+O(e^{-\frac{c}{h}})\big)}\right) \\
&= \frac{1}{2}\Big(a_{1,1}-\frac{1}{2}\Big(-2a_{1,1}+4\frac{a_{1,2}^2}{a_{2,2}}\Big)\big(1+O(e^{-\frac{c}{h}})\big)\Big) \\
&= \Big(a_{1,1}-\frac{a_{1,2}^2}{a_{2,2}}\Big)\big(1+O(e^{-\frac{c}{h}})\big)
\end{aligned}$$

and thus

$$\begin{aligned}
\eta_2([\widetilde{S}]_1)^2 = \Bigg(& h^{-\frac{3}{2}}\sum_{j,\, z_j\in\mathbf{j}(x_1)\cap\partial\Omega} C_{j,1}^2(1+r_1(h)) + h^{-1}\sum_{j,\, z_j\in\mathbf{j}(x_1)\cap\mathbf{j}(x_2)} C_{j,1}^2(1+r_2(h)) + h^{-\frac{1}{2}}r_3(h)\Bigg) \\
&\times e^{-\frac{2}{h}(f(z_1)-f(x_1))}
\end{aligned} \tag{C.261}$$

where for $i\in\{1,2\}$, $r_j(h)=O(h)$ admits a full expansion in h and $r_3(h)=O(h)$ admits a full expansion in $\sqrt{h}$. Let us recall that from (C.70) and by assumption,

$\mathbf{j}(x_1)\cap\mathbf{j}(x_2)=\mathbf{j}(x_1)\cap\Omega=\mathbf{j}(x_2)\cap\Omega=\overline{C_1}\cap\overline{C_2}\neq\emptyset$. Then (C.250) follows from (C.261) and the definition of the constants $C_{j,k}$'s (see (C.129)) together with (C.254).
Let us now prove items 2 and 3 in Proposition C.40. From (C.254) and (C.261), one has in the limit $h\to 0$:

$$\begin{aligned}\lambda_h &= \frac{h}{2}a_{1,1}\big(1+O(h)\big)\\ &= \frac{h}{2}\sum_{j=1}^{m_1^{\overline{\Omega}}}\langle\nabla\widetilde{u}_1,\widetilde{\psi}_j\rangle^2_{L^2_w}\big(1+O(h)\big).\end{aligned}$$

Therefore, from the proof of Lemma C.34, it holds when $h\to 0$:

$$\big\|\nabla(\pi_h^{(0)}-\widetilde{\pi}_h^{(0)})\widetilde{u}_1\big\|^2_{L^2_w}=\frac{2}{h}\lambda_h O(h).$$

Then, the results of Corollary C.35 hold with $\varepsilon_h=h$ (instead of (C.215)) and item 2 in Proposition C.40 follows directly from the estimates made in Section C.3.2.3 (replacing everywhere ε_h by h in Section C.3.2.3). Finally, using items 2 and 3 in Proposition C.40 follows from a direct adaptation of the proof of Corollary C.6 and Theorem C.3. ∎

C.4.2.2 On the optimality of the remainder terms in Theorems C.2 and C.3, and Corollary C.6

In this section, we discuss the remainder terms $O(h^{\frac{1}{4}})$ appearing in Theorem C.2 (see (C.23)), Corollary C.6 (see (C.27) and (C.28)) and Theorem C.3 (see (C.31) and (C.32)) under the assumption [**H-connexity**]. To this end, let us consider the following one-dimensional case. Let $z_1<z_2$ and $f\colon[z_1,z_2]\to\mathbb{R}$ be a C^∞ Morse function. Let us assume that $f(z_1)=f(z_2)$, $\{x\in[z_1,z_2],f'(x)=0\}=\{x_1,z,x_2\}$ with $z_1<x_1<z<x_2<z_2$ and $f(x_1)<f(x_2)<f(z)=f(z_1)$ (see Figure C.12). This implies $f'(z_1)<0$, $f'(z_2)>0$, x_1 is the global minimum of f in $[z_1,z_2]$, x_2 is a local minimum of f and z is a local maximum of f. Notice that in this example, all the assumptions of Proposition C.40 are satisfied and (see Definition C.2 and (C.19),(C.18) and (C.17)),

$$\arg\min_{\partial\Omega} f=\{z_1,z_2\}, C_1=(z_1,z),\ C_2=(z,z_2),\ \partial C_1\cap\partial\Omega=\{z_1\},\ k_1^{\partial C_1}=1 \text{ and } k_1^{\partial\Omega}=2.$$

Using (C.244) together with Laplace's method, one obtains for $x\in(z_1,z)$ in the limit $h\to 0$:

$$\mathbb{P}^x[X_{\tau_{(z_1,z_2)}}=z_1]=\frac{\sqrt{\frac{\pi}{|f''(z)|}}\sqrt{h}+\frac{1}{2f'(z_2)}h+O(h^{\frac{3}{2}})}{\sqrt{\frac{\pi}{|f''(z)}}\sqrt{h}+(\frac{1}{2f'(z_2)}+\frac{1}{2|f'(z_1)|})h+O(h^{\frac{3}{2}})}=1-\frac{\sqrt{|f''(z)|}}{2|f'(z_1)|\sqrt{\pi}}\sqrt{h}+O(h),$$

and thus:

$$\mathbb{P}^x[X_{\tau_{(z_1,z_2)}}=z_2]=\frac{\sqrt{|f''(z)|}}{2|f'(z_1)|\sqrt{\pi}}\sqrt{h}+O(h).$$

In this case, the exit through z_2 when $h\to 0$ is not exponentially small but is exactly of the order $\sqrt{h}$ even though z_2 is a generalized critical point of f on $\partial\Omega$ (i.e $f(z_2)\in\mathcal{U}_1^{\partial\Omega}$,

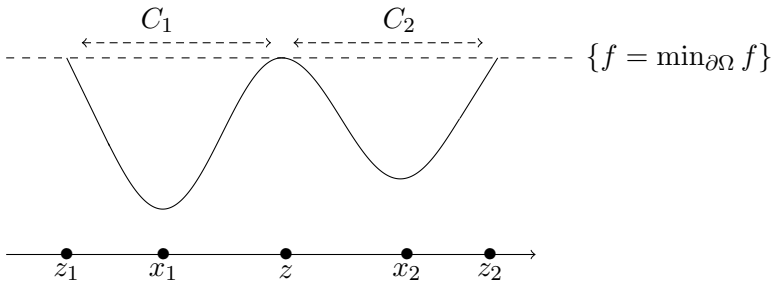

Figure C.12: A one dimensional case when [**H-connexity**] holds but not [**H-connexity+**].

see (C.14)) and $f(z_2) = \min_{\partial\Omega} f$.
Therefore, this shows that on the one hand the remainder terms $O(h^{\frac{1}{4}})$ in (C.27), (C.28), (C.31) and (C.32) are exactly $O(\sqrt{h})$ in this example and on the other hand the remainder terms given in item 3 of Proposition C.40 are optimal. Since the remainder terms given in item 3 of Proposition C.40 are obtained from those of item 2 of Proposition C.40, the remainder terms of item 3 of Proposition C.40 are optimal. This example also shows that when assuming only [**H-connexity**], the remainder terms $O(h^{\frac{1}{4}})$ in (C.27) and (C.31) which bound the exit of the process (C.1) through the points $z_{k_1^{\partial C_1}+1}, ..., z_{k_1^{\partial\Omega}}$ are not, in general exponentially small when $h \to 0$.

C.4.3 Generalization of the results of Section C.1.4

The aim this section is to exhibit a more general geometric setting for which the results of Theorems C.1, C.2, C.3 and Corollary C.6 are preserved. This setting covers in particular the case when f has local minima inside Ω which are higher in energy than $\min_{\partial\Omega} f$ (notice that this situation is not allowed under [**H-Boundary**]). To generalize the results of Section C.1.4, the main point is to define at a higher level of generality than the assumption [**H-Boundary**] an association between $\mathcal{U}_0^\Omega$ and $\mathcal{P}\big(\mathcal{U}_1^{\overline{\Omega}}\big)$, where $\mathcal{U}_0^\Omega$ and $\mathcal{U}_1^{\overline{\Omega}}$ are respectively the local minima of f in Ω and the generalized saddle points in $\overline{\Omega}$ of f (see Section C.1.3.2). This mapping aims at generalizing the map $\mathbf{j}$ constructed in Section C.2.3.3 under the assumptions [**H-Morse**] and [**H-Boundary**]. In all the following, we assume that

- [**H-Minima**] The set $\mathcal{U}_0^\Omega$ is not empty.

This section is organized as follows. One first defines, under [**H-Minima**] and [**H-Morse**], a collection of connected open sets indexed by the elements of $\mathcal{U}_0^\Omega$ and which plays a similar role as the connected components $(C_j)_{j\in\{1,...,N_1\}}$ of $\{f < \min_{\partial\Omega} f\}$ introduced in Definition C.2 under the assumption [**H-Boundary**]. Then, one constructs an association between $\mathcal{U}_0^\Omega$ and $\mathcal{P}\big(\mathcal{U}_1^{\overline{\Omega}}\big)$. Finally, generalizations of Theorems C.1, C.2, C.3 and Corollary C.6 are stated.

Connected components associated with the elements of $\mathcal{U}_0^\Omega$ and $\partial\Omega$

Let us recall that under [**H-Boundary**], the sets $(C_k)_{k\in\{1,\dots,N_1\}}$ are defined as the connected components $\{f < \min_{\partial\Omega} f\}$ (see Definition C.2). These sets were the starting point of the construction of the quasi-modes made in Section C.2. When assuming only [**H-Morse**], one needs to start with another set of connected components and to this end, one proceeds as follows.
Let assume that the assumption [**H-minima**] holds. Let us define for all $x \in \mathcal{U}_0^\Omega$ and $\lambda > f(x)$:

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

as well as

$$\lambda(x) := \sup\{\lambda > f(x) \text{ s.t. } \mathsf{C}(\lambda, x) \cap \partial\Omega = \emptyset\}, \text{ and } \mathsf{C}(x) := \mathsf{C}(\lambda(x), x). \tag{C.262}$$

Notice that under [**H-Morse**], for all $x \in \mathcal{U}_0^\Omega \subset \Omega$, $\lambda(x)$ is well defined. Indeed, for all $x \in \mathcal{U}_0^\Omega$, $\{\lambda > f(x) \text{ s.t. } \mathsf{C}(\lambda, x) \cap \partial\Omega = \emptyset\}$ is bounded by $\sup_{\overline{\Omega}} f + 1$ and non empty because for $\beta > 0$ small enough $\mathsf{C}(f(x) + \beta, x)$ is included in Ω (since $x \in \Omega$ and f is Morse).

Definition C.12. *Let us assume that the assumptions **[H-Morse]** and **[H-minima]** hold. The integer N_1 is defined by:*

$$\mathsf{N}_1 := \mathrm{Card}\big(\{\mathsf{C}(x),\, x \in \mathcal{U}_0^\Omega\}\big) \ \in \{1, \dots, m_0^\Omega\}, \tag{C.263}$$

where we recall $m_0^\Omega = \mathrm{Card}\,(\mathcal{U}_0^\Omega)$ (see (C.11)*) Moreover, the elements of $\{\mathsf{C}(x), x \in \mathcal{U}_0^\Omega\}$ are denoted by $\mathsf{C}_1, \dots, \mathsf{C}_{N_1}$.*

Remark C.19. *Notice that by definition, when **[H-Boundary]** holds, $\mathsf{N}_1 = N_1$ (see* (C.263)*) and the family $(\mathsf{C}_k)_{k=1,\dots,\mathsf{N}_1}$ introduced in Definition C.12 is exactly the set $(C_k)_{k=1,\dots,N_1}$ defined as the connected components of $\{f < \min_{\partial\Omega} f\}$ which are introduced in Definition C.2.*

The definition of a separating saddle point originally introduced in Definition C.3 under [**H-Morse**] and [**H-Boundary**] can be generalized in the setting of [**H-Morse**] and [**H-Minima**].

Definition C.13. *Assume **[H-Morse]** and **[H-Minima]**. Let $\mathsf{C}_1, \dots, \mathsf{C}_{N_1}$ be the connected sets introduced in Definition C.12.*

1. *A point $z \in U_1^{\overline{\Omega}}$ is a* separating saddle point *if*
   - *either $z \in \mathcal{U}_1^\Omega \cap \cup_{i=1}^{\mathsf{N}_1} \overline{\mathsf{C}_i}$ and for $r > 0$ small enough, the two connected components of $\{f < f(z)\} \cap B(z, r)$ are contained in different connected components of $\{f < f(z)\}$,*
   - *or $z \in \mathcal{U}_1^{\partial\Omega} \cap \cup_{i=1}^{\mathsf{N}_1} \partial\mathsf{C}_i$.*

   Notice that in the former case $z \in \Omega$ while in the latter case $z \in \partial\Omega$. The set of separating saddle points *is denoted by U_1^{ssp}.*

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

Let us recall that $\mathcal{U}_1^\Omega$ is the set of saddle points of f in Ω and $\mathcal{U}_1^{\partial\Omega}$ is the set of points $z \in \partial\Omega$ such that z is a local minima of $f|_{\partial\Omega}$ and $\partial_n f(z) > 0$, see Section C.1.3.2.

Remark C.20. *Notice that, according to Remark C.19, when **[H-boundary]** holds, the sets U_1^{ssp} and C_{crit} coincide respectively with $\mathcal{U}_1^{ssp}$ and $\mathcal{C}_{crit}$ introduced in Definition C.3.*

Let us now study the properties of $\mathsf{C}_1, \dots, \mathsf{C}_{N_1}$. The following lemma will be used in the first step of the construction of the map between points in $\mathcal{U}_0^\Omega$ and sets in $\mathcal{P}(\mathcal{U}_1^{\overline{\Omega}})$.

Lemma C.41. *Let us assume that **[H-Morse]** and **[H-Minima]** hold. Let $\mathsf{C}_1, \dots, \mathsf{C}_{\mathsf{N}_1}$ be the sets introduced in Definition C.12 and let $(k,l) \in \{1, \dots, \mathsf{N}_1\}^2$ with $k \neq \ell$. Then,*

$$\mathsf{C}_k \subset \Omega \ \text{ and } \ \mathsf{C}_k \cap \mathsf{C}_\ell = \emptyset.$$

In addition, one has

$$\partial\mathsf{C}_k \cap \partial\Omega \subset \mathsf{U}_1^{ssp} \cap \partial\Omega$$

and

$$\partial\mathsf{C}_k \cap \partial\mathsf{C}_\ell \subset \mathsf{U}_1^{ssp} \cap \Omega,$$

where the set U_1^{ssp} is introduced in item 1 in Definition C.13. Finally, $\partial\mathsf{C}_k \cap \mathsf{U}_1^{ssp} \neq \emptyset$.

The arguments used in the proof of Lemma C.41 are similar to those used in the proof of Proposition C.11.

Proof. For all $k \in \{1, \dots, \mathsf{N}_1\}$, the set C_k is a connected open set of $\overline{\Omega}$ since $\overline{\Omega}$ is locally connected and C_k is by definition a connected component of the open set $\{f < \lambda(x)\}$ for some $x \in \mathcal{U}_0^\Omega$ (see Definition C.12 and (C.262)). Notice that it holds in particular $\partial\mathsf{C}_k \subset \{f = \lambda(x)\}$.

Let $k \in \{1, \dots, \mathsf{N}_1\}$. Let us now show that C_k is included in Ω. From Definition C.12 and (C.262), there exists $x \in \mathcal{U}_0^\Omega \cap \mathsf{C}_k$ such that $\mathsf{C}_k = \mathsf{C}(\lambda(x), x)$ with $\lambda(x) > f(x)$. From Lemma C.10, it holds

$$\mathsf{C}(\lambda(x), x) = \cup_{\lambda \in (f(x), \lambda(x))} \mathsf{C}(\lambda, x).$$

Moreover, since $\lambda \mapsto \mathsf{C}(\lambda, x)$ is increasing on $(f(x), +\infty)$, by definition of $\lambda(x)$ (see (C.262)) one has that $\mathsf{C}(\lambda, x) \cap \partial\Omega = \emptyset$ for all $\lambda \in (f(x), \lambda(x))$. Therefore $\mathsf{C}(\lambda(x), x) \subset \Omega$ and thus $\mathsf{C}_k \cap \partial\Omega = \emptyset$.

Let us now show that the C_k's are two by two disjoint. To this end, let $(k, \ell) \in \{1, \dots, \mathsf{N}_1\}^2$ with $\ell \neq k$ and $\mathsf{C}_k \cap \mathsf{C}_\ell \neq \emptyset$. Therefore, since for $q \in \{k, \ell\}$, there exists $x_q \in \mathcal{U}_0^\Omega \cap \mathsf{C}_q$ such that $\mathsf{C}_q = C(\lambda(x_q), x_q)$ is a connected component of $\{f < \lambda(x_q)\}$ (see Definition C.12 and (C.262)), it holds $\mathsf{C}_k = \mathsf{C}_\ell$ if $\lambda(x_k) = \lambda(x_l)$. Let us prove that $\lambda(x_k) = \lambda(x_l)$ by contradiction and assume that, without loss of generality, $\lambda(x_k) < \lambda(x_l)$. Since $\mathsf{C}_k \cap \mathsf{C}_\ell \neq \emptyset$, this implies $\mathsf{C}_k \subset \mathsf{C}_\ell$. Therefore, for any $\varepsilon \in (0, \lambda(x_l) - \lambda(x_k))$, $\mathsf{C}(\lambda(x_k) + \varepsilon, x_k) \subset \mathsf{C}_\ell$ and by definition of $\lambda(x_k)$ (see (C.262)), $\mathsf{C}(\lambda(x_k) + \varepsilon, x_k)$ intersects $\partial\Omega$. This is in contradiction with the fact that $\mathsf{C}_\ell \subset \Omega$. Therefore, $\lambda(x_k) = \lambda(x_l)$ and thus $\mathsf{C}_k = \mathsf{C}_\ell$.

Let us now prove that for $k \in \{1, \dots, \mathsf{N}_1\}$, $\partial\mathsf{C}_k \cap \partial\Omega \subset \mathsf{U}_1^{ssp} \cap \partial\Omega$ which is equivalent, according to Definition C.13, to $\partial\mathsf{C}_k \cap \partial\Omega \subset \mathcal{U}_1^{\partial\Omega}$ (where $\mathcal{U}_1^{\partial\Omega}$ is defined in Section C.1.3.2). If $\partial\mathsf{C}_k \cap \partial\Omega \neq \emptyset$, let us consider $y \in \partial\mathsf{C}_k \cap \partial\Omega$. According to [15, Section 5.2], if y is not

a critical point of $f_{|\partial\Omega}$, then the hypersurfaces $\{f = f(y)\}$ and $\partial\Omega$ interest transversally in a neighborhood of y. This implies that for $r > 0$ small enough, $\{f < f(y)\} \cap B(y,r)$ is connected and $\{f < f(y)\} \cap B(y,r) \cap \partial\Omega \neq \emptyset$. Thus $\mathsf{C}_k \cap \partial\Omega \neq \emptyset$ which is impossible since $\mathsf{C}_k \subset \Omega$. Therefore y is a critical point of $f_{|\partial\Omega}$ and according to [15, Section 5.2], there are three possible different cases:

1. either y is local minimum of f
2. or y is a local minimum of $f_{|\partial\Omega}$ and $\partial_n f(y) > 0$,
3. or for $r > 0$ small enough, $\{f < f(y)\} \cap B(y,r)$ admits one or two connected components with non empty intersection with $\partial\Omega$.

The first case is not possible in our setting since $y \in \overline{\mathsf{C}_k}$ implies that y is not a local minimum of f. The third case is also not possible since $\mathsf{C}_k \subset \Omega$. Therefore y is a local minimum of $f_{|\partial\Omega}$ and $\partial_n f(y) > 0$. This proves $\partial\mathsf{C}_k \cap \partial\Omega \subset \mathsf{U}_1^{ssp} \cap \partial\Omega$.

Let us now prove that for all $(k,l) \in \{1,\dots,\mathsf{N}_1\}^2$ with $k \neq \ell$, $\partial\mathsf{C}_k \cap \partial\mathsf{C}_\ell \subset \mathsf{U}_1^{ssp} \cap \Omega$ which is equivalent to $\partial\mathsf{C}_k \cap \partial\mathsf{C}_\ell \subset \mathcal{U}_1^\Omega$ (where $\mathcal{U}_1^\Omega$ is the set of saddle points of f in Ω, see Section C.1.3.2). To this end, let us assume that $\partial\mathsf{C}_k \cap \partial\mathsf{C}_\ell \neq \emptyset$ for some $(k,l) \in \{1,\dots,\mathsf{N}_1\}^2$ with $k \neq \ell$. First, since for $q \in \{k,\ell\}$, there exists $x_q \in \mathcal{U}_0^\Omega \cap \mathsf{C}_q$ such that C_q is a connected component of $\{f < \lambda(x_q)\}$, one has necessarily $\lambda(x_\ell) = \lambda(x_k)$. Moreover, it holds $\partial\mathsf{C}_k \cap \partial\mathsf{C}_\ell \subset \Omega$. Indeed, if there exists $z \in \partial\mathsf{C}_k \cap \partial\Omega$, we know from the analysis above that $z \in \mathcal{U}_1^{\partial\Omega}$. It follows that for $r > 0$ small enough, $B(z,r) \cap \{f < \lambda(x_k)\}$ is connected and therefore $B(z,r) \cap \{f < \lambda(x_k)\} \subset \mathsf{C}_k$. This implies that $B(z,r) \cap \mathsf{C}_\ell = \emptyset$ (since we proved that for $k \neq l$, $\mathsf{C}_k \cap \mathsf{C}_\ell = \emptyset$) and hence $z \notin \overline{\mathsf{C}_\ell}$. Lastly, if there exists $z \in \partial\mathsf{C}_k \cap \partial\mathsf{C}_\ell \cap \Omega$, then one deduces from (C.51) that $z \in \mathcal{U}_1^\Omega$. Indeed, for all $r > 0$ small enough, $B(z,r) \cap \{f < \lambda(x_k)\}$ has two connected components respectively included in C_k and C_ℓ.

To conclude the proof of Lemma C.41, it remains to show that for all $k \in \{1,\dots,\mathsf{N}_1\}$, $\partial\mathsf{C}_k \cap \mathsf{U}_1^{ssp} \neq \emptyset$. Let us argue by contradiction and assume that $\partial\mathsf{C}_k \cap \mathsf{U}_1^{ssp} = \emptyset$. Since $(\partial\mathsf{C}_k \cap \partial\Omega) \cap \mathsf{U}_1^{ssp} = \emptyset$, one has $\overline{\mathsf{C}_k} \subset \Omega$ (indeed we proved above that $\mathsf{C}_k \subset \Omega$ and $\partial\mathsf{C}_k \cap \partial\Omega \subset \mathsf{U}_1^{ssp}$). Let us recall that $\mathsf{C}_k = \mathsf{C}(\lambda(x), x)$ for some $x \in \mathcal{U}_0^\Omega \cap \mathsf{C}_k$. Since $\overline{\mathsf{C}_k} \subset \Omega$ and $\partial\mathsf{C}_k \cap \mathsf{U}_1^{ssp} = \emptyset$, the same arguments as those used to prove (C.59) apply and lead to the fact that $\overline{\mathsf{C}_k}$ is a closed and open connected set in $\{f \leq \lambda(x)\}$. Thus,

$$\overline{\mathsf{C}_k} \text{ is a connected component of } \{f \leq \lambda(x)\}.$$

Let us now denote by $\mathsf{C}^+(\mu)$, for $\mu \geq \lambda(x)$, the connected component of $\{f \leq \mu\}$ containing $\overline{\mathsf{C}_k}$. It then holds, according to Lemma C.10,

$$\bigcap_{\mu > \lambda(x)} \mathsf{C}^+(\mu) = \mathsf{C}^+(\lambda(x)) = \overline{\mathsf{C}_k}.$$

Moreover, by definition of $\lambda(x)$ (see (C.262)), $\mathsf{C}^+(\mu)$ meets $\partial\Omega$ for all $\mu > \lambda(x)$. Hence, $\cap_{\mu>\lambda(x)} \mathsf{C}^+(\mu) \cap \partial\Omega = \overline{\mathsf{C}_k} \cap \partial\Omega$ is non empty as a decreasing intersection of non empty compact sets. This contradicts the fact that $\overline{\mathsf{C}_k} \subset \Omega$. In conclusion $\partial\mathsf{C}_k \cap \mathsf{U}_1^{ssp} \neq \emptyset$. This concludes the proof of Lemma C.41.

∎

Map between points in $\mathcal{U}_0^\Omega$ and sets in $\mathcal{P}(\mathcal{U}_1^{\overline{\Omega}})$

We are now in position to define the maps $\mathbf{j}_2 : \mathcal{U}_0^\Omega \to \mathcal{P}(\mathcal{U}_1^{\overline{\Omega}})$ and $\widetilde{\mathbf{j}}_2 : \mathcal{U}_0^\Omega \to \mathsf{C}_{crit}$ as we did in Section C.2.3.3. Let $\mathsf{C}_1, \dots, \mathsf{C}_{\mathsf{N}_1}$ as introduced in Definition C.12. The constructions of the maps $\mathbf{j}_2$ and $\widetilde{\mathbf{j}}_2$ are made recursively as follows:

1. Step 1. For each $k \in \{1, \dots, \mathsf{N}_1\}$, $x_{1,k}$ denotes one point in $\arg\min_{\overline{\mathsf{C}_k}} f = \arg\min_{\mathsf{C}_k} f$. Then we define, for all $k \in \{1, \dots, \mathsf{N}_1\}$,

$$\sigma_{1,k} := \max_{\overline{\mathsf{C}_k}} f, \quad \widetilde{\mathbf{j}}_2(x_{1,k}) := \mathsf{C}_k \in \mathsf{C}_{crit}, \quad \text{and} \quad \mathbf{j}_2(x_{1,k}) := \partial \mathsf{C}_k \cap \mathsf{U}_1^{ssp}.$$

   Note in particular that according to Lemma C.41,

$$\mathbf{j}_2(x_{1,k}) \neq \emptyset, \quad \partial \mathsf{C}_k \subset \{f = \sigma_{1,k}\} \quad \text{and} \quad \cup_{k=1}^{\mathsf{N}_1} \mathbf{j}_2(x_{1,k}) \cap \partial\Omega = \mathsf{U}_1^{ssp} \cap \partial\Omega.$$

2. Step 2. Let us now define the maps $\mathbf{j}_2$ and of $\widetilde{\mathbf{j}}_2$ on $\mathcal{U}_0^\Omega \setminus \{x_{1,1}, \dots, x_{1,\mathsf{N}_1}\}$. This is done by applying the procedure starting at the second step of Section C.2.3.3 with the family $(\mathsf{C}_k)_{k\in\{1,\dots,\mathsf{N}_1\}}$ instead of the family $(C_k)_{k\in\{1,\dots,N_1\}}$. This completes the definition of the maps $\mathbf{j}_2$ and of $\widetilde{\mathbf{j}}_2$ on $\mathcal{U}_0^\Omega$ with values respectively in $\mathcal{P}(\mathcal{U}_1^{\overline{\Omega}})$ and C_{crit}.

Notice that for all $x \in \mathcal{U}_0^\Omega \setminus \{x_{1,1}, \dots, x_{1,\mathsf{N}_1}\}$, it holds $\overline{\widetilde{\mathbf{j}}_2(x)} \subset \Omega$ and $\mathbf{j}_2(x) = \partial\widetilde{\mathbf{j}}_2(x) \cap \mathsf{U}_1^{ssp} \subset \mathcal{P}(\mathcal{U}_1^\Omega)$. Moreover, since for all $x \in \mathcal{U}_0^\Omega$, there exists $k \in \{1, ..., \mathsf{N}_1\}$ such that $\mathbf{j}_2(x) \subset \partial C_k \subset \{f = \lambda(x)\}$ (see Definition C.12 and (C.262)), one has $f(z) = f(y)$ for all $z, y \in \mathbf{j}_2(x)$ and

$$\max_{x\in\mathcal{U}_0^\Omega\setminus\{x_{1,1},\dots,x_{1,\mathsf{N}_1}\}} f(\mathbf{j}_2(x)) - f(x) < \max_{x\in\{x_{1,1},\dots,x_{1,\mathsf{N}_1}\}} f(\mathbf{j}_2(x)) - f(x). \tag{C.264}$$

Remark C.21. *Let us notice that when **[H-Boundary]** also holds, the maps $\mathbf{j}_2$ and $\widetilde{\mathbf{j}}_2$ are respectively equal to $\mathbf{j}$ and $\widetilde{\mathbf{j}}$ (see Remark C.19 together with the first step of the construction of $\mathbf{j}$ and $\widetilde{\mathbf{j}}$ in Section C.2.3.3).*

Generalization of Theorem C.1

Let us define the following assumptions:

- **[H-Connexity2]** The function f satisfies **[H-Morse]** and **[H-Minima]** and, up to reordering the wells $\mathsf{C}_1, \dots, \mathsf{C}_{N_1}$ defined above, it holds

$$\partial\mathsf{C}_1 \cap \partial\Omega \neq \emptyset \text{ and for all } k \in \{2, \dots, \mathsf{N}_1\}, \ f(\mathbf{j}_2(x_{1,k})) - f(x_{1,k}) < f(\mathbf{j}_2(x_{1,1})) - f(x_{1,1}).$$

- **[H-Connexity2+]** The function f satisfies **[H-Connexity2]** and

$$\partial\mathsf{C}_1 \cap \mathsf{U}_1^{ssp} \subset \partial\Omega.$$

Remark C.22. *Notice that under **[H-Connexity2]**, one has from* (C.264),

$$\max_{x\in\mathcal{U}_0^\Omega\setminus\{x_{1,1}\}} f(\mathbf{j}_2(x)) - f(x) < f(\mathbf{j}_2(x_{1,1})) - f(x_{1,1}).$$

*Thus, **[H-Connexity]** implies **[H-Connexity2]** (see Remarks C.19 and C.20 together with* (C.74) *and the fact that $N_0 = 1$ when **[H-Connexity]** holds). Notice also that **[H-Connexity+]** implies **[H-Connexity2+]**.*

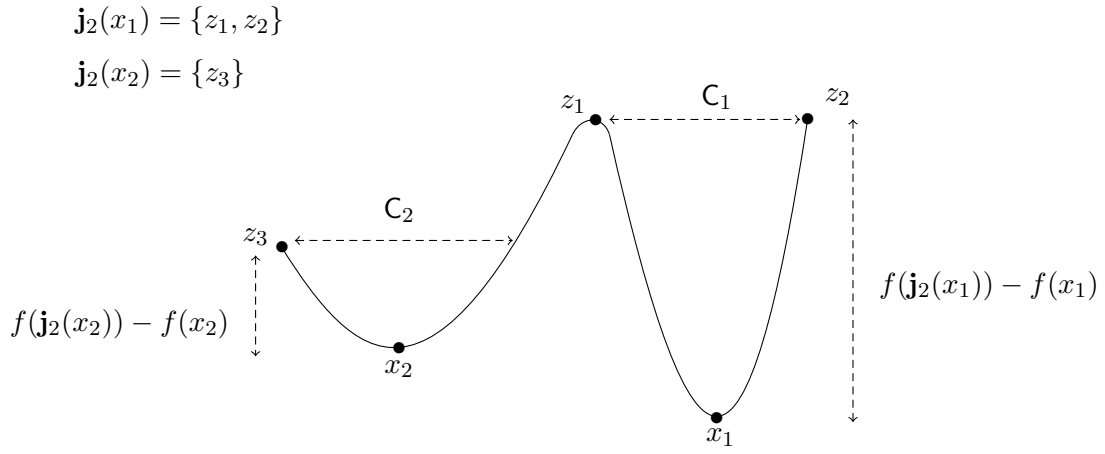

Figure C.13: A one dimensional example when [**H-connexity2**] holds. Notice that $\overline{\mathsf{C}_1} \cap \overline{\mathsf{C}_2} = \emptyset$ and $\partial\mathsf{C}_1 \cap \mathcal{U}_1^\Omega \cap \mathsf{U}_1^{ssp} = \{z_1\}$. In this example, [**H-Boundary**], [**H-connexity2+**] and [**H-connexity3**] do not hold.

In words, [**H-Connexity2**] ensures that $\mathsf{C}_1 \subset \Omega$ is the only deepest well (in terms of barriers $f(\mathbf{j}_2(x)) - f(x)$ for $x \in \mathcal{U}_0^\Omega$) among the wells $\widetilde{\mathbf{j}}_2(x)$ for $x \in \mathcal{U}_0^\Omega$ and that $\partial\mathsf{C}_1$ intersects $\partial\Omega$ (see for example Figure C.13). The stronger assumption [**H-Connexity2+**] ensures in addition that $\partial\mathsf{C}_1$ and $\mathcal{U}_1^\Omega \cap \mathsf{U}_1^{ssp}$ are disjoint, which implies in particular, using Lemma C.41, that $\overline{\mathsf{C}_1}$ is disjoint from the closure of any of the other wells $\mathsf{C}_2, \ldots, \mathsf{C}_{\mathsf{N}_1}$. However, under [**H-Connexity2**], $\overline{\mathsf{C}_1}$ can be such that for all $\ell \in \{2, ..., \mathsf{N}_1\}$, $\overline{\mathsf{C}_1} \cap \overline{\mathsf{C}_\ell} = \emptyset$, and $\partial\mathsf{C}_1 \cap \mathcal{U}_1^\Omega \cap \mathsf{U}_1^{ssp} \neq \emptyset$ (see for example Figure C.13). Notice that when [**H-Connexity2**] and $\partial\mathsf{C}_1 \subset \{f = \min_{\partial\Omega} f\}$ hold, one can easily check that [**H-Connexity2+**] is actually equivalent to $\overline{\mathsf{C}_1} \cap \cup_{k=2}^{\mathsf{N}_1} \overline{\mathsf{C}_k} = \emptyset$.

In order to generalize the statement of Theorem C.1 under [**H-Connexity2**] and [**H-Connexity2+**], we assume that the sets $\mathcal{U}_0^\Omega$ and $\mathcal{U}_1^{\partial\Omega}$ are labelled such that:

$$\{x_1, \ldots, x_{\mathsf{k}_0^{\mathsf{C}_1}}\} = \arg\min_{\overline{\mathsf{C}_1}} f \subset \mathcal{U}_0^\Omega \quad \text{and} \quad \{z_1, \ldots, z_{\mathsf{k}_1^{\partial\mathsf{C}_1}}\} = \partial\mathsf{C}_1 \cap \mathcal{U}_1^{\partial\Omega}, \tag{C.265}$$

where $\mathsf{k}_0^{\mathsf{C}_1} \in \{1, ..., k_0^\Omega\}$ (see (C.12)) and $\mathsf{k}_0^{\partial\mathsf{C}_1} \in \{1, ..., m_1^{\partial\Omega}\}$ (see (C.15)).

Remark C.23. *Notice that under the assumption [**H-connexity**], the integers* $\mathsf{k}_0^{\mathsf{C}_1}$ *and* $\mathsf{k}_1^{\partial C_1}$ *coincide respectively with* k_0^Ω *and* $k_1^{\partial C_1}$ *defined respectively by* (C.12) *and* (C.18).

One is now in position to state a more general result than Theorem C.1.

Theorem C.5. *The conclusions stated in Theorem C.1 remain valid if one replaces* $\{x_1, ..., x_{k_0^\Omega}\}$ *by* $\{x_1, \ldots, x_{\mathsf{k}_0^{\mathsf{C}_1}}\}$, $\{z_1, \ldots, z_{k_1^{\partial C_1}}\}$ *by* $\{z_1, \ldots, z_{\mathsf{k}_1^{\partial\mathsf{C}_1}}\}$ *and if one assumes [**H-Connexity2**] instead of [**H-Connexity**] and [**H-Connexity2+**] instead of [**H-Connexity+**].*

Proof. Let us explain how to prove Theorem C.5. First, the family of quasi modes for 0-forms and for 1-forms are constructed exactly as we did in Section C.2.4.1, using the

maps $\mathbf{j}_2$ instead of $\mathbf{j}$ and $\widetilde{\mathbf{j}}_2$ instead of $\widetilde{\mathbf{j}}$. We can then follow exactly the same analysis as the one made in Sections C.3.1.1 and C.3.1.2, replacing the number N_0 defined in (C.46) by 1 and using the maps $\mathbf{j}_2$ instead of $\mathbf{j}$ and $\widetilde{\mathbf{j}}_2$ instead of $\widetilde{\mathbf{j}}$. ∎

Generalization of Theorem C.2, Corollary C.6, and Theorem C.3

One can also easily generalize the statements of Theorem C.2, Corollary C.6, and Theorem C.3 following exactly the same analysis as done in Sections C.3.1.3, C.3.2, and C.3.3. The assumptions [**H-Connexity2**] and [**H-Connexity2+**] are nevertheless not sufficient to generalize these results following the same analysis since:

- to prove Proposition C.5 in Section C.3.1.3, one uses the fact that the point x_1, now defined by (C.265), is a global minimum of f (see indeed (C.212)),
- to prove Theorem C.2 in Section C.3.2, we use that the point z_1, now defined by (C.265), is a global minimum of $f\big|_{\partial\Omega}$ (see for example (C.223)).

Moreover, the same proofs as those made in Sections C.3.1.3, C.3.2, and C.3.3 work when $f(x_1) = \min_{\overline{\Omega}} f$ and $f(z_1) = \min_{\partial\Omega} f$. In view of these remarks, we define the following assumptions:

- [**H-Connexity3**] The function f satisfies [**H-Connexity2**] and
$$\partial\mathsf{C}_1 \subset \{f = \min_{\partial\Omega} f\}.$$
- [**H-Connexity3+**] The function f satisfies [**H-Connexity2+**] and
$$\partial\mathsf{C}_1 \subset \{f = \min_{\partial\Omega} f\}.$$

In Figure C.15, one gives a case when [**H-Connexity3**] but not [**H-Connexity3+**] and in Figure C.14, one gives a case when [**H-Connexity3+**] holds. Notice that under [**H-Connexity3**], the point x_1 defined by (C.265) satisfies $f(x_1) < \min_{\partial\Omega} f$ and hence $\arg\min_{\overline{\Omega}} f \subset \Omega$. Moreover, the point x_1 then necessarily belongs to $\arg\min_{\overline{\Omega}} f = \arg\min_{\Omega} f$ and $\arg\min_{\Omega} f \subset \mathsf{C}_1$. Indeed, for any $k \in \{1, ..., \mathsf{N}_1\}$, if there exists $x \in \arg\min_{\Omega} f \subset \{f < \min_{\partial\Omega} f\}$ such that $\mathsf{C}_k = \mathsf{C}(\lambda(x), x)$, then one has $\lambda(x) \geq \min_{\partial\Omega} f$ and thus
$$\lambda(x) - f(x) = f(\mathbf{j}_2(x_{1,k})) - f(x_{1,k}) \geq f(\mathbf{j}_2(x_{1,1})) - f(x_{1,1}),$$
since $\mathbf{j}_2(x_{1,1}) \subset \partial\mathsf{C}_1$ and by assumption $f(\mathbf{j}_2(x_{1,1})) = \min_{\partial\Omega} f$. This implies $\mathsf{C}_k = \mathsf{C}_1$ from the assumption [**H-Connexity2**]. We have then proved that if f satisfies [**H-Connexity3**] then
$$\arg\min_{\overline{\Omega}} f = \arg\min_{\Omega} f = \{x_1, \ldots, x_{\mathsf{k}_0^\Omega}\}.$$

Remark C.24. *Notice that under [**H-Connexity3**], $\mathcal{U}_0^\Omega \cap \{f \geq \min_{\partial\Omega} f\} \neq \emptyset$ may hold whereas this situation was excluded in [**H-Boundary**] (cf Figure C.14).*

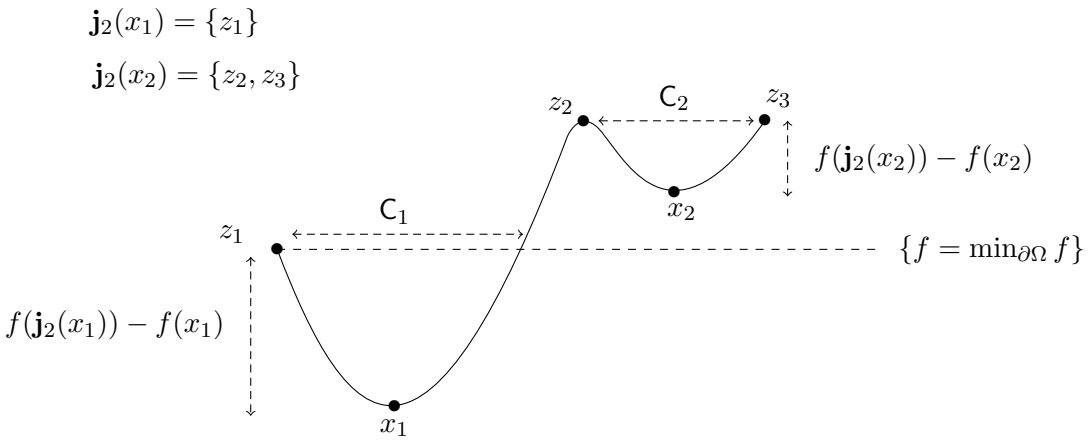

Figure C.14: A one dimensional example when [**H-connexity3+**] holds. In the figure $f(x_2) > \min_{\partial\Omega} f$. Thus, in this example, [**H-Boundary**] does not hold.

Before stating the generalized results, let us define under [**H-Connexity3**],

$$\{z_{\mathsf{k}_1^{\partial \mathsf{C}_1}+1}, \ldots, z_{k_1^{\partial\Omega}}\} := \mathcal{U}_1^{\partial\Omega} \cap \arg\min_{\partial\Omega} f \setminus \partial C_1 \tag{C.266}$$

where we recall, $k_1^{\partial\Omega}$ is defined in (C.17) and $\mathsf{k}_1^{\partial \mathsf{C}_1}$ by (C.265). Therefore, according to (C.265), it holds $\{z_1, \ldots, z_{\mathsf{k}_1^{\partial \mathsf{C}_1}}\} = \{z_1, \ldots, z_{k_1^{\partial\Omega}}\} \cap \partial C_1$. The same analysis as the one made in Sections C.3.1.3, C.3.2, and C.3.3 then leads to:

Theorem C.6. *The conclusions stated in Theorem C.2, Corollary C.6, and Theorem C.3 remain valid if one replaces the set* $\{x_1, ..., x_{k_0^\Omega}\}$ *by* $\{x_1, \ldots, x_{\mathsf{k}_0^{\mathsf{C}_1}}\}$, $\{z_1, \ldots, z_{k_1^{\partial C_1}}\}$ *by* $\{z_1, \ldots, z_{\mathsf{k}_1^{\partial \mathsf{C}_1}}\}$ *and if one assumes* ***[H-Connexity3]*** *instead of* ***[H-Connexity]*** *and* ***[H-Connexity3+]*** *instead of* ***[H-Connexity+]****.*

$\mathbf{j}_2(x_1) = \{z_1, z_2\}$

$\mathbf{j}_2(x_2) = \{z_2\}$

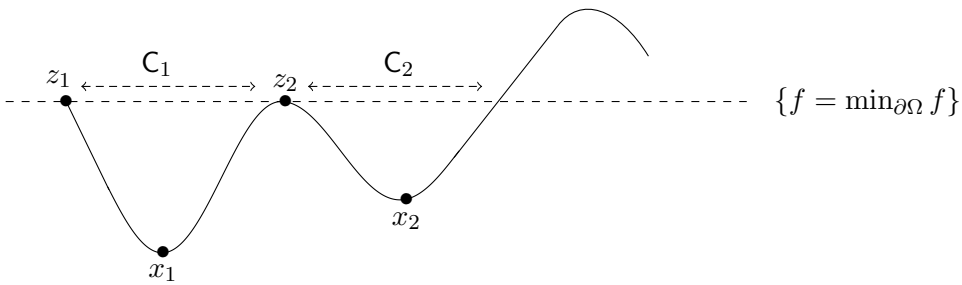

Figure C.15: A one dimensional example when [**H-connexity3**] holds but not [**H-connexity3+**]. Notice that in this example [**H-Boundary**] does not hold since the connected component $\partial\mathsf{C}_2$ of $\{f < \min_{\partial\Omega} f\}$ satisfies $\partial\mathsf{C}_2 \cap \partial\Omega = \emptyset$.

Bibliography of Chapter C

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