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# Quelques résultats d'analyse et de probabilités autour du laplacien de Witten

Dorian Le Peutrec

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# UNIVERSITÉ PARIS-SUD

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## Diplôme d'habilitation à diriger les recherches

Discipline : Mathématiques

*par*

**Dorian LE PEUTREC**

Quelques résultats d'analyse et de probabilités  
autour du laplacien de Witten

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# Liste des travaux effectués

## Travaux effectués depuis la rédaction de ce mémoire

*Sharp spectral asymptotics for non-reversible metastable diffusion processes.*

(Avec L. Michel)

Prépublication sur Arxiv, <https://arxiv.org/abs/1907.09166>, 48 pages (2019).

*Small eigenvalues of the Witten Laplacian with Dirichlet boundary conditions: the case with critical points on the boundary.* (Avec B. Nectoux)

Prépublication sur Arxiv, <https://arxiv.org/abs/1907.07517>, 61 pages (2019).

## Travaux présentés dans ce mémoire

*Repartition of the quasi-stationary distribution and first exit point density for a double-well potential.* (Avec B. Nectoux)

À paraître dans « SIAM Journal on Mathematical Analysis », version Arxiv :

<https://arxiv.org/abs/1902.06304>, 27 pages (2019).

*The exit from a metastable state: concentration of the exit point distribution on the low energy saddle points.* (Avec G. Di Gesù, T. Lelièvre et B. Nectoux)

Prépublication sur Arxiv, <https://arxiv.org/abs/1902.03270>, 113 pages (2019).

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*Part 1.* (Avec G. Di Gesù, T. Lelièvre et B. Nectoux)

Journal de Mathématiques Pures et Appliquées, article « in press » :

<https://doi.org/10.1016/j.matpur.2019.06.003>, 65 pages (2019).

*Part 2.* (Avec T. Lelièvre et B. Nectoux)

Soumis pour publication, 37 pages (2019).

*Exit event from a metastable state and Eyring-Kramers law for the overdamped Langevin dynamics.* (Avec T. Lelièvre et B. Nectoux)

Stochastic Dynamics Out of Equilibrium, IHPStochDyn 2017, Springer Proceedings in Mathematics & Statistics, 282, pages 331–363 (2019)

*Sharp asymptotics of the first exit point density.*

(Avec G. Di Gesù, T. Lelièvre et B. Nectoux)

Annals of PDE, 5(5), 174 pages (2019).

*On Witten Laplacians and Brascamp-Lieb's inequality on manifolds with boundary.*

Integral Equations Operator Theory, 87(3), pages 411–434 (2017).

*Small noise spectral gap asymptotics for a large system of nonlinear diffusions.*  
(Avec G. Di Gesù)  
Journal of Spectral Theory, 7(4), pages 939–984 (2017).

*Jump Markov models and transition state theory : the Quasi-Stationary Distribution approach.* (Avec G. Di Gesù, T. Lelièvre et B. Nectoux)  
Faraday Discussions, 195, pages 469–495 (2016).

*Precise Arrhenius law for  $p$ -forms : The Witten Laplacian and Morse-Barannikov complex.* (Avec F. Nier et C. Viterbo)  
Annales Henri Poincaré, 14(3), pages 567–610 (2013).

*Small eigenvalues of the Witten Laplacian acting on  $p$ -forms on a surface.*  
Asymptotic Analysis, 73(4), pages 187–201 (2011).

### **Travaux effectués en thèse**

*Small eigenvalues of the Neumann realization of the semiclassical Witten Laplacian.*  
Annales de la Faculté des Sciences de Toulouse, 19(3-4), pages 735–809 (2010).

*Local WKB construction for Witten Laplacians on manifolds with boundary.*  
Analysis & PDE, 3(3), pages 227–260 (2010).

*Small singular values of an extracted matrix of a Witten complex.*  
CUBO, A Mathematical Journal, 11(4), pages 49–57 (2009).

# Table des matières

Remerciements	i
Liste des travaux effectués	iii
Introduction	1
<b>1 Autour du laplacien de Witten</b>	<b>5</b>
1.1 Une déformation du laplacien de Hodge . . . . .	5
1.2 Premières propriétés spectrales . . . . .	7
1.2.1 Une version abstraite de la théorie de Hodge . . . . .	7
1.2.2 Application au laplacien de Witten . . . . .	9
1.2.3 Des conditions au bord naturelles . . . . .	13
1.3 Dynamique de Langevin sur-amortie et métastabilité . . . . .	18
1.3.1 Convergence vers l'équilibre . . . . .	18
1.3.2 Régime basse température et métastabilité . . . . .	21
1.3.3 Distribution quasi-stationnaire et métastabilité . . . . .	27
<b>2 Brascamp-Lieb's type inequalities</b>	<b>35</b>
2.1 The case without boundary . . . . .	35
2.2 Notions of Riemannian geometry . . . . .	37
2.3 Witten and weighted Laplacians . . . . .	40
2.4 Results in the case with boundary . . . . .	42
2.4.1 An integration by parts formula . . . . .	42
2.4.2 Consequences: Brascamp-Lieb's type inequalities . . . . .	44
<b>3 Low spectrum of the Witten Laplacian</b>	<b>49</b>
3.1 Landscape of the sublevel sets of a Morse function . . . . .	49
3.1.1 Separating saddle points . . . . .	50
3.1.2 Association between local minima and separating saddle points	51
3.1.3 The case with boundary . . . . .	52
3.1.4 A finer analysis of the landscape of the sublevel sets . . . . .	54
3.2 Sharp bounds on the small eigenvalues and prefactors . . . . .	56
3.2.1 The case of the Witten Laplacian acting on functions . . . . .	56
3.2.2 The case of the Witten Laplacian acting on forms . . . . .	59
3.3 Adapted quasimodes to the computation of the small singular values	60
3.3.1 "Global " quasimodes for functions . . . . .	61
3.3.2 Local quasimodes for 1-forms . . . . .	62
3.3.3 Reduction of the problem to some interaction matrix . . . . .	63
3.3.4 About the case of forms . . . . .	67
3.4 Study of a double-well potential in large dimension . . . . .	68



3.4.1	Description of the model and results . . . . .	68
3.4.2	Comments on the techniques used in this study . . . . .	73
3.5	Some perspectives . . . . .	74
3.5.1	Potentials with critical points on the boundary . . . . .	74
3.5.2	Non reversible overdamped Langevin dynamics . . . . .	75
3.5.3	The case of non Morse potentials . . . . .	76
<b>4</b>	<b>Exit from a metastable state: concentration of the first exit point distribution on the low energy saddle points</b>	<b>79</b>
4.1	The case of a confining well . . . . .	79
4.2	The case of more general wells . . . . .	82
4.2.1	Geometric hypotheses . . . . .	82
4.2.2	Local minima and saddle points of $f$ . . . . .	84
4.2.3	Main results on the exit point distribution . . . . .	85
4.2.4	About the hypotheses . . . . .	89
4.2.5	About the proofs . . . . .	94
4.3	Some perspectives . . . . .	95
4.3.1	Potentials with critical points on the boundary . . . . .	95
4.3.2	Non reversible overdamped Langevin dynamics . . . . .	96
<b>5</b>	<b>Exit from a metastable state: sharp asymptotics of the first exit point distribution</b>	<b>99</b>
5.1	Markov jump process and Eyring-Kramers law . . . . .	99
5.1.1	Kinetic Monte Carlo methods . . . . .	99
5.1.2	Eyring-Kramers law . . . . .	100
5.1.3	Markov jump process and quasi-stationary distribution . . . . .	101
5.2	Results for a confining well . . . . .	103
5.2.1	An adapted Agmon distance . . . . .	103
5.2.2	Main results . . . . .	103
5.2.3	About the hypotheses . . . . .	107
5.2.4	About the proofs . . . . .	110
5.3	Some perspectives . . . . .	114
5.3.1	The standard Eyring-Kramers law . . . . .	114
5.3.2	Case of the general Langevin dynamics . . . . .	115

# Introduction

Ce mémoire présente les travaux que j'ai effectués depuis ma thèse. Dans la continuité de ceux-ci, ils ont pour dénominateur commun la théorie spectrale d'un opérateur de Schrödinger auto-adjoint et positif (une fois muni d'un domaine opérateur approprié) au carrefour de différentes branches des mathématiques, le laplacien de Witten. Comme nous le verrons dans la suite, cet opérateur apparaît par exemple naturellement en topologie différentielle, en théorie de Hodge et en systèmes dynamiques via la théorie de Morse, ainsi qu'en théorie des processus de diffusion et en physique statistique via les dynamiques de Langevin. Il fut introduit par Witten en 1982 dans [Wit82] pour démontrer analytiquement les inégalités de Morse.

Sous la forme « opérateur de Schrödinger » que nous utiliserons par la suite, le laplacien de Witten s'écrit (lorsque l'espace ambiant est  $\mathbb{R}^d$ )

$$\Delta_{f,h}^{(0)} = -h^2 \Delta + |\nabla f|^2 - h \Delta f,$$

où  $f$  est une fonction régulière et  $h > 0$  le paramètre semi-classique. L'exposant <sup>(0)</sup> fait ici référence à la considération de cet opérateur agissant sur les fonctions, i.e. sur les 0-formes, cet opérateur étant plus généralement défini sur l'algèbre des formes différentielles. Sous cette forme générale, il jouit d'une structure algébrique riche, dite supersymétrique, due à sa forme de type « laplacien de Hodge », qui permet de l'analyser très précisément.

Pour être plus précis, ce que nous appellerons structure supersymétrique du laplacien de Witten dans ce mémoire est essentiellement la donnée des propriétés (C) et (E) ci-dessous. En notant  $d$  et  $d^*$  la différentielle extérieure et la codifférentielle (sur  $\mathbb{R}^d$  ou plus généralement sur une variété riemannienne), et

$$d_{f,h} := e^{-\frac{f}{h}}(h d)e^{\frac{f}{h}} \quad \text{et} \quad d_{f,h}^* := e^{\frac{f}{h}}(h d^*)e^{-\frac{f}{h}}$$

leurs déformations « à la Witten », le laplacien de Witten agissant sur les formes différentielles est défini par

$$\Delta_{f,h} := d_{f,h} d_{f,h}^* + d_{f,h}^* d_{f,h}.$$

Il s'écrit donc en particulier comme un carré,

$$(C) \quad \Delta_{f,h} = (d_{f,h} + d_{f,h}^*)^2,$$

et vérifie les relations d'entrelacement

$$(E) \quad \Delta_{f,h} d_{f,h} = d_{f,h} \Delta_{f,h} \quad \text{et} \quad \Delta_{f,h} d_{f,h}^* = d_{f,h}^* \Delta_{f,h}.$$

Les liens du laplacien de Witten avec la physique statistique sont rendus plus clairs par la formule de conjugaison suivante,

$$e^{\frac{f}{h}} \frac{1}{h} \Delta_{f,h}^{(0)} e^{-\frac{f}{h}} = -h\Delta + \nabla V \cdot \nabla, \quad \text{où } V := 2f,$$

montrant que le laplacien de Witten agissant sur les fonctions dans l'espace plat  $L^2(\mathbb{R}^d, dx)$  est unitairement équivalent (au facteur  $h$  près) au laplacien dit à poids

$$L_{V,h}^{(0)} := -h\Delta + \nabla V \cdot \nabla = h\nabla^* \nabla$$

agissant dans l'espace à poids  $L^2(\mathbb{R}^d, e^{-\frac{V}{h}} dx)$ , l'adjoint étant ici considéré formellement dans  $L^2(\mathbb{R}^d, e^{-\frac{V}{h}} dx)$  (l'espace ambiant peut aussi être une variété riemannienne  $\Omega$ , à bord ou non). Pour tout  $\omega \in \mathcal{C}_c^\infty(\mathbb{R}^d)$ , on a en particulier

$$\langle L_{V,h}^{(0)} \omega, \omega \rangle_{L^2(\mathbb{R}^d, e^{-\frac{V}{h}} dx)} = h \|\nabla \omega\|_{L^2(\mathbb{R}^d, e^{-\frac{V}{h}} dx)}^2,$$

d'où l'on déduit facilement que l'extension de Friedrichs de  $L_{V,h}^{(0)}$  agissant sur  $\mathcal{C}_c^\infty(\mathbb{R}^d)$  dans  $L^2(\mathbb{R}^d, e^{-\frac{V}{h}} dx)$ , toujours notée  $L_{V,h}^{(0)}$ , est associée à la forme quadratique  $Q_{V,h}^{(0)}$  de domaine  $H^1(\mathbb{R}^d, e^{-\frac{V}{h}} dx)$ , où :

$$\forall \omega \in H^1(\mathbb{R}^d, e^{-\frac{V}{h}} dx), \quad Q_{V,h}^{(0)}(\omega, \omega) = h \|\nabla \omega\|_{L^2(\mathbb{R}^d, e^{-\frac{V}{h}} dx)}^2.$$

Le noyau de  $L_{V,h}^{(0)}$  est donc non nul si et seulement si  $1 \in L^2(\mathbb{R}^d, e^{-\frac{V}{h}} dx)$ , i.e. si et seulement si  $e^{-\frac{V}{h}} \in L^1(\mathbb{R}^d, dx)$ , auquel cas il est engendré par 1.

Le laplacien à poids est le générateur infinitésimal du processus stochastique de Langevin sur-amorti

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

où  $X_t \in \mathbb{R}^d$  et  $(B_t)_{t \geq 0}$  est un mouvement brownien standard de dimension  $d$ . Ce processus est un modèle prototypique utilisé en physique statistique pour simuler l'évolution d'un système moléculaire à température fixée, auquel cas  $V$  est l'énergie potentielle et  $h$  est proportionnel à la température. Puisque l'évolution des observables est donnée par le semigroupe  $e^{-tL_{V,h}^{(0)}}$ , l'existence d'un équilibre pour la dynamique de Langevin sur-amortie équivaut à l'appartenance de  $e^{-\frac{V}{h}}$  à  $L^1(\mathbb{R}^d, dx)$ , auquel cas cette dynamique admet pour unique mesure (de probabilité) invariante

$$m_{V,h}(dx) := \left( \int_{\mathbb{R}^d} e^{-\frac{V}{h}} dx \right)^{-1} e^{-\frac{V}{h}} dx.$$

Les propriétés de retour à l'équilibre de la dynamique de Langevin sur-amortie sont donc intimement liées au comportement du bas spectre de  $L_{V,h}^{(0)}$ , ou de façon équivalente de  $\Delta_{f,h}^{(0)}$ . Dans la limite basse température  $h \rightarrow 0^+$ , lorsque  $e^{-\frac{V}{h}} \in L^1(\mathbb{R}^d, dx)$  pour tout  $h > 0$  assez petit, ce retour à l'équilibre est typiquement exponentiellement long, i.e. d'ordre  $\mathcal{O}(e^{\frac{C}{h}})$  pour un certain  $C > 0$  indépendant de  $h$ ; le processus est alors dit métastable. Du point de vue spectral, ce phénomène est caractérisé par l'existence de valeurs propres exponentiellement petites, i.e. d'ordre  $\mathcal{O}(e^{-\frac{C}{h}})$ , pour le laplacien de Witten  $\Delta_{f,h}^{(0)}$ .

Dans le premier chapitre introductif de ce mémoire, nous détaillons précisément la rapide présentation du laplacien de Witten faite ci-dessus et introduisons les problématiques traitées dans les chapitres suivants. Celles-ci portent sur les propriétés spectrales de cet opérateur et sur l'étude du phénomène de métastabilité de la dynamique de Langevin sur-amortie.

Le deuxième chapitre est consacré à notre travail [Lep17] sur l'obtention d'inégalités de type Brascamp-Lieb, pour les formes différentielles sur une variété riemannienne compacte à bord  $\Omega$ , à l'aide de la structure supersymétrique du laplacien de Witten. Il s'agit d'inégalités reposant sur des propriétés de convexité du potentiel  $V$  définissant le laplacien à poids qui généralisent dans ce cadre les inégalités de type Poincaré de la forme

$$\exists C > 0, \quad \forall \omega \in H^1(\Omega, e^{-V} d\text{Vol}_\Omega),$$

$$\|\omega - \left( \int_\Omega \omega e^{-V} d\text{Vol}_\Omega \right)\|_{L^2(\Omega, e^{-V} d\text{Vol}_\Omega)}^2 \leq \frac{1}{C} \|\nabla \omega\|_{L^2(\Omega, e^{-V} d\text{Vol}_\Omega)}^2,$$

équivalentes à la minoration du trou spectral de  $L_{V,1}^{(0)}$  (par  $C$ ). Mis à part le chapitre introductif de ce mémoire, c'est le seul chapitre dans lequel nous nous intéressons au laplacien de Witten et à son homologue le laplacien à poids lorsque  $h$  est fixé (égal à 1) et non à leurs comportements asymptotiques à la limite  $h \rightarrow 0^+$ .

Le troisième chapitre de ce mémoire porte sur l'obtention d'asymptotiques précises à la limite  $h \rightarrow 0^+$ , dites de type Eyring-Kramers en référence à la cinétique chimique, pour les valeurs propres exponentiellement petites non nulles du laplacien de Witten. Nous y expliquons la stratégie générale utilisée dans différents travaux des quinze dernières années permettant *in fine* de prouver de telles asymptotiques, i.e. des asymptotiques de la forme

$$A h^p e^{-\frac{C}{h}} (1 + o(1)), \quad \text{où } A > 0, C > 0 \text{ et } p \in \mathbb{R} \text{ sont explicites,}$$

avec des méthodes d'analyse semi-classique. À partir de ce troisième chapitre, les potentiels  $f$  considérés seront toujours de type Morse, assurant l'existence de formules précises du type précédent. Nos travaux réalisés depuis la thèse concernés par ce chapitre sont :

- [DLLN19b]<sup>1</sup>, en collaboration avec Giacomo Di Gesù, Tony Lelièvre et Boris Nectoux, dans le cas des 0-formes et de variétés à bord avec des conditions au bord de Dirichlet,
- [Lep11] et [LNV13], le second en collaboration avec Francis Nier et Claude Viterbo, dans le cas général des formes différentielles sur une variété sans bord,
- et [DL17], en collaboration avec Giacomo Di Gesù, portant sur l'étude d'un potentiel explicite en grande dimension.

Les deux derniers chapitres sont principalement consacrés à nos travaux [DLLN19a] et [DLLN17b] en collaboration avec Giacomo Di Gesù, Tony Lelièvre et Boris Nectoux, et dans une moindre mesure à [LN19a], en collaboration avec Boris Nectoux. Ils

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1. Cet article constitue la première partie de la prépublication [DLLN19a], qui a été divisée en deux parties thématiques pour publication.

portent sur l'étude de l'évènement de sortie, à la limite basse température  $h \rightarrow 0^+$ , du processus de Langevin sur-amorti d'un domaine borné  $\Omega$  de  $\mathbb{R}^d$  (ou d'une variété riemannienne compacte à bord). Ces travaux sont par ailleurs aussi résumés dans les articles de type compte rendu [DLLN17a, LLN18] et la prépublication [DLLN19a] a été divisé en deux parties pour publication, avec pour première partie [DLLN19b]. Dans ces travaux et ces deux derniers chapitres, nous cherchons à analyser précisément, lorsque  $h \rightarrow 0^+$ , l'évènement de sortie du processus de Langevin sur-amorti de  $\Omega$ , caractérisé par le temps de sortie et le lieu de sortie de ce domaine, lorsque le processus est initialement distribué selon une distribution naturelle appelée distribution quasi-stationnaire.

Cette distribution est définie à partir de l'état fondamental de la réalisation de Dirichlet  $L_{V,h}^{D,(0)}$  du laplacien à poids  $L_{V,h}^{(0)}$  sur  $\Omega$ . L'évènement de sortie du processus, initialement distribué selon la distribution quasi-stationnaire, est de plus entièrement caractérisé en termes de propriétés spectrales de  $L_{V,h}^{D,(0)}$ . À partir des résultats obtenus partant de cette distribution naturelle, nous considérons aussi l'évènement de sortie partant de conditions initiales déterministes.

Les deux derniers chapitres de ce mémoire sont plus précisément organisés comme suit. Le quatrième chapitre concerne les lieux de sorties les plus probables pour la dynamique de Langevin sur-amortie, i.e. les lieux de  $\partial\Omega$  au voisinage desquels la probabilité de sortie du processus ne tend pas vers 0 à la limite  $h \rightarrow 0^+$ . Nous y présentons notamment des hypothèses géométriques générales sur le comportement de la fonction de Morse  $V$  sur le domaine  $\Omega$  assurant que l'ensemble des lieux de sortie les plus probables soit contenu dans  $\arg \min_{\partial\Omega} V = (V|_{\partial\Omega})^{-1}(\min_{\partial\Omega} V)$ . Cela généralise ainsi de nombreux résultats obtenus pour des dynamiques très générales, mais pour lesquelles  $\Omega$  est un puits confinant du potentiel  $V$ , à des domaines  $\Omega$  beaucoup plus généraux.

Enfin, le cinquième et dernier chapitre concerne l'analyse précise globale, i.e. sur tout  $\partial\Omega$ , du lieu de sortie de la dynamique de Langevin sur-amortie à la limite  $h \rightarrow 0^+$  lorsque  $\Omega$  est un puits confinant du potentiel  $V$ . Les résultats obtenus permettent en particulier de justifier dans ce cadre la validité asymptotique de la loi d'Eyring-Kramers, utilisée en pratique dans de nombreux algorithmes de simulation moléculaire.

# Chapitre 1

## Autour du laplacien de Witten

### 1.1 Une déformation du laplacien de Hodge

Dans cette première section, nous introduisons quelques notations de géométrie riemannienne et l'opérateur différentiel « laplacien de Witten », qui est une déformation du laplacien de Hodge à partir d'une fonction régulière  $f$ , sur une variété riemannienne lisse. Nous définissons ici cet opérateur comme opérateur agissant sur les distributions, ou plus précisément sur les courants de de Rham. Nous le considérerons par la suite en tant qu'opérateur non borné avec différents domaines dans l'espace de Hilbert des formes différentielles de carré intégrable.

Introduisons donc une variété riemannienne lisse orientée et connexe  $(\Omega, g = \langle \cdot, \cdot \rangle)$  de dimension  $d$ . On suppose de plus que :

- la variété  $\Omega$  est compacte, de bord  $\partial\Omega$  éventuellement non vide,
- ou la variété  $\Omega$  est l'espace  $\mathbb{R}^d$  muni de sa métrique plate usuelle.

Le fibré cotangent (resp. tangent) de  $\Omega$  est noté  $T^*\Omega$  (resp.  $T\Omega$ ) et le fibré des formes différentielles (non régulières) est noté  $\Lambda T^*\Omega = \bigoplus_{p=0}^d \Lambda^p T^*\Omega$ . Lorsque  $\partial\Omega$  est non vide, les fibrés  $T^*\partial\Omega$ ,  $T\partial\Omega$  et  $\Lambda T^*\partial\Omega = \bigoplus_{p=0}^{d-1} \Lambda^p T^*\partial\Omega$  sont définis de la même façon. Le produit scalaire sur  $\Lambda^p T^*\Omega$  hérité de  $g$  sera noté  $\langle \cdot, \cdot \rangle_{\Lambda^p}$ . L'espace des sections  $\mathcal{C}^\infty$ ,  $L^2$ , etc. sur  $O = \Omega$  ou  $O = \partial\Omega$  de l'un des fibrés  $E$  définis ci-dessus sera noté  $\mathcal{C}^\infty(O, E)$ ,  $L^2(O, E)$ , etc.. La notation plus compacte  $\Lambda^p \mathcal{C}^\infty(\Omega)$ ,  $\Lambda^p L^2(\Omega)$ ,  $\Lambda L^2(\Omega)$  etc. sera également utilisée à la place de  $\mathcal{C}^\infty(\Omega, \Lambda^p T^*\Omega)$ ,  $L^2(\Omega, \Lambda^p T^*\Omega)$ ,  $L^2(\Omega, \Lambda T^*\Omega)$  etc.. Les espaces  $L^2$  considérés sont définis à partir des mesures riemanniennes naturelles  $\mu$  sur  $\Omega$  et  $\mu_{\partial\Omega}$  sur  $\partial\Omega$ . Le produit scalaire  $\Lambda^p L^2(\Omega)$  et la norme correspondant à  $\mu$  seront notés  $\langle \cdot, \cdot \rangle_{\Lambda^p L^2}$  et  $\| \cdot \|_{\Lambda^p L^2}$ , ou plus simplement  $\langle \cdot, \cdot \rangle_{L^2}$  et  $\| \cdot \|_{L^2}$  quand aucune confusion n'est possible.

Pour  $p \in \{0, \dots, d\}$ , soit  $\mathcal{D}'^{(p)}(\Omega)$  l'espace des courants de de Rham (i.e. des distributions) agissant sur l'espace  $\Lambda^p \mathcal{C}_c^\infty(\Omega)$  des formes différentielles régulières de degré  $p$  à support compact dans  $\Omega \setminus \partial\Omega^1$  et  $\mathcal{D}'(\Omega) = \bigoplus_{p=0}^d \mathcal{D}'^{(p)}(\Omega)$ . On note  $d : \mathcal{D}'(\Omega) \rightarrow \mathcal{D}'(\Omega)$  la différentielle extérieure et  $d^* : \mathcal{D}'(\Omega) \rightarrow \mathcal{D}'(\Omega)$  son adjoint formel. Le laplacien de Hodge  $\Delta_H : \mathcal{D}'(\Omega) \rightarrow \mathcal{D}'(\Omega)$  est alors l'opérateur différentiel défini par la relation

$$\Delta_H := d^*d + dd^* = (d + d^*)^2,$$

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1. Remarquons qu'avec la notation adoptée dans cette partie, on a toujours  $\partial\Omega \subset \Omega$ .

la dernière égalité découlant de la propriété  $d^2 = (d^*)^2 = 0$ . Lorsque  $\Omega = \mathbb{R}^d$ , le laplacien de Hodge agissant sur les 0-formes est donc l'opposé du laplacien usuel  $\Delta$ .

Étant donnée une fonction régulière  $f : \Omega \rightarrow \mathbb{R}$ , les opérateurs différentiels déformés « à la Witten »  $d_f : \mathcal{D}'(\Omega) \rightarrow \mathcal{D}'(\Omega)$  et  $d_f^* : \mathcal{D}'(\Omega) \rightarrow \mathcal{D}'(\Omega)$  sont définis par les relations

$$d_f := e^{-f} d e^f \quad \text{et} \quad d_f^* := e^f d^* e^{-f}, \quad (1.1.1)$$

et le laplacien de Witten  $\Delta_f : \mathcal{D}'(\Omega) \rightarrow \mathcal{D}'(\Omega)$  est alors défini de façon analogue au laplacien de Hodge par la relation

$$\Delta_f := d_f^* d_f + d_f d_f^* = (d_f + d_f^*)^2. \quad (1.1.2)$$

Notons d'ores et déjà la structure supersymétrique du laplacien de Witten (et donc aussi du laplacien de Hodge) sur laquelle nous reviendrons plus longuement dans les parties suivantes : pour tout  $u$  dans  $\mathcal{D}'^{(p)}(\Omega)$ , on a

$$\Delta_f^{(p+1)} d_f^{(p)} u = d_f^{(p)} \Delta_f^{(p)} u \quad \text{et} \quad \Delta_f^{(p-1)} d_f^{(p-1),*} u = d_f^{(p-1),*} \Delta_f^{(p)} u,$$

où l'exposant  $(p)$  signifie que nous considérons l'action de l'opérateur différentiel concerné sur les courants de dimension  $p$ .

Notons de plus  $\wedge$  et  $\mathbf{i}$  les produits extérieur et intérieur,  $\nabla$  le gradient et  $\mathcal{L}$  la dérivée de Lie (d'adjoint formel  $\mathcal{L}^*$ ). Notons aussi  $\sharp : \xi \mapsto \xi^\sharp$  l'isomorphisme canonique de  $T^*\Omega$  sur  $T\Omega$ , défini par la relation  $\langle \xi^\sharp, X \rangle := \xi(X)$  pour tout  $X \in T\Omega$ , et  $\flat : X \mapsto X^\flat$  son isomorphisme inverse. D'après les relations

$$\begin{aligned} (df \wedge)^* &= \mathbf{i}_{\nabla f} \quad \text{au sens des opérateurs bornés dans } \Lambda L^2(\Omega), \\ d_f &= d + df \wedge, \\ d_f^* &= d^* + \mathbf{i}_{\nabla f}, \\ \mathcal{L}_X &= d \circ \mathbf{i}_X + \mathbf{i}_X \circ d \quad \text{et} \quad \mathcal{L}_X^* = d^* \circ (X^\flat \wedge \cdot) + X^\flat \wedge d^*, \end{aligned}$$

le laplacien de Witten est simplement l'opérateur de type Schrödinger suivant :

$$\Delta_f = \Delta_H + |\nabla f|^2 + (\mathcal{L}_{\nabla f} + \mathcal{L}_{\nabla f}^*). \quad (1.1.3)$$

Sa restriction aux courants de dimension 0, i.e. aux distributions usuelles, a en particulier la forme

$$\Delta_f^{(0)} = d_f^{(0),*} d_f^{(0)} = \Delta_H + |\nabla f|^2 + \Delta_H f.$$

Mentionnons également la formule suivante (cf. [Jam12, Lep17] et le chapitre 2 pour plus de détails) satisfaite par le laplacien de Witten :

$$\Delta_f^{(p)} = \Delta_H + |\nabla f|^2 + 2 \text{Hess}^{(p)} f + \Delta_H f. \quad (1.1.4)$$

Dans la suite, nous nous intéresserons particulièrement au laplacien de Witten semi-classique, c'est-à-dire à l'opérateur différentiel suivant, où  $h$  est un réel strictement positif :

$$\Delta_{f,h} := h^2 \Delta_{\frac{f}{h}} = h^2 \Delta_H + |\nabla f|^2 + h (\mathcal{L}_{\nabla f} + \mathcal{L}_{\nabla f}^*) \quad (1.1.5)$$

$$= (d_{f,h} + d_{f,h}^*)^2, \quad (1.1.6)$$

où

$$d_{f,h} := h d_{\frac{f}{h}} = e^{-\frac{f}{h}} h d e^{\frac{f}{h}} = h d + df \wedge \quad (1.1.7)$$

et

$$d_{f,h}^* := h d_{\frac{f}{h}}^* = e^{\frac{f}{h}} h d^* e^{-\frac{f}{h}} = h d^* + \mathbf{i}_{\nabla f}. \quad (1.1.8)$$

## 1.2 Premières propriétés spectrales

Commençons cette section par une présentation abstraite de la théorie de Hodge à laquelle nous ferons référence lorsque, appliquée au laplacien de Witten, nous évoquerons la structure supersymétrique de cet opérateur. Cette présentation est en partie inspirée de [JMM09, GMM11] où les auteurs considèrent notamment le laplacien de Hodge sur des domaines de  $\mathbb{R}^d$  ou des variétés riemanniennes lipschitziennes. Elle diffère légèrement de celle suivie en général dans les travaux présentés dans ce texte, à l'exception de [DLLN17b, Section 4.1] (où nous renvoyons en particulier à la section 4.1.1 à ce sujet).

### 1.2.1 Une version abstraite de la théorie de Hodge

La proposition suivante réunit différents résultats spectraux impliquant les décompositions de type théorie de Hodge énoncées dans le corollaire 1.2.2. Pour une preuve, nous renvoyons par exemple à [GMM11, Section 2] (et plus précisément aux propositions 2.3 et 2.4, au corollaire 2.5 et au théorème 2.8).

**Proposition 1.2.1.** *Soit  $(H, \|\cdot\|_H)$  un espace de Hilbert et  $T : D(T) \subset H \rightarrow H$  un opérateur non borné fermé à domaine dense tel que*

$$\text{Ran } T \subset \text{Ker } T \quad \text{et} \quad D(T) \cap D(T^*) \quad \text{s'injecte de façon compacte dans } H,$$

où  $D(T) \cap D(T^*)$  est muni de la norme du graphe

$$\|u\|_{D(T) \cap D(T^*)} := \sqrt{\|u\|_H^2 + \|Tu\|_H^2 + \|T^*u\|_H^2}.$$

Nous avons alors les propriétés suivantes :

i) *L'opérateur  $(T + T^*, D(T) \cap D(T^*))$  est auto-adjoint à résolvante compacte et vérifie*

$$\text{Ker } (T + T^*) = \text{Ker } T \cap \text{Ker } T^*.$$

*En particulier, l'espace vectoriel  $D(T) \cap D(T^*)$  est dense dans  $H$  et  $T + T^*$  est un opérateur auto-adjoint de Fredholm d'indice 0, c-à-d*

$$\text{Ker } T \cap \text{Ker } T^* \quad \text{est de dimension finie et} \quad \text{Ran } (T + T^*) = (\text{Ker } T \cap \text{Ker } T^*)^\perp.$$

ii) *L'opérateur  $\Delta := TT^* + T^*T$  muni du domaine*

$$D(\Delta) := \{u \in D(T) \cap D(T^*) \text{ t.q. } Tu \in D(T^*) \text{ et } T^*u \in D(T)\}$$

*est un opérateur auto-adjoint positif dont le noyau vérifie*

$$\text{Ker } \Delta = \text{Ker } T \cap \text{Ker } T^* = \text{Ker } (T + T^*).$$

*En particulier,  $\Delta$  a une résolvante compacte (puisque  $D(\Delta)$  muni de la norme du graphe s'injecte continûment dans  $D(T) \cap D(T^*)$ ) et est l'extension de Friedrichs associée à la forme quadratique fermée positive  $Q$  sur  $D(T) \cap D(T^*)$  définie par*

$$Q(u, v) := \langle Tu, Tv \rangle_H + \langle T^*u, T^*v \rangle_H.$$



Dans la proposition précédente, en supposant uniquement  $\text{Ran } T \subset \text{Ker } T$ , c-à-d sans l'hypothèse d'injection compacte, il est toujours vrai que  $(T+T^*, D(T) \cap D(T^*))$  et  $(\Delta, D(\Delta))$  sont auto-adjoints et vérifient

$$\text{Ker } \Delta = \text{Ker } T \cap \text{Ker } T^* = \text{Ker } (T + T^*).$$

Cette hypothèse de compacité est de plus vérifiée dans tous nos travaux présentés dans ce mémoire. Cela découle du fait que nous y considérons toujours des variétés différentielles compactes  $\Omega$ , pour lesquelles  $D(T) \cap D(T^*)$  est au moins inclus dans l'espace de Sobolev  $\Lambda H^{\frac{1}{2}}(\Omega)$  (et à l'exception d'une partie assez technique de [DLLN17b] expliquée dans la section 5.2.4, toujours inclus dans  $\Lambda H^1(\Omega)$ ) et du théorème d'injection compacte de Rellich (cf. la partie suivante pour plus de détails). Cette hypothèse tombe par contre en général en défaut lorsque  $\Omega = \mathbb{R}^d$  mais des hypothèses classiques supplémentaires de confinement à l'infini permettent de se ramener à un cadre proche (cf. la partie 1.3.2 et le chapitre 3).

Signalons aussi que la démonstration de [GMM11] repose largement sur le fait que l'opérateur  $(\Delta, D(\Delta))$  tel que défini au point ii) est auto-adjoint, ce qui avait déjà été remarqué par Gaffney dès 1955 dans [Gaf55].

Enfin, notons les conséquences suivantes de la proposition 1.2.1 soulignant plus précisément ce que nous entendons par structure supersymétrique de l'opérateur  $\Delta$  : lorsque  $T$  vérifie les hypothèses de la proposition 1.2.1, les relations suivantes sont vérifiées pour tous  $z \in \mathbb{C} \setminus \text{Sp } (\Delta)$ ,  $u \in D(T)$  et  $u' \in D(T^*)$  :

$$(z - \Delta)^{-1} T u = T (z - \Delta)^{-1} u \quad \text{et} \quad (z - \Delta)^{-1} T^* u' = T^* (z - \Delta)^{-1} u'. \quad (1.2.1)$$

Démontrons la première relation, la seconde se démontrant de façon analogue. Considérons pour cela  $u \in D(T)$  et définissons  $v = (z - \Delta)^{-1} u$  pour un  $z \in \mathbb{C} \setminus \text{Sp } (\Delta)$  arbitraire. On a alors  $v \in D(\Delta)$  et  $(z - \Delta)v = u \in D(T)$ , ce qui implique  $\Delta v = T^* T v + T T^* v \in D(T)$  et donc, puisque  $\text{Ran } T \subset \text{Ker } T$ ,  $T^* T v \in D(T)$ . On a en particulier  $T v \in D(T T^*)$ , donc aussi  $T v \in D(\Delta)$ , et les relations suivantes sont vérifiées :

$$(z - \Delta) T v = z T v - T T^* T v = T (z - \Delta) v = T u \quad \text{et donc} \quad T v = (z - \Delta)^{-1} T u,$$

d'où la première relation de (1.2.1).

Une conséquence presque immédiate de (1.2.1) est la suivante : pour n'importe quelle valeur propre  $\lambda$  de  $\Delta$  et n'importe quel vecteur propre associé  $u \in D(\Delta)$ , les éléments  $T u \in D(\Delta)$  et  $T^* u \in D(\Delta)$  appartiennent à  $D(\Delta)$  et

$$T \Delta u = \Delta T u = \lambda T u \quad \text{et} \quad T^* \Delta u = \Delta T^* u = \lambda T^* u \quad (1.2.2)$$

Remarquons aussi que si de plus  $\lambda \neq 0$ , alors l'un au moins des deux éléments  $T u, T^* u$  est non nul (puisque alors  $u \notin \text{Ker } \Delta = \text{Ker } T \cap \text{Ker } T^*$ ).

Nous concluons cette partie par le corollaire suivant de la proposition 1.2.1 sur la décomposition de Hodge dans ce cadre.

**Corollaire 1.2.2.** *Supposons les hypothèses de la proposition 1.2.1 satisfaites et définissons  $\Delta := T T^* + T^* T$  de la même façon. Nous avons alors les décompositions orthogonales suivantes :*

$$H = \text{Ran } T \oplus^\perp \text{Ran } T^* \oplus^\perp \text{Ker } \Delta$$

et, pour  $\mathbf{T} = T$  ou  $\mathbf{T} = T^*$ ,

$$\text{Ker } \mathbf{T} = \text{Ran } \mathbf{T} \oplus^\perp \text{Ker } \Delta.$$

En particulier, les opérateurs  $T$  et  $T^*$  ont leurs images fermées et

$$\text{Ker } T/\text{Ran } T \simeq \text{Ker } T^*/\text{Ran } T^* \simeq \text{Ker } \Delta.$$

## 1.2.2 Application au laplacien de Witten

Nous supposons dans cette partie que  $\Omega$  est compacte et que sa frontière  $\partial\Omega$  est vide. Le cas  $\partial\Omega$  non vide est l'objet de la partie suivante.

Soit  $f : \Omega \rightarrow \mathbb{R}$  une fonction régulière et l'opérateur différentiel non borné dans  $\Lambda L^2(\Omega)$  suivant (cf. (1.1.1)) :

$$\begin{aligned} d_f \text{ muni du domaine } \quad D(d_f) &:= \{u \in \Lambda L^2(\Omega), d_f u \in \Lambda L^2(\Omega)\} \\ &= \{u \in \Lambda L^2(\Omega), du \in \Lambda L^2(\Omega)\}. \end{aligned}$$

Lorsque  $f = 0$ , on le notera simplement  $(d, D(d))$  au lieu de  $(d_0, D(d_0))$ . Il s'agit d'un opérateur fermé à domaine dense satisfaisant la relation  $\text{Ran } d_f \subset \text{Ker } d_f$  et son adjoint est simplement l'opérateur différentiel

$$\begin{aligned} d_f^* \text{ muni du domaine } \quad D(d_f^*) &= \{u \in \Lambda L^2(\Omega), d_f^* u \in \Lambda L^2(\Omega)\} \\ &= \{u \in \Lambda L^2(\Omega), d^* u \in \Lambda L^2(\Omega)\}. \end{aligned}$$

Par conséquent, puisque

$$D(d_f) \cap D(d_f^*) = D(d) \cap D(d^*) = \Lambda H^1(\Omega),$$

la dernière égalité découlant de l'ellipticité du laplacien de Hodge, l'opérateur  $d_f$  muni du domaine  $D(d_f)$  vérifie les hypothèses de la proposition 1.2.1. Le laplacien de Witten  $\Delta_f = d_f d_f^* + d_f^* d_f$  (cf. (1.1.2)) muni du domaine

$$D(\Delta_f) = \{u \in D(d_f) \cap D(d_f^*) \text{ t.q. } d_f u \in D(d_f^*) \text{ et } d_f^* u \in D(d_f)\} = \Lambda H^2(\Omega)$$

est donc auto-adjoint positif et à résolvante compacte dans  $\Lambda L^2(\Omega)$ . La dernière égalité se déduit encore de résultats classiques de régularité elliptique, impliquant par exemple que l'opérateur  $(\Delta_f, \Lambda H^2(\Omega))$  est auto-adjoint, d'où l'on déduit l'égalité des opérateurs auto-adjoints comparables  $(\Delta_f, \Lambda H^2(\Omega)) \subset (\Delta_f, D(\Delta_f))$ . Notons aussi que par densité de  $\Lambda \mathcal{C}^\infty(\Omega)$  dans  $\Lambda H^2(\Omega)$ , le laplacien de Witten  $\Delta_f$  muni du domaine  $\Lambda \mathcal{C}^\infty(\Omega)$  est essentiellement auto-adjoint dans  $\Lambda L^2(\Omega)$ .

En introduisant maintenant, pour un réel  $h > 0$  quelconque, les opérateurs semi-classiques associés  $d_{f,h} = h d_{\frac{f}{h}}$ ,  $d_{f,h}^* = h d_{\frac{f}{h}}^*$  et  $\Delta_{f,h} = h^2 \Delta_{\frac{f}{h}}$  (cf. (1.1.5)–(1.1.8)), il découle du corollaire 1.2.2 le fait remarquable suivant souligné par Witten dans son célèbre article [Wit82] : pour tout  $h > 0$ ,

$$\begin{aligned} \text{Ker } \Delta_{f,h} &\simeq \text{Ker } d_{f,h}/\text{Ran } d_{f,h} = \text{Ker } (e^{-\frac{f}{h}} h d e^{\frac{f}{h}})/\text{Ran } (e^{-\frac{f}{h}} h d e^{\frac{f}{h}}) \\ &\simeq \text{Ker } d/\text{Ran } d \\ &\simeq \text{Ker } \Delta_0, \end{aligned}$$

où  $\Delta_0$  n'est autre que la réalisation auto-adjointe du laplacien de Hodge. En particulier, pour tout  $p \in \{0, \dots, d\}$ , la dimension de  $\text{Ker } \Delta_{f,h}^{(p)}$  est indépendante de  $f$  et de  $h$ , et on a plus précisément la relation suivante :

$$\dim \text{Ker } \Delta_{f,h}^{(p)} = \dim \text{Ker } \Delta_0^{(p)} = \mathbf{b}_p(\Omega), \quad (1.2.3)$$

où, d'après le théorème de Hodge-de Rham, le nombre de Betti  $\mathbf{b}_p(\Omega)$  est la dimension du  $p$ -ième groupe de cohomologie singulière réelle de  $\Omega$ .

Nous avons de plus le résultat d'analyse semi-classique fondamental suivant énoncé par Witten dans [Wit82] puis rigoureusement démontré par Helffer-Sjöstrand dans [HS85c]. Avant de l'énoncer, rappelons d'abord que la fonction régulière  $f$  est dite de Morse si ses points critiques sont non dégénérés et que l'indice d'un point critique non dégénéré  $a$  de  $f$  est le nombre de valeurs propres négatives de  $\text{Hess } f(a)$ .

**Théorème 1.2.3.** *Supposons la fonction régulière  $f : \Omega \rightarrow \mathbb{R}$  de Morse et notons, pour  $p \in \{0, \dots, d\}$ ,  $\mathbf{m}_p \in \mathbb{N}$  le nombre de points critiques de  $f$  d'indice  $p$ . Il existe alors  $h_0 > 0$  et  $C > 0$  tels que, pour tous  $h \in (0, h_0]$  et  $p \in \{0, \dots, d\}$ , on a*

$$\text{Sp}(\Delta_{f,h}^{(p)}) \cap [0, Ch] = \text{Sp}(\Delta_{f,h}^{(p)}) \cap [0, e^{-\frac{C}{h}}]$$

et

$$\text{Card}(\text{Sp}(\Delta_{f,h}^{(p)}) \cap [0, Ch]) = \mathbf{m}_p,$$

où les valeurs propres sont comptées avec multiplicité.

Le théorème 1.2.3 et l'équation 1.2.3 soulignent le lien entre certaines caractéristiques de la fonction de Morse  $f$  sur  $\Omega$  (les indices de ses points critiques) et certains invariants topologiques de cette variété (ses nombres de Betti). Ces résultats conduisent notamment aux inégalités de Morse – l'objet de l'article de Witten [Wit82] était justement leur démonstration par une approche analytique! – que l'on peut par exemple énoncer comme suit :

**Théorème 1.2.4.** *Soient  $f : \Omega \rightarrow \mathbb{R}$  une fonction de Morse et, pour  $p \in \{0, \dots, d\}$ ,  $\mathbf{m}_p \in \mathbb{N}$  le nombre de points critiques de  $f$  d'indice  $p$  et  $\mathbf{b}_p(\Omega)$  la dimension du  $p$ -ième groupe de cohomologie de de Rham de  $\Omega$ . On a alors les relations suivantes :*

$$\forall p \in \{0, \dots, d\}, \quad \mathbf{b}_p(\Omega) \leq \mathbf{m}_p \quad (\text{inégalités faibles de Morse})$$

et

$$\sum_{p=0}^d (-1)^p (\mathbf{m}_p - \mathbf{b}_p(\Omega)) = 0.$$

Démontrons ici le théorème 1.2.4, cela n'étant plus très long compte tenu de ce qui précède. D'abord, les inégalités faibles de Morse s'obtiennent immédiatement du théorème 1.2.3 et de (1.2.3) :

$$\begin{aligned} \forall p \in \{0, \dots, d\}, \quad \mathbf{b}_p(\Omega) &= \dim \text{Ker } \Delta_{f,h}^{(p)} \\ &\leq \text{Card}(\text{Sp}(\Delta_{f,h}^{(p)}) \cap [0, Ch]) = \mathbf{m}_p. \end{aligned} \quad (1.2.4)$$

Ensuite, en définissant  $F_h^{(p)} := \text{Ran } \mathbf{1}_{[0, Ch]}(\Delta_{f,h}^{(p)})$  pour  $p \in \{0, \dots, d\}$  et  $h \in (0, h_0]$ , il découle du théorème 1.2.3 et de la propriété de supersymétrie (1.2.2) que la suite

$$\{0\} \longrightarrow F_h^{(0)} \xrightarrow{d_{F_h^{(0)}}} F_h^{(1)} \xrightarrow{d_{F_h^{(1)}}} \dots \longrightarrow F_h^{(n)} \xrightarrow{d_{F_h^{(n)}}} \{0\} \quad (1.2.5)$$

est un complexe de cochaîne (de dimension finie), ce qui signifie que  $\text{Ran } d|_{F_h^{(p)}} \subset \text{Ker } d|_{F_h^{(p+1)}}$  pour  $p \in \{0, \dots, d-1\}$ . Puisque, pour tout  $p \in \{0, \dots, d\}$ , on a

$$\dim F_h^{(p)} = \mathbf{m}_p \quad \text{et} \quad \mathbf{b}_p(\Omega) = \dim \text{Ker } \Delta_{f,h}^{(p)} = \dim \text{Ker } (d|_{F_h^{(p)}}) / \text{Ran } (d|_{F_h^{(p-1)}}),$$

il vient, d'après le théorème du rang,

$$\sum_{p=0}^d (-1)^p (\mathbf{m}_p - \mathbf{b}_p(\Omega)) = 0,$$

ce qui termine la démonstration du théorème 1.2.4.

Dans la suite de ce mémoire, et en particulier dans le chapitre 3, nous nous intéresserons notamment à la forme précise des valeurs propres exponentiellement petites du laplacien de Witten exhibées dans le théorème 1.2.3 : nous chercherons à comprendre précisément les échelles exponentielles en jeu ainsi que les valeurs des préfacteurs, i.e. à obtenir des formules du type Eyring-Kramers, c-à-d de la forme

$$\lambda_{k,h}^{(p)} = A_{k,p} h^{\ell_{k,p}} e^{-\frac{C_{k,p}}{h}} (1 + o(1)), \quad \text{où } A_{k,p} \in \mathbb{R}^+, \ell_{k,p} \in \mathbb{R} \text{ et } C_{k,p} > 0. \quad (1.2.6)$$

Ici,  $0 \leq \lambda_{1,h}^{(p)} \leq \dots \leq \lambda_{\mathbf{m}_p,h}^{(p)}$  sont, pour  $p \in \{0, \dots, d\}$  et  $k \in \{1, \dots, \mathbf{m}_p\}$ , les valeurs propres exponentiellement petites (comptées avec multiplicité) du laplacien de Witten  $\Delta_{f,h}^{(p)}$ .

Les coefficients  $C_{k,p}$  apparaissant dans la relation (1.2.6) donnent les équivalents logarithmiques des valeurs propres  $\lambda_{k,h}^{(p)}$  non nulles au sens où ils vérifient (en supposant (1.2.6) valide) :

$$\forall p \in \{0, \dots, d\}, \forall k \in \{1, \dots, \mathbf{m}_p\}, \quad C_{k,p} = - \lim_{h \rightarrow 0^+} h \ln \lambda_{k,h}^{(p)}.$$

Dans la suite, nous les appellerons souvent les taux d'Arrhenius des valeurs propres  $\lambda_{k,h}^{(p)}$ , en référence à la loi d'Arrhenius dans le cadre de la théorie des cinétiques de réaction créée par Arrhenius à la fin du 19<sup>ème</sup> siècle (cf. [Arr89] ou [HTB90] pour une revue de la littérature ; nous renvoyons aussi à la partie 1.3.2 de cette introduction soulignant le rapport entre les petites valeurs propres de  $\Delta_{f,h}^{(0)}$  et la cinétique chimique, et justifiant au passage la référence à Eyring et à Kramers). Ces coefficients dépendent de la topologie des ensembles de sous-niveau de la fonction de Morse  $f$  et correspondent à certaines barrières d'énergie caractérisant cette topologie. Nous renvoyons à la partie 1.3.2 et surtout au chapitre 3 pour plus de détails à ce sujet. Les préfacteurs<sup>2</sup>  $A_{k,p}$  (et les exposants  $\ell_{k,p}$ ) dépendent quant à eux du comportement de  $f$  aux bornes de ces barrières d'énergie caractéristiques (et plus précisément, concernant les  $A_{k,p}$ , des dérivées partielles de  $f$  d'ordre  $\leq 2$  en certains points critiques dont les énergies délimitent ces barrières). Cela sera aussi plus clair à partir de la partie 1.3.2.

L'analyse semi-classique des petites valeurs propres de  $\Delta_{f,h}^{(p)}$  est une question délicate, notamment en raison de l'effet tunnel entre les  $\mathbf{m}_p$  puits quantiques associés aux points critiques d'indice  $p$  avec les puits quantiques associés aux autres points critiques, faiblement résonnants selon la terminologie adoptée dans [HS85b, HS85a].

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2. Ils sont nommés facteurs pré-exponentiels en cinétique chimique.

L'exploitation de la structure supersymétrique du laplacien de Witten joue un rôle fondamental dans notre analyse, en nous permettant en particulier de nous ramener à l'étude de l'interaction de  $d_{f,h}$  avec les modes propres de  $\Delta_{f,h}^{(p+1)}$  et de  $d_{f,h}^*$  avec les modes propres de  $\Delta_{f,h}^{(p-1)}$  (cf. (1.2.5) et la partie 3.3).

L'étude des petites valeurs propres du laplacien de Witten  $\Delta_{f,h}^{(p)}$  est l'objet du chapitre 3 et nous y renvoyons notamment aux théorèmes 3.2.1 et 3.2.2 concernant le cas des fonctions, i.e.  $p = 0$  (voir aussi (1.2.7) ci-dessous et (1.3.22) dans la partie 1.3.2), et au théorème 3.2.3 concernant les  $p$ -formes générales. L'avant-dernière section 3.4 du chapitre 3 porte par ailleurs sur notre travail [DL17] concernant l'étude de  $\Delta_{f,h}^{(0)}$  en grande dimension lorsque  $f$  est un potentiel double puits explicite naturellement associé à l'équation d'Allen-Cahn stochastique unidimensionnelle (cf. (3.4.2)). Nous renvoyons à la section 3.4 pour plus de détails à ce sujet.

En physique statistique, la compréhension fine du bas spectre de  $\Delta_{f,h}^{(0)}$  constitue la première étape de la description précise de la métastabilité du processus de Langevin sur-amorti. Nous reviendrons plus longuement sur la notion de métastabilité et sur ses liens avec le bas spectre de  $\Delta_{f,h}^{(0)}$  dans la section 1.3 de cette introduction ainsi que dans les chapitres 4 et 5. Les premiers résultats généraux dans ce sens ont d'abord été établis dans  $\mathbb{R}^d$  par Bovier-Gaynard-Klein dans [BGK05] par la théorie du potentiel puis par Helffer-Klein-Nier dans [HKN04], dans  $\mathbb{R}^d$  ou sur une variété compacte sans bord, par des méthodes d'analyse semi-classique. Ces méthodes semi-classiques ont ensuite été adaptées aux cas de variétés compactes à bord avec des conditions au bord de type Dirichlet dans [HN06, DLLN19b]<sup>3</sup> et de type Neumann dans [Lep10] (ces conditions au bord sont l'objet de la partie suivante), au cas du laplacien de Witten discret dans [Dig13], ou encore à l'étude de marches aléatoires semi-classiques dans [BHM15]. Dans le cadre plus général des opérateurs de Kramers-Fokker-Planck<sup>4</sup> (cf. partie 5.3.2) s'appliquant aussi au laplacien de Witten, les résultats de l'article [HHS11] de Hérou-Hitrik-Sjöstrand conduisent en particulier, dans  $\mathbb{R}^d$  ou sur une variété compacte sans bord, à une généralisation des résultats de [HKN04] : il y est notamment donné, pour une fonction de Morse  $f$  générale (sous des hypothèses de confinement classiques à l'infini lorsque  $\Omega = \mathbb{R}^d$ ), un encadrement précis des petites valeurs propres de  $\Delta_{f,h}^{(0)}$  à la limite  $h \rightarrow 0^+$  du type :

$$\exists C \geq 1, \forall k \in \{1, \dots, \mathbf{m}_0\}, \frac{1}{C} h^{\ell_k} e^{-\frac{C_k}{h}} \leq \lambda_{k,h}^{(0)} \leq C h^{\ell_k} e^{-\frac{C_k}{h}}, \quad (1.2.7)$$

où les  $\ell_k$  et  $C_k$  sont explicités. Les résultats de [HHS11] conduisent donc en particulier à l'obtention, dans le cas général, de tous les taux d'Arrhenius. En utilisant les techniques de [HKN04], Michel a aussi récemment donné dans [Mic19] une généralisation complète des résultats de [HKN04] où les auteurs, en plus des hypothèses de confinement classiques à l'infini sur la fonction de Morse  $f$ , font des hypothèses supplémentaires génériques sur  $f$ . Signalons aussi les travaux probabilistes antérieurs [HKS89, Mic95, Mat95] donnant les taux d'Arrhenius des petites valeurs propres de  $\Delta_{f,h}^{(0)}$  sous des hypothèses beaucoup plus faibles sur la fonction  $f$ , mais excluant donc ainsi la possibilité d'obtenir les préfacteurs précis.

Mentionnons de plus ici que, même si l'on ne s'intéresse qu'au comportement de  $\Delta_{f,h}^{(0)}$  lorsque  $h \rightarrow 0^+$ , la compréhension de  $\Delta_{f,h}^{(p)}$ ,  $p \in \{1, \dots, d\}$ , et en particulier

3. Le second article correspond à la première partie de la prépublication [DLLN19a].

4. Ces opérateurs ne sont pas elliptiques mais seulement hypoelliptiques en général ; cela rend leur analyse beaucoup plus délicate.

celle de  $\Delta_{f,h}^{(1)}$ , fournit via la structure supersymétrique un outil puissant pour mener à bien l'analyse. Citons notamment, en plus des travaux déjà évoqués [HKN04, HN06, Lep10, Dig13, BHM15, Mic19, DLLN19b], les articles [Sjö96, Hel98, Joh00, Hel02, KT04, HN04, HN05, LN15, Lep17, DLLN17b, MZ18] dans cet esprit et sur les connexions entre le laplacien de Witten et la physique statistique.

Le cas des petites valeurs propres du laplacien de Witten  $\Delta_{f,h}^{(p)}$ ,  $p \in \{0, \dots, d\}$ , agissant sur des formes différentielles de degrés quelconques sera aussi étudié dans le chapitre 3 s'appuyant sur les travaux [Lep11] dans le cadre de surfaces compactes sans bord et surtout [LNV13] dans la cadre de variétés compactes sans bord de dimensions quelconques. Outre l'utilité évoquée ci-dessus d'étudier  $\Delta_{f,h}^{(p)}$  pour comprendre certaines propriétés de physique statistique liées à  $\Delta_{f,h}^{(0)}$ , la compréhension du bas spectre de  $\Delta_{f,h}^{(p)}$  est aussi une question naturelle en géométrie (cf. par exemple [Zha01, BL08]) et en systèmes dynamiques (cf. [DR17], où les auteurs montrent que ce spectre converge à la limite  $h \rightarrow 0^+$  vers le spectre de Pollicott-Ruelle du flot gradient de  $f$  agissant sur des espaces de Sobolev appropriés). Le bas spectre de  $\Delta_{f,h}^{(p)}$  est par ailleurs intimement lié à l'homologie persistante de la fonction  $f$  sur la variété  $\Omega$  : les taux d'Arrhenius des petites valeurs propres non nulles de  $\Delta_{f,h}^{(p)}$  communes à celles de  $\Delta_{f,h}^{(p+1)}$  donnent les longueurs des codes barres (non infinies) de l'homologie persistante d'indice  $p$  de  $f$  (voir la section 3.1.4 pour plus de détails à ce propos et l'article de revue [EH08] sur l'homologie persistante).

### 1.2.3 Des conditions au bord naturelles

Cette partie a pour but d'introduire les conditions au bord de type Dirichlet ou Neumann brièvement évoquées dans la partie précédente. Par « naturelle », nous entendons des conditions au bord qui préservent la structure supersymétrique de cet opérateur (cf. (1.2.1) et (1.2.2) dans la partie 1.2.1).

Nous supposons dans cette partie que  $\Omega$  est compact et que sa frontière  $\partial\Omega$  est non vide. Commençons par rappeler les notions usuelles de traces tangentielle et normale dans ce cadre.

Nous noterons  $\vec{n}$  la normale extérieure sur  $\partial\Omega$  et  $\vec{n}^\flat$  sa 1-forme duale canonique (i.e. définie par  $\vec{n}_p^\flat(X_p) = \langle \vec{n}_p, X_p \rangle_p$  pour tout  $p \in \partial\Omega$  et  $X_p \in T_p\Omega$ ). L'orientation est choisie de sorte que

$$\mu_{\partial\Omega} = \mathbf{i}_{\vec{n}} \mu.$$

Pour tout  $\omega \in \Lambda^p H^1(\Omega)$ , la partie tangentielle de  $\omega$  sur  $\partial\Omega$  est la forme  $\mathbf{t}\omega \in H^{\frac{1}{2}}(\partial\Omega, \Lambda^p T^*\Omega|_{\partial\Omega})$  définie par :

$$\forall \sigma \in \partial\Omega, \quad (\mathbf{t}\omega)_\sigma(X_1, \dots, X_p) := \omega_\sigma(X_1^T, \dots, X_p^T),$$

où  $X_i = X_i^T \oplus x_i^\perp \vec{n}_\sigma$  est la décomposition de  $X_i$  au point  $\sigma$  selon ses composantes tangentielle et normale à  $\partial\Omega$ . De façon plus concise :

$$\mathbf{t}\omega = \mathbf{i}_{\vec{n}}(\vec{n}^\flat \wedge \omega).$$

La partie normale de  $\omega$  sur  $\partial\Omega$  est alors définie par :

$$\mathbf{n}\omega := \omega|_{\partial\Omega} - \mathbf{t}\omega = \vec{n}^\flat \wedge (\mathbf{i}_{\vec{n}}\omega) \in H^{\frac{1}{2}}(\partial\Omega, \Lambda^p T^*\Omega|_{\partial\Omega}).$$

Pour  $\mathbf{b} \in \{\mathbf{t}, \mathbf{n}\}$ , nous pouvons maintenant définir les espaces suivants qui seront utiles par la suite :

$$\Lambda^p H_{\mathbf{b}}^1(\Omega) := \{ \omega \in \Lambda^p H^1(\Omega), \mathbf{b}\omega = 0 \text{ (sur } \partial\Omega) \} . \quad (1.2.8)$$

Notons que l'on a en particulier  $\Lambda^0 H_{\mathbf{t}}^1(\Omega) = H_0^1(\Omega)$  et  $\Lambda^0 H_{\mathbf{n}}^1(\Omega) = H^1(\Omega)$ .

Ramenons-nous, comme dans la partie précédente, à la proposition 1.2.1 pour définir un laplacien de Witten auto-adjoint supersymétrique, ici avec des conditions au bord de type Neumann ou Dirichlet. On définit pour cela les espaces fonctionnels suivants :

$$\text{pour } \mathbf{d} = d \text{ ou } \mathbf{d} = d^*, \quad \Lambda^p H^{\mathbf{d}}(\Omega) := \{ \omega \in \Lambda^p L^2(\Omega), \mathbf{d}\omega \in \Lambda L^2(\Omega) \} . \quad (1.2.9)$$

En nous basant sur la formule de Green classique, valable pour tous  $\omega \in \Lambda^{p-1} H^1(\Omega)$  et  $\eta \in \Lambda^p H^1(\Omega)$  (pour  $p \in \{1, \dots, d\}$ ),

$$\langle d\omega, \eta \rangle_{\Lambda^p L^2} - \langle \omega, d^* \eta \rangle_{\Lambda^{p-1} L^2} = \begin{cases} \int_{\partial\Omega} \langle \omega, \mathbf{i}_{\vec{n}} \eta \rangle_{\Lambda^{p-1}} d\mu_{\partial\Omega} = \int_{\partial\Omega} \langle \mathbf{t}\omega, \mathbf{i}_n \eta \rangle_{\Lambda^{p-1}} d\mu_{\partial\Omega} \\ \int_{\partial\Omega} \langle \vec{n}^{\flat} \wedge \omega, \eta \rangle_{\Lambda^p} d\mu_{\partial\Omega} = \int_{\partial\Omega} \langle \vec{n}^{\flat} \wedge \omega, \mathbf{n}\eta \rangle_{\Lambda^p} d\mu_{\partial\Omega} \end{cases} ,$$

on peut généraliser les espaces définis dans (1.2.8) de la façon suivante. Pour  $\omega \in \Lambda^p H^d(\Omega)$ , on définit  $\vec{n}^{\flat} \wedge \omega \in \Lambda^{p+1} H^{-\frac{1}{2}}(\partial\Omega)$  par :

$$\forall g \in \Lambda^{p+1} H^{\frac{1}{2}}(\partial\Omega), \quad \langle \vec{n}^{\flat} \wedge \omega, g \rangle_{H^{-\frac{1}{2}}(\partial\Omega), H^{\frac{1}{2}}(\partial\Omega)} = \langle d\omega, G \rangle_{L^2} - \langle \omega, d^* G \rangle_{L^2}, \quad (1.2.10)$$

où  $G$  est un élément de  $\Lambda^{p+1} H^1(\Omega)$  dont la trace dans  $\Lambda^{p+1} H^{\frac{1}{2}}(\partial\Omega)$  est  $g$ . Par densité de  $\Lambda C^\infty(\Omega)$  dans  $\Lambda^p H^d(\Omega)$  muni de la norme du graphe associée, cette définition est indépendante de l'extension  $G$  choisie. De même, pour  $\omega \in \Lambda^p H^{d^*}(\Omega)$ , on définit  $\mathbf{i}_{\vec{n}} \omega \in \Lambda^{p-1} H^{-\frac{1}{2}}(\partial\Omega)$  par

$$\forall g \in \Lambda^{p-1} H^{\frac{1}{2}}(\partial\Omega), \quad \langle \mathbf{i}_{\vec{n}} \omega, g \rangle_{H^{-\frac{1}{2}}(\partial\Omega), H^{\frac{1}{2}}(\partial\Omega)} = \langle \omega, dG \rangle_{L^2} - \langle d^* \omega, G \rangle_{L^2}, \quad (1.2.11)$$

où  $G$  est une extension quelconque de  $g$  dans  $\Lambda^{p-1} H^1(\Omega)$ . Lorsque  $\omega$  appartient à  $\Lambda^p H^1(\Omega)$ , les définitions précédentes coïcident avec les définitions usuelles de  $\vec{n}^{\flat} \wedge \omega$  et de  $\mathbf{i}_{\vec{n}} \omega$ . On a en particulier pour de tels  $\omega$  :

$$(\vec{n}^{\flat} \wedge \omega = 0 \text{ ssi } \omega \in \Lambda^p H_{\mathbf{t}}^1(\Omega)) \quad \text{et} \quad (\mathbf{i}_{\vec{n}} \omega = 0 \text{ ssi } \omega \in \Lambda^p H_{\mathbf{n}}^1(\Omega)) .$$

Plus généralement, on peut maintenant définir

$$\Lambda^p H_{\mathbf{t}}^d(\Omega) := \{ \omega \in \Lambda^p H^d(\Omega), \vec{n}^{\flat} \wedge \omega = 0 \text{ (sur } \partial\Omega) \} \quad (1.2.12)$$

et

$$\Lambda^p H_{\mathbf{n}}^{d^*}(\Omega) := \{ \omega \in \Lambda^p H^{d^*}(\Omega), \mathbf{i}_{\vec{n}} \omega = 0 \text{ (sur } \partial\Omega) \} . \quad (1.2.13)$$

Introduisons maintenant une fonction régulière  $f : \Omega \rightarrow \mathbb{R}$ . Comme dans la partie précédente, on définit l'opérateur non borné dans  $\Lambda L^2(\Omega)$  suivant :

$$\begin{aligned} d_f \text{ muni du domaine } \quad D(d_f) &:= \Lambda H_{\mathbf{t}}^d(\Omega) \\ &= \{ u \in \Lambda L^2(\Omega), d_f u \in \Lambda L^2(\Omega) \text{ et } \vec{n}^{\flat} \wedge u = 0 \} . \end{aligned}$$

On peut de nouveau vérifier qu'il s'agit d'un opérateur fermé satisfaisant la relation  $\text{Ran } d_f \subset \text{Ker } d_f$  et dont l'adjoint est l'opérateur différentiel

$$d_f^* \text{ muni du domaine } D(d_f^*) = \Lambda^p H^{d^*}(\Omega) = \{u \in \Lambda L^2(\Omega), d_f^* u \in \Lambda L^2(\Omega)\}.$$

Par conséquent, puisque (cf. (1.2.8), (1.2.9) et (1.2.12))

$$D(d_f) \cap D(d_f^*) = \Lambda H_{\mathfrak{t}}^d(\Omega) \cap \Lambda^p H^{d^*}(\Omega) = \Lambda H_{\mathfrak{t}}^1(\Omega), \quad (1.2.14)$$

l'opérateur  $(d_f, D(d_f))$  vérifie les hypothèses de la proposition 1.2.1. La dernière égalité ci-dessus peut être démontrée de façon indirecte par identification d'opérateurs auto-adjoints comparables en utilisant les résultats de [HN06] (cf. ci-dessous). Elle repose sur la relation d'ellipticité suivante (cf. [Sch95, Corollary 2.1.6]),

$$\exists C > 0, \forall \omega \in \Lambda H_{\mathfrak{t}}^1(\Omega), \quad \|\omega\|_{H^1} \leq C(\|\omega\|_{L^2} + \|d\omega\|_{L^2} + \|d^*\omega\|_{L^2}), \quad (1.2.15)$$

qui généralise des estimées obtenues par Gaffney dans [Gaf51]. Le laplacien de Witten  $\Delta_f = d_f d_f^* + d_f^* d_f$  muni du domaine

$$D(\Delta_f) = \{u \in \Lambda H_{\mathfrak{t}}^1(\Omega) \text{ t.q. } d_f u \in D(d_f^*) \text{ et } d_f^* u \in D(d_f)\}$$

est donc auto-adjoint positif et à résolvante compacte dans  $\Lambda L^2(\Omega)$ . Par comparaison avec le laplacien de Witten  $\Delta_f$  muni du domaine

$$D(\Delta_f) = \{\omega \in \Lambda H^2(\Omega), \mathfrak{t}\omega = 0 \text{ et } \mathfrak{t}d_f^*\omega = 0\},$$

auto-adjoint d'après [HN06], il y a égalité des domaines et donc des domaines des formes quadratiques associées (d'où (1.2.14)).

Dans la suite, on notera  $\Delta_f^{\mathfrak{t}}$  ou  $\Delta_f^D$  cet opérateur auto-adjoint de type Dirichlet. Comme

$$\Lambda \mathcal{C}_{\mathfrak{t}}^\infty(\Omega) := \{u \in \Lambda \mathcal{C}^\infty(\Omega) \text{ t.q. } \mathfrak{t}u = 0\}$$

est dense dans  $\Lambda H_{\mathfrak{t}}^1(\Omega)$ , il s'agit aussi de l'extension de Friedrichs de  $\Delta_f$  agissant sur  $\Lambda \mathcal{C}_{\mathfrak{t}}^\infty(\Omega)$ ; c'est le point de vue adopté dans [HN06]. Notons aussi qu'agissant sur les fonctions,  $\Delta_f^{D,(0)}$  est la réalisation de Dirichlet classique de domaine  $H^2(\Omega) \cap H_0^1(\Omega)$ . Il est néanmoins important de remarquer que l'opérateur auto-adjoint  $\Delta_f$  avec conditions au bord de Dirichlet complètes, i.e. muni du domaine  $\Lambda H^2(\Omega) \cap \Lambda H_0^1(\Omega)$ , n'est pas supersymétrique. En effet, considérons par exemple une fonction propre  $u$  associée à la plus petite valeur propre de  $\Delta_f^{D,(0)}$ . Les résultats classiques sur les opérateurs elliptiques permettent de montrer que cette valeur propre est strictement positive, simple, que  $u$  a un signe sur  $\Omega \setminus \partial\Omega$  et une dérivée normale ne s'annulant jamais le long de  $\partial\Omega$ . En particulier, la 1-forme  $d_f u$  n'appartient pas à  $\Lambda^1 H_0^1(\Omega)$  (mais elle appartient bien sûr à  $\Lambda^1 H_{\mathfrak{t}}^1(\Omega)$  d'après ce qui précède)!

De la même façon,

$$d_f \text{ muni du domaine } D(d_f) := \Lambda H^d(\Omega) = \{u \in \Lambda L^2(\Omega), d_f u \in \Lambda L^2(\Omega)\}$$

est un opérateur fermé satisfaisant la relation  $\text{Ran } d_f \subset \text{Ker } d_f$ , d'adjoint

$$d_f^* \text{ muni du domaine } D(d_f^*) = \Lambda^p H_{\mathfrak{n}}^{d^*}(\Omega),$$

et on a

$$D(d_f) \cap D(d_f^*) = \Lambda H^d(\Omega) \cap \Lambda H_{\mathfrak{n}}^{d^*}(\Omega) = \Lambda H_{\mathfrak{n}}^1(\Omega), \quad (1.2.16)$$



la dernière égalité reposant sur l'inégalité de Gaffney suivante (cf. [Sch95, Theorem 2.1.7]) :

$$\exists C > 0, \forall \omega \in \Lambda H_{\mathbf{n}}^1(\Omega), \quad \|\omega\|_{H^1} \leq C(\|\omega\|_{L^2} + \|d\omega\|_{L^2} + \|d^*\omega\|_{L^2}). \quad (1.2.17)$$

Le laplacien de Witten  $\Delta_f = d_f d_f^* + d_f^* d_f$  muni du domaine

$$D(\Delta_f) = \{u \in \Lambda H_{\mathbf{n}}^1(\Omega) \text{ t.q. } d_f u \in D(d_f^*) \text{ et } d_f^* u \in D(d_f)\}$$

est donc auto-adjoint positif à résolvante compacte dans  $\Lambda L^2(\Omega)$ , et par comparaison avec le laplacien de Witten  $\Delta_f$  muni du domaine

$$D(\Delta_f) = \{\omega \in \Lambda H^2(\Omega), \mathbf{n}\omega = 0 \text{ et } \mathbf{n}d_f\omega = 0\},$$

auto-adjoint d'après [Lep10], il y a égalité des domaines, ce qui conduit aussi à (1.2.16).

Dans la suite, on notera  $\Delta_f^{\mathbf{n}}$  ou  $\Delta_f^N$  cet opérateur auto-adjoint de type Neumann. Par densité de

$$\Lambda \mathcal{C}_{\mathbf{n}}^\infty(\Omega) := \{u \in \Lambda \mathcal{C}^\infty(\Omega) \text{ t.q. } \mathbf{n}u = 0\}$$

dans  $\Lambda H_{\mathbf{n}}^1(\Omega)$ , il s'agit encore de l'extension de Friedrichs de  $\Delta_f$  agissant sur  $\Lambda \mathcal{C}_{\mathbf{n}}^\infty(\Omega)$ , point de vue adopté dans [Lep10]. Notons aussi qu'agissant sur les fonctions,  $\Delta_f^{N,(0)}$  n'est pas la réalisation de Neumann classique de l'opérateur différentiel considéré mais sa réalisation de type Neumann-Robin de domaine

$$\{\omega \in H^2(\Omega), \partial_n \omega + \omega \partial_n f = 0\}.$$

Comme dans la partie précédente, en considérant maintenant les laplaciens de Witten semi-classiques  $\Delta_{f,h}^{\mathbf{b}} = h^2 \Delta_f^{\frac{\mathbf{b}}{h}}$  pour  $h > 0$  et  $\mathbf{b} \in \{\mathbf{t}, \mathbf{n}\}$  (cf. (1.1.5)–(1.1.8)), on a ici, pour tout  $h > 0$ , d'après le corollaire 1.2.2,

$$\text{Ker } \Delta_{f,h}^{\mathbf{b}} \simeq \text{Ker } \Delta^{\mathbf{b}},$$

où  $\Delta^{\mathbf{b}}$  est le laplacien de Hodge  $\Delta_0^{\mathbf{b}}$ , et donc, pour tout  $p \in \{0, \dots, d\}$  et  $h > 0$  :

$$\dim \text{Ker } \Delta_{f,h}^{\mathbf{b},(p)} = \dim \text{Ker } \Delta^{\mathbf{b},(p)} = \mathbf{b}_p^{\mathbf{b}}(\Omega). \quad (1.2.18)$$

Ici, d'après le théorème de Hodge-de Rham dans le cadre de variétés à bord (voir par exemple [Gue04], [Gil95, Theorem 2.7.3] ou [Tay96, Section 5.9]) :

- le nombre de Betti  $\mathbf{b}_p^{\mathbf{n}}(\Omega)$  est la dimension du  $p$ -ième groupe de cohomologie absolue réelle de  $\Omega$ ,
- le nombre de Betti  $\mathbf{b}_p^{\mathbf{t}}(\Omega)$  est la dimension du  $p$ -ième groupe de cohomologie relative réelle de  $(\Omega, \partial\Omega)$ .

De plus, une généralisation du théorème 1.2.3 est démontrée dans [HN06] pour  $\Delta_{f,h}^D$  et dans [Lep10] pour  $\Delta_{f,h}^N$ . Pour l'énoncer précisément, supposons que  $f$  est une fonction de Morse dans  $\Omega$ , que  $\nabla f$  ne s'annule pas sur  $\partial\Omega$  et que  $f|_{\partial\Omega}$  est aussi de Morse. On définit alors, pour  $p \in \{0, \dots, d\}$ ,

$$\mathcal{U}_{\Omega}^{(p)} := \{\text{points critiques d'indice } p \text{ de } f \text{ dans } \Omega\}, \quad (1.2.19)$$

ainsi que

$$\mathcal{U}_{\partial\Omega}^{N,(p)} := \{\text{points critiques } z \text{ d'indice } p \text{ de } f|_{\partial\Omega} \text{ t.q. } \partial_n f(z) < 0\} \quad (1.2.20)$$

et

$$\mathcal{U}_{\partial\Omega}^{D,(p)} := \{\text{points critiques } z \text{ d'indice } p-1 \text{ de } f|_{\partial\Omega} \text{ t.q. } \partial_n f(z) > 0\}. \quad (1.2.21)$$

Sous les hypothèses précédentes, les éléments de l'ensemble défini par (1.2.20) (resp. par (1.2.21)) jouent du point de vue topologique le rôle de points critiques d'indice  $p$  de  $f$  pour l'homologie absolue de  $\Omega$  (respectivement pour l'homologie relative de  $(\Omega, \partial\Omega)$ ). On a plus précisément d'après [HN06, Lep10] :

**Théorème 1.2.5.** *Supposons que  $f : \Omega \rightarrow \mathbb{R}$  est de Morse, que  $\nabla f \neq 0$  sur  $\partial\Omega$  et que  $f|_{\partial\Omega}$  est de Morse. Pour  $B \in \{N, D\}$  et  $p \in \{0, \dots, d\}$ , on définit (cf. (1.2.19)–(1.2.21))*

$$\mathbf{m}_p^B := \text{Card} \mathcal{U}_{\Omega}^{(p)} + \text{Card} \mathcal{U}_{\partial\Omega}^{B,(p)} = \mathbf{m}_p + \text{Card} \mathcal{U}_{\partial\Omega}^{B,(p)} \in \mathbb{N}$$

le nombre de points critiques généralisés de  $f$  d'indice  $p$ . Pour  $B \in \{N, D\}$ , il existe alors  $h_0 > 0$  et  $C > 0$  tels que, pour tous  $h \in (0, h_0]$  et  $p \in \{0, \dots, d\}$ , on a<sup>5</sup>

$$\text{Sp}(\Delta_{f,h}^{B,(p)}) \cap [0, Ch] = \text{Sp}(\Delta_{f,h}^{B,(p)}) \cap [0, h^{\frac{3}{2}}]$$

et

$$\text{Card}(\text{Sp}(\Delta_{f,h}^{B,(p)}) \cap [0, Ch]) = \mathbf{m}_p^B.$$

Il existe de plus  $c > 0$  tel que pour tous  $h \in (0, h_0]$  et  $p \in \{0, 1\}$ , on a

$$\text{Sp}(\Delta_{f,h}^{B,(p)}) \cap [0, Ch] \subset [0, e^{-\frac{c}{h}}].$$

Cela conduit en particulier à des inégalités de Morse dans ce cadre (nous renvoyons aussi [CL95, Lau11] à ce sujet). Enfin, il est montré dans [HN06, Lep10] que sous des hypothèses additionnelles génériques sur la fonction  $f$ , les petites valeurs propres de  $\Delta_{f,h}^{B,(0)}$  satisfont à la limite  $h \rightarrow 0^+$  des formules de type Eyring-Kramers, i.e. de la forme (1.2.6).

Dans notre travail [DLLN19b], nous généralisons notamment ces derniers résultats de [HN06] concernant le cas de conditions au bord de type Dirichlet. En nous inspirant de l'analyse de [HHS11] (cf. partie précédente), nous y montrons par exemple que pour une fonction de Morse  $f$  générale satisfaisant les hypothèses du théorème 1.2.5, les petites valeurs propres  $0 < \lambda_{1,h}^{(0)} < \lambda_{2,h}^{(0)} \leq \dots \leq \lambda_{\mathbf{m}_0,h}^{(0)}$  de  $\Delta_{f,h}^{D,(0)}$  satisfont asymptotiquement :

$$\exists C \geq 1, \forall k \in \{1, \dots, \mathbf{m}_0^D = \mathbf{m}_0\}, \frac{1}{C} h^{\ell_k} e^{-\frac{C_k}{h}} \leq \lambda_{k,h}^{(0)} \leq C h^{\ell_k} e^{-\frac{C_k}{h}}, \quad (1.2.22)$$

où les  $\ell_k$  et  $C_k$  sont explicités. Cela conduit en particulier à l'obtention de tous les taux d'Arrhenius dans ce cas. Nous renvoyons au théorème 3.2.2 dans le chapitre 3 pour un énoncé plus précis.

5. Dans [HN06, théorème 3.2.3] et [Lep10, théorème 3.1.5], il est en fait seulement précisé que pour tout  $h > 0$  assez petit,  $\text{Sp}(\Delta_{f,h}^{B,(p)}) \cap [0, h^{\frac{3}{2}}]$  a dimension  $\mathbf{m}_p^B$ . Les preuves de ces résultats montrent néanmoins bien que les valeurs propres restantes sont de taille  $h$ .

Comme nous l'avons déjà indiqué dans la partie précédente, nous reviendrons plus en détail sur les résultats fins sur le bas spectre du laplacien de Witten, que ce soit dans le cas sans bord ou avec des conditions au bord de type Dirichlet ou Neumann, dans le chapitre 3. La théorie spectrale asymptotique de  $\Delta_{f,h}^{D,(0)}$  est par ailleurs au coeur de l'analyse de nos travaux [DLLN17b, DLLN19b, LN19a] portant sur la dynamique de Langevin sur-amortie et résumés dans les chapitres 4 et 5. Nous y reviendrons longuement dans la partie 1.3.3 de ce chapitre introductif.

## 1.3 Dynamique de Langevin sur-amortie et méta-stabilité

Plaçons nous pour commencer ici dans  $\Omega = \mathbb{R}^d$  et considérons la dynamique de Langevin sur-amortie

$$dX_t = -\nabla V(X_t)dt + \sqrt{2h} dB_t, \quad (1.3.1)$$

où  $X_t \in \Omega = \mathbb{R}^d$ ,  $h$  est un paramètre strictement positif,  $V : \Omega = \mathbb{R}^d \rightarrow \mathbb{R}$  est une fonction régulière vérifiant  $Z_h := \int_{\Omega} e^{-\frac{V}{h}} d\mu < +\infty$  et  $(B_t)_{t \geq 0}$  est un mouvement brownien standard de dimension  $d$ . Cette dynamique est prototypique de modèles utilisés en physique statistique pour simuler l'évolution d'un système moléculaire à température fixée (cf. par exemple [Cha43] ou [SM79, Sections 2 et 3]), auquel cas  $V$  est l'énergie potentielle,  $h = k_B T$  est proportionnel à la température ( $k_B$  est la constante de Boltzmann) et la dimension  $d$  est typiquement trois fois le nombre d'atomes du système.

### 1.3.1 Convergence vers l'équilibre

On suppose dans cette partie que le paramètre  $h > 0$  apparaissant dans (1.3.1) vérifie  $h = 1$ . Le générateur infinitésimal du semigroupe markovien donnant l'évolution de (1.3.1) est alors l'opérateur différentiel de type Ornstein-Uhlenbeck

$$L_V^{(0)} := -\Delta + \nabla V \cdot \nabla = \Delta_H + \mathcal{L}_{\nabla V}, \quad (1.3.2)$$

parfois appelé laplacien à poids<sup>6</sup>(ou encore laplacien de Bakry-Émery) dans la littérature (cf. par exemple [KM17]). Cet opérateur est un modèle important de la théorie des processus de diffusion de Bakry-Émery et nous renvoyons en particulier à ce propos à l'article précurseur de Bakry-Émery [BE85] ainsi qu'au livre [BGL14] pour un aperçu de la littérature associée. Le générateur de l'évolution des densités de probabilité du processus  $(X_t)_{t \geq 0}$  est quant à lui donné par l'adjoint formel de  $L_V^{(0)}$ ,

$$L_V^{(0),\dagger} := -\Delta - \operatorname{div}(\cdot \nabla V). \quad (1.3.3)$$

Autrement dit, la densité de probabilité  $(\rho(t, \cdot))_{t \geq 0}$  du processus  $(X_t)_{t \geq 0}$  vérifie l'équation de Fokker-Planck suivante, aussi dite de (Kramers-)Smoluchowski dans ce cadre (cf. [Ris89]),

$$\partial_t \rho = \Delta \rho + \operatorname{div}(\rho \nabla V). \quad (1.3.4)$$

6. Il s'agit en effet du laplacien de type Hodge  $d^*d$  agissant sur les fonctions, où l'adjoint  $d^*$  est considéré par rapport au produit scalaire de l'espace à poids  $L^2(\Omega, e^{-V} d\mu)$ .

La dynamique de Langevin sur-amortie admet de plus comme mesure invariante, puisque  $L_V^{(0)\dagger} e^{-V} = 0$ , la mesure de Boltzmann-Gibbs

$$m_V(d\mu) := \left( \int_{\Omega} e^{-V} d\mu \right)^{-1} e^{-V} d\mu = Z_1^{-1} e^{-V} d\mu, \quad (1.3.5)$$

et  $L_V^{(0)}$  agissant sur  $\mathcal{C}_c^{\infty}(\mathbb{R}^d)$  est symétrique dans l'espace à poids  $L^2(\Omega, m_V)$ .

Autorisons plus généralement  $\Omega$  à être ( $\mathbb{R}^d$  ou) une variété riemannienne orientée compacte et connexe de dimension  $d$  sans bord et définissons en général  $L_V^{(0)}$  par la dernière relation de (1.3.2). On remarque que le laplacien de Witten

$$\Delta_f^{(0)} = \Delta_H + |\nabla f|^2 + \Delta_H f$$

associé à  $f := \frac{V}{2}$  est unitairement équivalent à l'opérateur  $L_V^{(0)}$  agissant dans l'espace à poids  $L^2(\Omega, m_V)$  en vertu de la relation

$$\Delta_f^{(0)} = e^{-\frac{V}{2}} L_V^{(0)} e^{\frac{V}{2}} \quad \text{où} \quad V = 2f. \quad (1.3.6)$$

Il est ainsi équivalent d'étudier l'opérateur  $\Delta_{\frac{V}{2}}^{(0)}$  ou l'opérateur  $L_V^{(0)}$  qui a donc en particulier une extension supersymétrique naturelle définie sur l'algèbre des formes différentielles sur l'espace à poids  $\Lambda L^2(\Omega, m_V)$  définie, pour tout  $p \in \{0, \dots, d\}$ , par

$$L_V^{(p)} := e^{\frac{V}{2}} \Delta_{\frac{V}{2}}^{(p)} e^{-\frac{V}{2}} = \Delta_H^{(p)} + \mathcal{L}_{\nabla V}. \quad (1.3.7)$$

Pour souligner plus précisément le lien avec la théorie des processus de diffusion de Bakry-Émery, les opérateurs  $L_V^{(0)}$  et  $L_V^{(1)}$  sont liés à l'opérateur carré du champ de Bakry-Émery  $\Gamma$  et à son itéré  $\Gamma_2$  via les relations

$$\int_{\Omega} \Gamma(\omega) dm_V = \int_{\Omega} (L_V^{(0)} \omega) \omega dm_V = \int_{\Omega} \langle d\omega, d\omega \rangle_{\Lambda^1} dm_V = \|\nabla \omega\|_{L^2(\Omega, m_V)}^2 \quad (1.3.8)$$

et

$$\int_{\Omega} \Gamma_2(\omega) dm_V = \int_{\Omega} (L_V^{(0)} \omega)^2 dm_V = \int_{\Omega} \langle L_V^{(1)} d\omega, d\omega \rangle_{\Lambda^1} dm_V, \quad (1.3.9)$$

où  $\omega \in \mathcal{C}_c^{\infty}(\Omega)$  (cf. en particulier [BGL14] pour plus de matériel et de références sur le carré du champ).

De plus, que  $\Omega$  soit  $\mathbb{R}^d$  ou variété riemannienne orientée compacte et connexe de dimension  $d$  sans bord, l'opérateur  $L_V^{(0)}$  agissant sur l'espace  $\mathcal{C}_c^{\infty}(\Omega)$  (qui n'est autre que  $\mathcal{C}^{\infty}(\Omega)$  lorsque  $\Omega$  n'est pas  $\mathbb{R}^d$ ) est essentiellement auto-adjoint dans l'espace de Hilbert  $L^2(\Omega, m_V)$  et sa fermeture dans cet espace, que nous noterons toujours  $L_V^{(0)}$ , est positive avec  $\lambda_1 = 0$  pour valeur propre simple, associée aux fonctions constantes (cela découle du fait que  $e^{-V} \in L^1(\Omega)$ ). Le caractère essentiellement auto-adjoint se déduit de la relation (1.3.7) et :

- de l'analyse faite dans la partie 1.2.2 lorsque  $\Omega$  est compacte,
- du fait que le laplacien de Witten  $\Delta_{\frac{V}{2}}^{(0)}$  agissant sur  $\mathcal{C}_c^{\infty}(\mathbb{R}^d)$  est essentiellement auto-adjoint dans  $L^2(\mathbb{R}^d)$ , étant positif et à potentiel régulier (cf. par exemple [Hel13, Theorem 9.15]), lorsque  $\Omega = \mathbb{R}^d$ .

En remarquant que le domaine de la forme quadratique associée à  $L_V^{(0)}$  est l'espace de Sobolev à poids  $H^1(\Omega, m_V)$ , on déduit de ce qui précède et du principe du Max-Min que pour tout  $C \in \mathbb{R}^{+*}$ , l'inégalité de type Poincaré (cf. (1.3.8))

$$\forall \omega \in H^1(\Omega, m_V), \quad \|\omega - (\int_{\Omega} \omega dm_V)\|_{L^2(\Omega, m_V)}^2 \leq \frac{1}{C} \|\nabla \omega\|_{L^2(\Omega, m_V)}^2 \quad (1.3.10)$$

est satisfaite si et seulement si

$$\text{Sp}(L_V^{(0)}) \cap (0, C) = \emptyset. \quad (1.3.11)$$

L'inégalité (1.3.10) est donc vérifiée pour (au moins) un  $C > 0$  si et seulement si 0 appartient au spectre discret de  $L_V^{(0)}$ , auquel cas le  $C$  optimal est donné par  $\lambda_2 := \inf(\text{Sp}(L_V^{(0)}) \setminus \{0\})$ . C'est en particulier toujours le cas lorsque  $\Omega$  est compacte puisqu'alors le laplacien de Witten, et donc le laplacien à poids, est à résolvante compacte (cf. partie 1.2.2). Dans ce cas, on a l'estimation en variance suivante, valable pour tous  $t \geq 0$  et  $\omega \in L^2(\Omega, m_V)$ <sup>7</sup> :

$$\|e^{-tL_V^{(0)}} \omega - (\int_{\Omega} \omega dm_V)\|_{L^2(\Omega, m_V)} \leq \|\omega - (\int_{\Omega} \omega dm_V)\|_{L^2(\Omega, m_V)} e^{-\lambda_2 t}. \quad (1.3.12)$$

De plus, lorsque la loi de probabilité  $\rho_0$  de  $X_0$  admet une densité  $\mu_0$  par rapport à  $m_V$  dans  $L^2(\Omega, m_V)$ , alors, pour tout  $t \geq 0$ , la loi de probabilité  $\rho_t$  de  $X_t$  admet la densité par rapport à  $m_V$  dans  $L^2(\Omega, m_V)$  donnée par  $\mu_t = e^{-tL_V^{(0)}} \mu_0$ . Il découle ainsi de (1.3.12) que pour tout  $t \geq 0$ , on a :

$$\begin{aligned} \|\rho_t - m_V\|_{VT} &= \|\mu_t - 1\|_{L^1(\Omega, m_V)} \\ &\leq \|\mu_t - 1\|_{L^2(\Omega, m_V)} \leq \|\mu_0 - 1\|_{L^2(\Omega, m_V)} e^{-\lambda_2 t}, \end{aligned} \quad (1.3.13)$$

où  $\|\cdot\|_{VT}$  désigne la distance en variation totale. Remarquons au passage que lorsque  $\Omega$  est compacte, supposer que  $\rho_0$  admet une densité  $L^2$  par rapport à  $m_V$  n'est pas vraiment restrictif puisque, par l'effet régularisant de l'équation parabolique de (Kramers-)Smoluchowski (1.3.4), on se ramène automatiquement à ce cas pour tout  $t > 0$ . Nous renvoyons par exemple à [Roy07, BGL14] pour plus de détails au sujet de ce paragraphe.

Montrons maintenant comment la structure supersymétrique du laplacien de Witten, ou de façon équivalente du laplacien à poids, peut donner des informations sur la constante  $C > 0$  de l'inégalité (1.3.10). Si l'on sait par exemple que  $L_V^{(1)} \geq c$  pour un certain réel  $c > 0$ , on peut alors conclure que  $\lambda_2 := \inf(\text{Sp}(L_V^{(0)}) \setminus \{0\})$  est strictement positive et vérifie  $\lambda_2 \geq c$ . L'inégalité de Poincaré (1.3.10) est donc en particulier satisfaite lorsque  $C = c$ . Notons que lorsque  $\Omega$  est compact, cela découle simplement de la propriété supersymétrique (1.2.2) qui conduit facilement à  $\text{Sp}(L_V^{(0)}) \setminus \{0\} \subset \text{Sp}(L_V^{(1)})$ . Cette dernière relation est de plus toujours satisfaite lorsque  $\Omega = \mathbb{R}^d$  et  $L_V^{(1)} \geq c > 0$  mais devient alors plus difficile à démontrer (cf. [Joh00, Theorem 1.3]). Ce type de raisonnement, qui remonte au moins à l'article de Helffer-Sjöstrand [HS94], est au coeur de nombreux articles étudiant le comportement asymptotique des fonctions de corrélations en mécanique statistique et nous

7. Cette relation est aussi vraie lorsque  $\lambda_2 = 0$  mais n'implique évidemment pas dans ce cas la convergence vers 0 du terme de droite.

renvoyons par exemple à [Sjö96, NS97, Hel98, BJS00, BM03, BM04] pour d'autres références.

Dans ce cadre, les potentiels uniformément strictement convexes sur  $\mathbb{R}^d$  jouent un rôle important puisqu'il s'agit des potentiels les plus simples pour lesquels le raisonnement précédent est valable. Cela se déduit encore très facilement de la structure supersymétrique en remarquant que l'on a simplement

$$L_V^{(0)} = -\Delta + \nabla V \cdot \nabla \quad \text{et} \quad L_V^{(1)} = L_V^{(0)} \otimes \text{Id} + \text{Hess } V \geq \text{Hess } V \quad (1.3.14)$$

lorsque  $\Omega = \mathbb{R}^d$ . Dans ce cas, la relation  $L_V^{(1)} \geq c > 0$  est donc en particulier assurée par l'hypothèse  $\text{Hess } V \geq c$  sur  $\mathbb{R}^d$ .

Dans ce cas convexe, l'inégalité de Poincaré (1.3.10) est un cas particulier de l'inégalité plus générale de Brascamp-Lieb (cf. l'équation (2.1.1) du chapitre suivant et [BL76]) sur laquelle porte le chapitre 2 de ce mémoire s'appuyant sur notre travail [Lep17]. Nous y généralisons en particulier ce type d'inégalité à des formes différentielles de degré quelconque sur des variétés riemanniennes orientées compactes et connexes à bord (cf. théorème 2.4.2 au chapitre 2), pour les conditions au bord naturelles de type Dirichlet ou Neumann définies dans la partie 1.2.3. Par ailleurs, lorsque l'on se restreint à des fonctions dans ce cadre plus général, on peut préciser nos résultats (cf. corollaire 2.4.4 au chapitre 2) pour aboutir à des formules qui, à notre connaissance, n'avaient été établies à ce niveau de généralité par d'autres méthodes que dans le très intéressant récent travail [KM17]. Nous renvoyons au chapitre 2 pour plus de détails et de références à ce sujet.

### 1.3.2 Régime basse température et métastabilité

Intéressons-nous maintenant au régime semi-classique basse température  $h \rightarrow 0^+$  de la dynamique de Langevin sur-amortie (1.3.1),

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

Nous supposons que  $V$  est un potentiel de Morse tendant vers l'infini à l'infini, suffisamment vite pour que  $Z := \int_{\Omega} e^{-\frac{V}{h}} d\mu$  soit fini pour au moins un  $h > 0$  et donc pour tout  $h > 0$  assez petit. Le terme  $-\nabla V(X_t)$  envoie typiquement (i.e. en dehors d'un ensemble de mesure nulle) le processus  $(X_t)_{t \geq 0}$  vers les minima locaux de  $V$  tandis que, sous l'effet du terme de bruit  $\sqrt{2h} dB_t$ , celui-ci peut « sauter » d'un bassin d'attraction de la dynamique  $\dot{x} = -\nabla V(x)$  vers un autre. Dans le régime  $h \rightarrow 0^+$ , le bruit est très faible et le processus  $(X_t)_{t \geq 0}$  reste donc piégé pendant une très longue période dans un puits du potentiel  $V$ , appelé état métastable, avant de visiter une autre région de l'espace. Ce passage d'une région métastable à une autre correspond typiquement à un changement de conformation macroscopique du système. D'après ce phénomène, correspondant essentiellement à celui d'effet tunnel en analyse semi-classique, le processus  $(X_t)_{t \geq 0}$  est dit métastable. Pour être un peu plus précis, on dira qu'un domaine  $\Omega_0 \subset \mathbb{R}^n$  est métastable pour la mesure de probabilité  $\mu$  supportée dans  $\Omega_0$  si, lorsque  $X_0$  est distribué selon  $\mu$ , ce que l'on notera  $X_0 \sim \mu$ , le processus (1.3.1) atteint un équilibre local dans  $\Omega_0$  bien avant de s'en échapper. Cela sera précisé dans la partie 1.3.3 ci-dessous à l'aide de la notion de distribution quasi-stationnaire (cf. définition 1.3.4).

La métastabilité conduit ainsi à une séparation des échelles de temps, ce qui constitue l'un des obstacles majeurs à l'obtention de l'évolution macroscopique d'un

système métastable à partir de simulations effectuées au niveau microscopique. En effet, de nombreuses transitions ne peuvent pas être observées en pratique en intégrant directement les trajectoires du processus (1.3.1), les temps de simulations numériques accessibles étant trop courts. L'étude de ce phénomène est un domaine très actif de la recherche scientifique en dynamique moléculaire et nous renvoyons en particulier à [LS16] pour un aperçu de ce sujet.

Pour surmonter cette difficulté, certains algorithmes, très utilisés aujourd'hui, en particulier pour des applications en science des matériaux, utilisent le fait que l'évènement de sortie d'une région métastable peut être bien approché par un processus de sauts de Markov dont les taux de transition sont calculés à l'aide de la formule d'Eyring-Kramers. Ces algorithmes utilisent notamment trois idées pour générer de manière plus efficace les évènements de sortie des états métastables : considérer des répliques en parallèle (algorithme *parallel replica*, cf. [Vot98, LLLP12]), modifier le potentiel dans le domaine pour favoriser la sortie (algorithme *hyperdynamics*, cf. [Vot97, LN15]) ou augmenter la température (algorithme *temperature accelerated dynamics*, cf. [SV00, AL14]).

Pour appréhender un peu plus précisément la notion de métastabilité, regardons d'abord ce que nous dit la partie précédente lorsque  $h = 1$  est remplacé par  $h \rightarrow 0^+$ . Le générateur infinitésimal donnant l'évolution de (1.3.1) est maintenant donné par

$$L_{V,h}^{(0)} := -h \Delta + \nabla V \cdot \nabla = h \Delta_{\mathbb{H}}^{(0)} + \mathcal{L}_{\nabla V}, \quad (1.3.15)$$

et  $L_{V,h}^{(0)}$  agissant sur  $\mathcal{C}_c^\infty(\mathbb{R}^d)$  est essentiellement auto-adjoint dans l'espace à poids  $L^2(\Omega, m_{V,h})$ , où  $m_{V,h}$  est la mesure invariante définie par

$$m_{V,h}(d\mu) := \left( \int_{\Omega} e^{-\frac{V}{h}} d\mu \right)^{-1} e^{-\frac{V}{h}} d\mu = Z_h^{-1} e^{-\frac{V}{h}} d\mu. \quad (1.3.16)$$

De nouveau, et ce qui suit reste aussi valable lorsque  $\Omega$  est une variété riemannienne orientée compacte et connexe de dimension  $d$  sans bord, on a équivalence unitaire, au facteur  $h$  près, entre  $L_{V,h}^{(0)}$  agissant dans  $L^2(\Omega, m_{V,h})$  et  $\Delta_{\frac{V}{2},h}^{(0)}$  agissant dans  $L^2(\Omega)$ , d'après la relation

$$\Delta_{\frac{V}{2},h}^{(0)} = e^{-\frac{V}{2h}} h L_{V,h}^{(0)} e^{\frac{V}{2h}}, \quad (1.3.17)$$

et on définit plus généralement, pour tout  $p \in \{0, \dots, d\}$ ,

$$L_{V,h}^{(p)} := h \Delta_{\mathbb{H}}^{(p)} + \mathcal{L}_{\nabla V} = e^{\frac{V}{2h}} \Delta_{\frac{V}{2},h}^{(p)} e^{-\frac{V}{2h}}. \quad (1.3.18)$$

En particulier, en définissant  $\lambda_{2,h} := \inf(\text{Sp}(L_{V,h}^{(0)}) \setminus \{0\})$ , les relations (1.3.12) et (1.3.13) restent vraies en remplaçant  $m_V$  par  $m_{V,h}$  et  $\lambda_2$  par  $\lambda_{2,h}$ . Il faut par contre remplacer le facteur  $\frac{1}{C}$  apparaissant dans (1.3.10) par  $\frac{h}{C}$  puisque :

$$\forall \omega \in H^1(\Omega, m_{V,h}), \quad \int_{\Omega} (L_{V,h}^{(0)} \omega) \omega dm_{V,h} = h \|\nabla \omega\|_{L^2(\Omega, m_{V,h})}^2.$$

Lorsque  $\Omega$  est compacte, la relation (1.3.17) et le théorème 1.2.3 conduisent en particulier à l'existence de  $h_0 > 0$  et de  $C > 0$  tels que pour tout  $h \in (0, h_0]$ ,

$$\text{Sp}(L_{V,h}^{(0)}) \cap [0, C] = \text{Sp}(L_{V,h}^{(0)}) \cap [0, e^{-\frac{C}{h}}] \quad (1.3.19)$$

et

$$\dim \operatorname{Sp} (L_{V,h}^{(0)}) \cap [0, C] = \mathbf{m}_0, \quad (1.3.20)$$

où  $\mathbf{m}_0$  est le nombre de minima locaux de  $f$ . Lorsque  $\Omega = \mathbb{R}^d$ , les hypothèses additionnelles de confinement suivantes,

$$\text{en dehors d'un compact } K, \quad |\nabla f| \geq \frac{1}{C} \quad \text{et} \quad |\operatorname{Hess} f| \leq C |\nabla f|^2,$$

garantissent (avec (1.3.17)) l'inclusion du spectre essentiel de  $L_{V,h}^{(0)}$  dans  $[\frac{C_1}{h}, +\infty)$  pour un certain  $C_1 > 0$  et les relations (1.3.19), (1.3.20) restent valides (cf. [HKN04, Proposition 2.2]). On en déduit le comportement asymptotique de l'évolution d'un état  $\omega \in L^2(\Omega, m_{V,h})$  suivant :

- si  $\omega$  est un vecteur propre associé à la valeur propre 0, i.e. si  $\omega \in \operatorname{Ran} (x \mapsto 1)$ , alors cet état est stable :

$$\text{pour tout } t \geq 0, \quad e^{-tL_{V,h}^{(0)}} \omega = \omega,$$

- si  $\omega$  appartient à l'espace spectral  $\operatorname{Ran} \mathbf{1}_{(C,+\infty)}(L_{V,h}^{(0)})$ , alors  $\omega$  a un temps de vie court, d'ordre au plus  $\frac{1}{C}$  :

$$\text{pour tout } t \geq 0, \quad \|e^{-tL_{V,h}^{(0)}} \omega\|_{L^2(\Omega, m_{V,h})} \leq \|\omega\|_{L^2(\Omega, m_{V,h})} e^{-Ct},$$

- enfin, si  $\omega$  est un vecteur propre associé à  $\lambda_{p,h}$ , l'une des valeurs propres  $0 < \lambda_{2,h} \leq \dots \leq \lambda_{\mathbf{m}_0,h}$  de  $L_{V,h}^{(0)}$  dans  $(0, C]$ , alors, comme  $0 < \lambda_{p,h} \leq e^{-\frac{C}{h}}$ ,  $\omega$  est métastable, i.e. a un temps de vie exponentiellement long d'ordre  $\frac{1}{\lambda_{p,h}}$  :

$$\text{pour tout } t \geq 0, \quad e^{-tL_{V,h}^{(0)}} \omega = e^{-\lambda_{p,h}t} \omega.$$

Les travaux [BEGK04, BGK05] de Bovier, Eckhoff, Gaynard et Klein, utilisant la théorie du potentiel dans  $\mathbb{R}^d$ , conduisent par ailleurs à une caractérisation probabiliste précise des temps de vie  $\frac{1}{\lambda_{p,h}}$  (pour  $p \in \{2, \dots, \mathbf{m}_0\}$ ) de ces états métastables sous des hypothèses additionnelles génériques sur la fonction de Morse  $V$ . Décrivons cela précisément ci-dessous.

On suppose que  $\{x_1\} = \operatorname{argmin}_{\mathbb{R}^n} V$  et, pour  $k \in \{2, \dots, \mathbf{m}_0\}$  et  $B_k = \{x \in \{x_1, \dots, x_{\mathbf{m}_0}\} \setminus \{x_k\}, V(x) \leq V(x_k)\}$ <sup>8</sup>, on note  $\mathcal{P}(x_k, B_k)$  l'ensemble des courbes  $\gamma \in \mathcal{C}^0([0, 1], \mathbb{R}^n)$  telles que  $\gamma(0) = x_k$  et  $\gamma(1) \in B_k$ . Supposons aussi que :

1. pour tout  $k \in \{2, \dots, \mathbf{m}_0\}$ , il existe un unique point selle  $z_k$  tel que  $V(z_k) = \inf_{\gamma \in \mathcal{P}(x_k, B_k)} \sup_{t \in [0, 1]} V(\gamma(t))$ <sup>9</sup>,
2. les valeurs  $(V(z_k) - V(x_k))_{k \in \{2, \dots, \mathbf{m}_0\}}$  sont toutes distinctes.

Sous ces hypothèses,  $x_k \in \{x_2, \dots, x_{\mathbf{m}_0}\} \mapsto z_k$  définit une application injective et on réordonne alors les  $k \in \{2, \dots, \mathbf{m}_0\}$  de sorte que la suite  $(V(z_k) - V(x_k))_{k \in \{2, \dots, \mathbf{m}_0\}}$  soit strictement décroissante (une illustration est donnée par la figure 1.1). On a alors (d'après [BEGK04, BGK05]) :

8.  $B_k$  est donc l'ensemble des minima locaux de  $f$  d'énergie inférieure à celle de  $x_k$ .

9. Pour une fonction de Morse quelconque, il y a toujours au moins un tel point  $z_k$ ; nous renvoyons au chapitre 3 pour plus de détails à ce sujet.



- i) pour tout  $k \in \{2, \dots, \mathbf{m}_0\}$ , le temps moyen  $\tau_{k,h}$  mis par le processus  $(X_t)_{t \geq 0}$ , partant de  $x_k$ , pour atteindre  $B_k$ , est donné par la formule de type Eyring-Kramers suivante lorsque  $h \rightarrow 0^+$  :

$$\tau_{k,h} = \frac{2\pi}{|\lambda(z_k)|} \frac{\sqrt{|\det \text{Hess } V(z_k)|}}{\sqrt{|\det \text{Hess } V(x_k)|}} e^{\frac{V(z_k) - V(x_k)}{h}} (1 + o(1)), \quad (1.3.21)$$

où  $\lambda(z_k)$  est la valeur propre négative de  $\text{Hess } V(z_k)$ ,

- ii) il existe  $c > 0$  tel que pour tout  $k \in \{2, \dots, \mathbf{m}_0\}$ , on a lorsque  $h \rightarrow 0^+$  :

$$\begin{aligned} \lambda_{k,h} &= \frac{1}{\tau_{k,h}} (1 + O(e^{-\frac{c}{h}})) \\ &= \frac{|\lambda(z_k)|}{2\pi} \frac{\sqrt{|\det \text{Hess } V(x_k)|}}{\sqrt{|\det \text{Hess } V(z_k)|}} e^{-\frac{V(z_k) - V(x_k)}{h}} (1 + o(1)). \end{aligned} \quad (1.3.22)$$

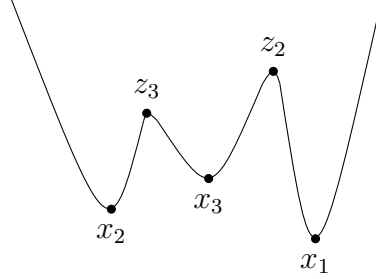


FIGURE 1.1 – Classement des minima et points selles sur un exemple 1D

Les hypothèses précédentes impliquent donc en particulier l'existence d'une cascade d'événements, se produisant sur différentes échelles de temps, permettant au processus  $(X_t)_{t \geq 0}$ , partant de  $x_k$  (pour  $k \in \{2, \dots, \mathbf{m}_0\}$ ), d'atteindre le minimum global  $x_1$  de  $V$  dans  $\mathbb{R}^n$  (cf. figure 1.1). Nous renvoyons également à [Eck05] pour des résultats similaires, à [HKN04] pour une autre preuve de (1.3.22) (également valable lorsque  $\Omega$  est compacte et sans bord) à l'aide d'outils d'analyse semi-classique ainsi qu'à [HHS11, Mic19] pour une généralisation des résultats obtenus dans [HKN04]<sup>10</sup>. Cette approche semi-classique est l'objet du chapitre 3. Signalons aussi notre travail [DL17] pour un résultat du type (1.3.22) pour un certain potentiel double puits en grande dimension (cf. section 3.4 pour plus de détails), [LMS19] généralisant [BEGK04] à certaines dynamiques non réversibles (i.e. non gradient) lorsque  $V$  a deux minima locaux, ainsi que [HKS89, Mic95, MS14, BD16] pour des résultats connexes. Dans le cas à bord, nous renvoyons à [HN06, Lep10, DLLN19b, LN19a] pour des résultats précis du type (1.3.22) (voir aussi (1.2.22) à la fin de la partie 1.2.3 et les théorèmes 3.2.1 et 3.2.2 du chapitre 3)<sup>11</sup>. Enfin, nous renvoyons à l'article de revue [Ber13] sur ce sujet.

10. Mentionnons aussi ici notre travail plus récent [LM19], non présenté dans ce mémoire, généralisant ces résultats à certaines dynamiques non réversibles (i.e. non gradient) pour des potentiels  $V$  multi-puits.

11. Par ailleurs, notre travail plus récent [LN19b], non présenté dans ce mémoire, généralise les résultats de [HN06, DLLN19b] à des potentiels  $V$  admettant des points critiques sur  $\partial\Omega$ .

De telles estimées sont par exemple utilisées dans [SS13, Sch98] pour construire des dynamiques markoviennes de saut en projetant le générateur infinitésimal  $L_{V,h}^{(0)}$  de la diffusion (1.3.1) sur l'espace engendré par ses  $\mathbf{m}_0$  petites valeurs propres par une méthode de Galerkin. Cela conduit à une très bonne approximation de  $L_{V,h}^{(0)}$  à la limite  $h \rightarrow 0^+$ .

La formule (1.3.21) remonte au moins à l'article de cinétique chimique de Kramers [Kra40] paru en 1940 (et même en fait à quelques années avant, comme cela est expliqué dans l'article de revue [HTB90]) où elle est formellement obtenue en dimension 1 et y est comparée à une formule similaire notamment obtenue par Eyring dans [Eyr35] en 1935 par une autre méthode de calcul des cinétiques de réaction (cf. [Kra40, page 295] ou [HTB90] pour une revue de la littérature).

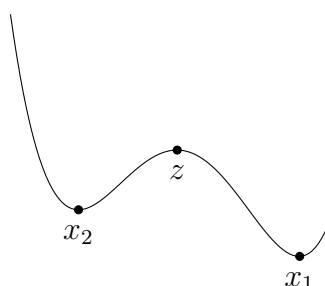


FIGURE 1.2 – Allure du potentiel  $V$  considéré par Kramers dans [Kra40, Fig. 1]

Avec nos notations, la formule (17) donnée par Kramers dans [Kra40] pour un potentiel double puits comme représenté à la figure 1.2 se réécrit en effet comme suit : lorsque  $0 < h \ll V(z) - V(x_2)$ ,

$$r_{21} = \frac{\sqrt{|V'''(z)| V''(x_2)}}{2\pi} e^{-\frac{V(z)-V(x_2)}{h}} (1 + o(1)), \quad (1.3.23)$$

où  $r_{21}$  est le taux de réaction qui, si l'on cite [Kra40], « denotes the chance in unit time that a particle which originally was caught at  $A$  (ici  $A = x_2$ ) escapes to  $B$  (ici  $B = x_1$ ) ». En d'autres termes, d'après [Kra40], le temps pour atteindre  $x_1$  partant de  $x_2$  suit une loi exponentielle de paramètre  $r_{21}$ , où, d'après (1.3.23),  $r_{21}$  satisfait la formule (1.3.22) donnée pour  $\lambda_{2,h}$  dans ce cadre (en dimension 1, un point selle est un maximum local). Par conséquent, l'inverse de  $r_{21}$ , qui représente donc d'après [Kra40] le temps moyen, partant de  $x_2$ , pour atteindre  $x_1$ , est donné d'après Kramers par la formule (1.3.21). Signalons que le préfacteur dans (1.3.23) (comme d'ailleurs dans (1.3.21) et dans (1.3.22)) est *in fine* obtenu par la méthode de Laplace en comparant  $V$  au voisinage de  $x_2$  et de  $z$  avec son polynôme de Taylor d'ordre 2<sup>12</sup>.

Il est important de remarquer ici que les résultats présentés ci-dessus ne fournissent, à la limite  $h \rightarrow 0^+$ , que certains taux de réaction du système et ne justifient donc pas la validité asymptotique de la « loi complète » d'Eyring-Kramers, utilisée en pratique dans les algorithmes de simulation moléculaire comme ceux déjà cités (cf. [Vot97, Vot98, SV00]). Cette loi prend en effet en compte tous les taux de réaction du système alors que dans les résultats cités ci-dessus, rien n'est par exemple

12. En fait, dans son article [Kra40], Kramers suppose simplement que  $V$  est quadratique au voisinage de  $x_2$  et au voisinage de  $z$ .

dit sur ce qu'il se passe partant du minimum global de  $V$ . Nous renvoyons à la partie suivante pour une définition de la loi d'Eyring-Kramers et au chapitre 5 pour plus de détails à ce propos.

Dans notre travail [DLLN17b] présenté dans le chapitre 5, nous démontrons justement la validité asymptotique de la loi d'Eyring-Kramers (cf. en particulier les corollaires 5.2.7 et 5.2.8). Plus précisément, nous y montrons que cette loi correspond bien, dans l'asymptotique  $h \rightarrow 0^+$ , à la loi de sortie d'un état métastable  $\Omega$  lorsque  $\Omega$  est un puits confinant du potentiel  $V$  (i.e. tel que  $V$  admet un unique point critique, un minimum, dans  $\Omega$  et  $\partial_n V > 0$  sur  $\partial\Omega$ ) et le processus  $(X_t)_{t \geq 0}$  solution de (1.3.1) est initialement distribué selon une distribution de probabilité naturelle supportée dans  $\Omega$  appelée distribution quasi-stationnaire. Néanmoins, comme sous ces hypothèses  $V$  n'admet pas de véritable point selle sur  $\partial\Omega$ , les méthodes de Laplace conduisant au calcul des préfacteurs mènent à des formules différant légèrement de (1.3.22) et de (1.3.23). Pour être plus précis, nous justifions en fait dans [DLLN17b] la validité asymptotique de la loi d'Eyring-Kramers construite à partir du taux de réaction formellement obtenu par Kramers en dimension 1 dans [Kra40] pour un potentiel double puits comme représenté à la figure 1.3. Dans ce cas, la formule donnée dans [Kra40, Page 293] pour le taux de transition  $r_{21}$  de  $x_2$  vers  $x_1$  se réécrit avec nos notations

$$r_{21} = \frac{V''(x_2) \sqrt{V(z) - V(x_2)}}{2\sqrt{\pi h}} (1 + o(1)).$$

Comme Kramers suppose en outre  $V$  quadratique sur  $[x_2, z]$ , ce qui mène à

$$V'(z) = \sqrt{V(z) - V(x_2)} \sqrt{2V''(x_2)} \quad (\text{cf. figure 1.3}),$$

le taux de transition  $r_{21}$  s'écrit encore comme suit (voir les taux du corollaire 5.2.8, l'équation (1.3.33) de la partie suivante et la discussion associée)

$$r_{21} = \frac{V'(z) \sqrt{V''(x_2)}}{2\sqrt{2\pi h}} e^{-\frac{V(z) - V(x_2)}{h}} (1 + o(1)). \quad (1.3.24)$$

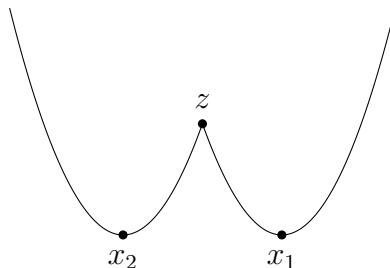


FIGURE 1.3 – Allure du potentiel  $V$  considéré par Kramers dans [Kra40, Fig. 2]. Le potentiel  $V(z + \cdot)$  est ici symétrique.

Dans la partie suivante, dernière partie de ce chapitre introductif, nous définissons la distribution quasi-stationnaire et donnons ses premières propriétés.

### 1.3.3 Distribution quasi-stationnaire et métastabilité

Nous présentons dans cette partie la distribution quasi-stationnaire du processus de Langevin sur-amorti et ses connexions avec la métastabilité. Cet objet est au coeur de l'analyse de nos travaux [DLLN17b, DLLN19a, LN19a]<sup>13</sup>, portant sur l'évènement de sortie d'un domaine métastable pour le processus de Langevin sur-amorti, sur lesquels portent les chapitres 4 et 5 de ce mémoire et par ailleurs résumés dans les articles de type compte rendu [DLLN17a, LLN18]. Pour des résultats plus généraux sur les distributions quasi-stationnaires que ceux présentés ici, nous renvoyons par exemple à [CCL<sup>+</sup>09, CMS13, CV17].

Dans toute cette partie, le domaine  $\Omega_0 \subset \mathbb{R}^d$  est supposé ouvert, régulier et borné<sup>14</sup>. Pour le processus  $(X_t)_{t \geq 0}$  solution de (1.3.1) et initialement distribué dans  $\Omega_0$ , on définit

$$\tau_{\Omega_0} := \inf\{t \geq 0, X_t \notin \Omega_0\}$$

le temps de première sortie de  $\Omega_0$  pour  $(X_t)_{t \geq 0}$ . L'évènement de sortie de  $\Omega_0$  est caractérisé par le couple de variables aléatoires  $(\tau_{\Omega_0}, X_{\tau_{\Omega_0}})$ .

Une distribution quasi-stationnaire associée à la dynamique de Langevin sur-amortie (1.3.1) et à  $\Omega_0$  se définit alors comme suit :

**Définition 1.3.1.** *Soit  $\Omega_0 \subset \mathbb{R}^d$  et  $(X_t)_{t \geq 0}$  la dynamique solution de (1.3.1). Une distribution quasi-stationnaire associée à  $(X_t)_{t \geq 0}$  et à  $\Omega_0$  est une mesure de probabilité  $\nu_h$  supportée dans  $\Omega_0$  telle que, pour tout ensemble mesurable  $A \subset \Omega_0$  et pour tout  $t \geq 0$ ,*

$$\nu_h(A) = \frac{\int_{\Omega_0} \mathbb{P}_x[X_t \in A, t < \tau_{\Omega_0}] \nu_h(d\mu)}{\int_{\Omega_0} \mathbb{P}_x[t < \tau_{\Omega_0}] \nu_h(d\mu)},$$

où l'indice  $x$  dans  $\mathbb{P}_x$  indique ici que le processus commence initialement en  $x$ .

Autrement dit,  $\nu_h$  est une distribution quasi-stationnaire si, lorsque  $X_0$  est distribué selon  $\nu_h$ , alors, pour tout  $t > 0$ , le processus  $X_t$  conditionné à ne pas avoir quitté  $\Omega_0$  jusqu'au temps  $t$  est toujours distribué selon  $\nu_h$ .

Considérons maintenant l'espace de Hilbert à poids

$$L_w^2(\Omega_0) := \left\{ u : \Omega_0 \rightarrow \mathbb{R}, \int_{\Omega_0} u^2 e^{-\frac{V}{h}} d\mu < +\infty \right\}$$

et définissons les espaces de Sobolev à poids  $H_w^k(\Omega_0)$  de la même façon. D'après l'analyse du laplacien de Witten sur des variétés à bord faite dans la partie 1.2.3, la réalisation de Dirichlet  $L_{V,h}^{D,(0)}$  du générateur infinitésimal de la dynamique (1.3.1) définie par (cf. (1.3.17))

$$L_{V,h}^{D,(0)} = e^{\frac{V}{2h}} \frac{1}{h} \Delta_{\frac{V}{2},h}^{D,(0)} e^{-\frac{V}{2h}}$$

13. La prépublication [DLLN19a] a été divisée en deux parties pour publication, avec pour première partie [DLLN19b].

14. Dans les chapitres 4 et 5, on utilisera simplement la notation  $\Omega$  et non  $\Omega_0$ . La notation  $\Omega_0$  permet néanmoins ici d'éviter les confusions avec la notation  $\Omega$  des parties précédentes.

est auto-adjointe, à résolvante compacte et positive dans  $L_w^2(\Omega_0)$ . Son domaine est simplement

$$D(L_{V,h}^{D,(0)}) = \{u \in H_w^1(\Omega_0), u = 0 \text{ sur } \partial\Omega_0\} \cap H_w^2(\Omega_0) := H_{w,0}^1(\Omega_0) \cap H_w^2(\Omega_0)$$

et il s'agit aussi de l'extension de Friedrichs de  $L_{V,h}^{(0)}$  agissant sur  $\mathcal{C}_c^\infty(\Omega_0)$ .

De même, le générateur infinitésimal  $L_{V,h}^{(0),\dagger} = -h\Delta - \operatorname{div}(\cdot \nabla V)$  de l'évolution de la densité de probabilité du processus  $(X_t)_{t \geq 0}$  (cf. (1.3.3)) muni du domaine

$$D(L_{V,h}^{(0),\dagger}) = H_0^1(\Omega_0, e^{\frac{V}{h}} d\mu) \cap H^2(\Omega_0, e^{\frac{V}{h}} d\mu)$$

est auto-adjoint, à résolvante compacte et positif dans  $L^2(\Omega_0, e^{\frac{V}{h}} d\mu)$  (toujours d'après la relation (1.3.17)). En notant  $L_{V,h}^{D,(0),\dagger}$  cette réalisation de Dirichlet auto-adjointe, on a de plus clairement

$$\operatorname{Sp}(L_{V,h}^{D,(0),\dagger}) = \operatorname{Sp}(L_{V,h}^{D,(0)}) =: \{\lambda_{k,h}, k \in \mathbb{N}^*\} \quad (1.3.25)$$

et

$$L_{V,h}^{D,(0)} u_k = \lambda_{k,h} u_k \quad \text{si et seulement si} \quad L_{V,h}^{D,(0),\dagger} u_k e^{-\frac{V}{h}} = \lambda_{k,h} u_k e^{-\frac{V}{h}}. \quad (1.3.26)$$

Par la théorie classique des opérateurs elliptiques (cf. par exemple [GT01]), la première valeur propre  $\lambda_{1,h}$  de  $L_{V,h}^{D,(0)}$  (ou encore de  $L_{V,h}^{D,(0),\dagger}$ ) est strictement positive, simple et toute fonction propre associée  $u_h$  appartient à  $\mathcal{C}^\infty(\overline{\Omega}_0)$  et a un signe sur  $\Omega_0$ . On a par ailleurs la proposition suivante donnant l'existence d'une distribution quasi-stationnaire associée à la dynamique de Langevin sur-amortie et à  $\Omega_0$  (cf. [LLL12, Proposition 2]) :

**Proposition 1.3.2.** *Soit  $u_h$  une fonction propre principale de  $L_{V,h}^{D,(0)}$ . La mesure de probabilité*

$$\nu_h(d\mu) := \nu_h(x) d\mu := \frac{u_h(x) e^{-\frac{V(x)}{h}}}{\int_{\Omega_0} u_h e^{-\frac{V}{h}} d\mu} d\mu \quad (1.3.27)$$

*est alors une distribution quasi-stationnaire (indépendante du choix de  $u_h$ ) associée à la dynamique (1.3.1) et à  $\Omega_0$ .*

En termes du générateur infinitésimal  $L_{V,h}^{(0),\dagger} = -h\Delta - \operatorname{div}(\cdot \nabla V)$  de l'évolution de la densité de probabilité du processus  $(X_t)_{t \geq 0}$ , cela signifie encore que la fonction propre principale de  $L_{V,h}^{D,(0),\dagger}$  normalisée dans  $L^1(\Omega_0, e^{\frac{V}{h}} d\mu)$  est la densité (par rapport à la mesure de Lebesgue) d'une distribution quasi-stationnaire associée à la dynamique (1.3.1) et à  $\Omega_0$ .

Nous avons de plus le résultat suivant, impliquant en particulier l'unicité de la distribution quasi-stationnaire associée à la dynamique (1.3.1) et à  $\Omega_0$  (cf. [LLL12, Proposition 6]). Notons au passage qu'il implique donc aussi que la mesure invariante  $m_{V,h}$  (définie dans (1.3.16)) restreinte à  $\Omega_0$ , i.e.  $\frac{1}{m_{V,h}(\Omega_0)} m_{V,h}|_{\Omega_0}$ , n'est pas la distribution quasi-stationnaire associée à la dynamique (1.3.1) et à  $\Omega_0$  !

**Proposition 1.3.3.** *Soient  $\nu_h$  la mesure de probabilité définie par (1.3.27) et  $(X_t)_{t \geq 0}$  la dynamique solution de (1.3.1). Supposons que  $X_0$  est distribué dans  $\Omega_0$  et que sa loi de probabilité admet une densité  $\mu_0$  par rapport à  $m_{V,h}$  dans  $L^2(\Omega_0, m_{V,h})$ . Il existe alors une constante  $C(\mu_0, h) > 0$  telle que, pour tout  $t \geq 0$ ,*

$$\|\text{Loi}(X_t | t < \tau_{\Omega_0}) - \nu_h\|_{VT} \leq C(\mu_0, h) e^{-(\lambda_{2,h} - \lambda_{1,h})t} \xrightarrow[t \rightarrow +\infty]{} 0. \quad (1.3.28)$$

Ici,  $\text{Loi}(X_t | t < \tau_{\Omega_0})$  désigne la loi de probabilité de  $X_t$  conditionné à ne pas avoir quitté  $\Omega_0$ , i.e. à l'évènement  $\{t < \tau_{\Omega_0}\}$  (et  $\|\cdot\|_{VT}$  la distance en variation totale). La relation (1.3.28) est en quelque sorte une généralisation de la relation (1.3.13) dans ce cadre. D'ailleurs, comme  $\Omega_0$  est borné, l'hypothèse sur la densité de la loi de  $X_0$  n'est en fait pas restrictive puisque l'on s'y ramène immédiatement par effet régularisant de l'évolution en temps.

Soit  $(X_t)_{t \geq 0}$  le processus solution de (1.3.1) avec  $X_0$  distribué dans  $\Omega_0$ . Si  $\tau_{\Omega_0}$  est suffisamment grand, alors d'après la proposition 1.3.3, le processus  $(X_t)_{t \geq 0}$  atteindra un équilibre local, donné par la distribution quasi-stationnaire, avant de sortir de  $\Omega_0$ . Dans ce cas, subordonné à la distribution de  $X_0$ , il est donc pertinent d'étudier l'évènement de sortie  $(\tau_{\Omega_0}, X_{\tau_{\Omega_0}})$  du domaine  $\Omega_0$  pour la dynamique de Langevin sur-amortie lorsque le processus  $(X_t)_{t \geq 0}$  solution de (1.3.1) est initialement distribué selon la distribution quasi-stationnaire associée. Néanmoins, le domaine  $\Omega_0$  peut très bien être « mal » choisi de sorte que, pour (presque) toute condition initiale du type  $X_0 = x \in \Omega_0$ , le temps de séjour moyen  $\mathbb{E}_x[\tau_{\Omega_0}]$  du processus  $(X_t)_{t \geq 0}$  dans  $\Omega_0$  soit trop court pour permettre à  $(X_t)_{t \geq 0}$  d'atteindre (en moyenne) l'équilibre local donné par la distribution quasi-stationnaire avant de quitter  $\Omega_0$  (voir par exemple l'exemple b) dans la première partie de la section 4.2.4). Cette distribution n'est alors pas d'un grand intérêt.

Ces considérations nous conduisent à proposer la définition suivante d'un domaine  $\Omega_0$  métastable.

**Définition 1.3.4.** *Soit  $(X_t)_{t \geq 0}$  la dynamique solution de (1.3.1), supposée initialement distribuée dans  $\Omega_0$ .*

- i) On dit que le domaine  $\Omega_0$  est métastable pour  $X_0$  si, à la limite  $h \rightarrow 0^+$ , la convergence dans (1.3.28) a lieu bien avant le temps de (premier) séjour moyen  $\mathbb{E}[\tau_{\Omega_0}]$  de  $(X_t)_{t \geq 0}$  dans  $\Omega_0$ .*
- ii) Plus généralement, on dit que le domaine  $\Omega_0$  est métastable s'il existe un ouvert  $\mathcal{V} \subset \Omega_0$  tel que  $\Omega_0$  est métastable pour  $X_0 = x$  pour tout  $x \in \mathcal{V}$ .*

Pour un domaine  $\Omega_0$  métastable (pour  $X_0$ ), il est donc raisonnable de supposer que le processus  $(X_t)_{t \geq 0}$  est initialement distribué selon la distribution quasi-stationnaire  $\nu_h$ . Par ailleurs, lorsque le processus  $(X_t)_{t \geq 0}$  solution de (1.3.1) est initialement distribué selon  $\nu_h$ , l'évènement de sortie  $(\tau_{\Omega_0}, X_{\tau_{\Omega_0}})$  du domaine  $\Omega_0$  est caractérisé par la proposition suivante (cf. [LLLP12, Proposition 3]) :

**Proposition 1.3.5.** *Considérons  $(X_t)_{t \geq 0}$  la dynamique solution de (1.3.1) et  $\nu_h$  la distribution quasi-stationnaire associée (cf. (1.3.27)). Supposons de plus que  $X_0$  est distribué selon  $\nu_h$ . Alors :*

- i) les variables aléatoires  $\tau_{\Omega_0}$  et  $X_{\tau_{\Omega_0}}$  sont indépendantes,*
- ii) la variable aléatoire  $\tau_{\Omega_0}$  suit une loi exponentielle de paramètre  $\lambda_{1,h}$  (la valeur propre principale de  $L_{V,h}^{D,(0)}$ ), d'où en particulier  $\mathbb{E}_{\nu_h}[\tau_{\Omega_0}] = \frac{1}{\lambda_{1,h}}$ ,*

iii) la loi de la variable aléatoire  $X_{\tau_{\Omega_0}}$  a une densité par rapport à la mesure de Lebesgue sur  $\partial\Omega_0$  donnée par

$$z \in \partial\Omega_0 \longmapsto -\frac{h}{\lambda_{1,h}} \frac{\partial_n u_h(z) e^{-\frac{V(z)}{h}}}{\int_{\Omega_0} u_h e^{-\frac{V}{h}} d\mu}, \quad (1.3.29)$$

où  $\partial_n = \vec{n} \cdot \nabla$  désigne dérivée normale au bord et  $\vec{n}$  la normale extérieure à  $\partial\Omega_0$ .

Dans nos travaux [DLLN19a, LN19a]<sup>15</sup> résumés dans le chapitre 4, nous essayons d'analyser la métastabilité d'un domaine  $\Omega_0$  via l'étude des lieux de sortie les plus probables de ce domaine pour la dynamique de Langevin sur-amortie (cf. définition 4.1.1).

Lorsque  $X_0 = x \in \Omega_0$  et  $\Omega_0$  est un puits confinant du potentiel  $V$ , i.e. tel que

- $V$  admet un unique point critique, un minimum (non dégénéré), dans  $\Omega_0$
- et  $\partial_n V > 0$  sur  $\partial\Omega_0$ ,

il est bien connu qu'à la limite  $h \rightarrow 0^+$ ,  $X_{\tau_{\Omega_0}}$  se concentre sur  $\arg \min_{\partial\Omega_0} V$ . Lorsque  $V|_{\partial\Omega_0}$  atteint son minimum en un unique point (de  $\partial\Omega_0$ ), cela découle des travaux de Freidlin-Wentzell dans le cadre de leur théorie des grandes déviations développée dans les années 70 (cf. leur ouvrage [FW12] pour un aperçu général de leurs résultats et plus précisément le théorème 2.1 du chapitre 4 sur ce point). Leurs résultats conduisent également aux estimées logarithmiques suivantes (cf. [FW12, théorème 5.1 du chapitre 6]) : pour tout  $x \in \Omega_0$  tel que  $V(x) < \min_{\partial\Omega_0} V$  et pour tous  $\gamma > 0$  et  $\delta_0 > 0$ , il existe  $\delta \in (0, \delta_0]$  tel que pour tous  $h > 0$  suffisamment petit et  $y \in \partial\Omega_0$ ,

$$e^{-\frac{V(y) - \min_{\partial\Omega_0} V}{h}} e^{-\frac{\gamma}{h}} \leq \mathbb{P}_x[|X_{\tau_{\Omega_0}} - y| < \delta] \leq e^{-\frac{V(y) - \min_{\partial\Omega_0} V}{h}} e^{\frac{\gamma}{h}}. \quad (1.3.30)$$

À l'aide de calculs formels, Matkowsky-Schuss ont ensuite obtenu la formule énoncée ci-dessous dans [MS77], par la suite notamment rigoureusement démontrée dans [FW12, Kam78, Kam79, Day84, Day87, Per90] : pour tous  $x \in \Omega_0$  et  $F \in \mathcal{C}^\infty(\partial\Omega_0, \mathbb{R})$ , on a à la limite  $h \rightarrow 0^+$ ,

$$\mathbb{E}_x[F(X_{\tau_{\Omega_0}})] = \frac{\int_{\partial\Omega_0} F \partial_n V e^{-\frac{V}{h}} d\mu_{\partial\Omega_0}}{\int_{\partial\Omega_0} \partial_n V e^{-\frac{V}{h}} d\mu_{\partial\Omega_0}} + o(1). \quad (1.3.31)$$

Voir aussi [IS15, IS17] pour des résultats plus récents utilisant des techniques similaires à celles de [Kam78, Kam79, Per90].

La relation (1.3.31) implique en particulier la concentration de  $X_{\tau_{\Omega_0}}$  sur l'ensemble  $\arg \min_{\partial\Omega_0} V$  et donne également, par la méthode de Laplace, les probabilités asymptotiques de sortie au voisinage de chaque élément de  $\arg \min_{\partial\Omega_0} V$ . Contrairement à la relation (1.3.30), elle ne donne par contre aucune information sur la probabilité (partant de  $x \in \Omega_0$ ) de sortir au voisinage d'un point n'appartenant pas à  $\arg \min_{\partial\Omega_0} V$  si ce n'est qu'elle tend vers 0. Mentionnons aussi ici que d'après la formule de Feynman-Kac, la fonction  $x \in \Omega_0 \rightarrow \mathbb{E}_x[F(X_{\tau_{\Omega_0}})]$  est, du point de

15. Nous rappelons que [DLLN19a] a été divisé en deux parties pour publication, avec pour première partie [DLLN19b].

vue des équations aux dérivées partielles, la solution du problème de Dirichlet non homogène (cf. (1.3.15))

$$\begin{cases} L_{V,h}^{(0)} u = 0 & \text{dans } \Omega \\ u = F & \text{sur } \partial\Omega. \end{cases} \quad (1.3.32)$$

Dans l'optique d'analyser la métastabilité d'un domaine  $\Omega_0$ , ce type de comportement naturel – i.e. attendu pour un domaine  $\Omega_0$  convenable – nous conduit d'après la définition 1.3.4 à nous poser dans [DLLN19a] les questions suivantes :

- Quel cadre géométrique pour le potentiel  $V$  nous assure-t-il, lorsque  $X_0$  est initialement distribué selon la distribution quasi-stationnaire  $\nu_h$ , que la loi de  $X_{\tau_{\Omega_0}}$  se concentre sur une partie de  $\arg \min_{\partial\Omega_0} V$  ?
- Quelles conditions sur  $V$  nous assurent-elles que ces résultats s'étendent à un ensemble d'intérieur non vide de conditions initiales déterministes dans  $\Omega_0$  ?

Dans le travail [DLLN19a]<sup>16</sup>, nous étendons en particulier à un cadre très général les résultats obtenus pour un puits confinant du potentiel  $V$  dans [FW12, Kam78, Kam79, Day84, Day87, Per90] (cf. théorème 4.2.3 et la relation (4.2.20) généralisant (1.3.31) au chapitre 4). Ces travaux couvrent cependant aussi le cas non gradient, i.e. le cas de dynamiques de la forme<sup>17</sup>

$$dX_t = b(X_t)dt + \sqrt{2h} dB_t,$$

où  $b$  est un champ vectoriel tel que  $\Omega_0$  soit confinant pour la dynamique  $\dot{x} = b(x)$ , i.e. tel que :

- $\Omega_0$  contient un unique point singulier, asymptotiquement stable et non dégénéré, pour la dynamique
- et  $b \cdot \vec{n} < 0$  sur  $\partial\Omega_0$ .

Enfin, notre travail [LN19a] concerne l'étude fine d'un potentiel double puits dégénéré. Nous renvoyons au chapitre 4 pour plus de détails et de références à ce sujet.

Dans le travail [DLLN17b], résumé dans le chapitre 5, nous justifions la validité asymptotique, i.e. à la limite  $h \rightarrow 0^+$ , de la « loi complète » d'Eyring-Kramers (cf. partie précédente) lorsque :

- $\Omega_0$  est un puits confinant du potentiel  $V$ , i.e. tel que  $V$  admet un unique point critique, un minimum non dégénéré, dans  $\Omega_0$  et  $\partial_n V > 0$  sur  $\partial\Omega_0$ ,
- la fonction  $V|_{\partial\Omega_0}$  est une fonction de Morse,
- $X_0$  est distribué selon  $\nu_h$ .

Nous y montrons aussi sa validité asymptotique pour des conditions initiales déterministes d'énergie suffisamment basse. Expliquons ici cela un peu plus précisément ; nous renvoyons au chapitre 5 pour de plus amples détails.

Nous nous intéressons donc aux taux de réaction associés à l'évènement de sortie de  $\Omega_0$  pour la dynamique de Langevin sur-amortie  $(X_t)_{t \geq 0}$  initialement distribuée

16. Le premier article tiré de cette prépublication, [DLLN19b], s'intéresse au cas  $X_0 \sim \nu_h$ , et le second aux conditions initiales déterministes.

17. Le générateur infinitésimal est alors l'opérateur différentiel  $-h\Delta - b \cdot \nabla$ .



dans  $\Omega_0$ . Notons  $(\Omega_i)_{i=1,\dots,n}$  les domaines voisins de  $\Omega_0$ , chacun correspondant à un état macroscopique du système, et supposons que :

$$\text{pour tout } i \in \{1, \dots, n\}, \quad \{z_i\} = \arg \min_{\partial\Omega_0 \cap \partial\Omega_i} V$$

(cf. figure 1.4, apparaissant aussi dans le chapitre 5).

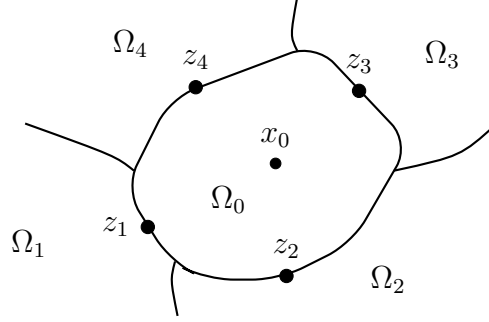


FIGURE 1.4 – Le domaine  $\Omega_0$  et ses domaines voisins  $(\Omega_i)_{i=1,\dots,4}$ ;  $x_0$  est le minimum global de  $V$  dans  $\Omega_0$  et, pour  $i \in \{1, 2, 3, 4\}$ ,  $\{z_i\} = \operatorname{argmin}_{\partial\Omega_0 \cap \partial\Omega_i} V$ .

Les méthodes numériques basées sur l'hypothèse que l'événement de sortie d'une région métastable est bien approché par un processus de sauts de Markov dont les taux de transition sont calculés à l'aide de la formule d'Eyring-Kramers nous conduisent à la définition suivante (cf. [HTB90, Vot05] et la première section du chapitre 5 pour plus de détails) :

**Définition 1.3.6.** Soit  $(X_t)_{t \geq 0}$  la dynamique solution de (1.3.1), supposée initialement distribuée dans  $\Omega_0$ . Nous dirons que l'événement de sortie de  $(X_t)_{t \geq 0}$  de  $\Omega_0$  suit la loi d'Eyring-Kramers associée aux taux de transitions  $(k_{0i})_{i \in \{1,\dots,n\}}$  si :

- i) les variables aléatoires  $\tau_{\Omega_0}$  et  $X_{\tau_{\Omega_0}}$  sont indépendantes,
- ii) la variable aléatoire  $\tau_{\Omega_0}$  suit une loi exponentielle de paramètre  $\sum_{i=1}^n k_{0i}$ , d'où en particulier  $\mathbb{E}[\tau_{\Omega_0}] = \frac{1}{\sum_{i=1}^n k_{0i}}$ ,
- iii) pour tout  $i \in \{1, \dots, n\}$ , la probabilité que  $X_{\tau_{\Omega_0}}$  appartienne à  $\partial\Omega_0 \cap \partial\Omega_i$  vaut  $\frac{k_{0i}}{\sum_{i=1}^n k_{0i}}$ ,
- iv) les taux de transitions satisfont la formule d'Eyring-Kramers « exacte » (cf. partie précédente et ci-dessous).

Le point ii) de cette définition est la simple traduction de la remarque suivante : si, pour  $i \in \{1, \dots, n\}$ ,  $k_{0i}$  est le taux de transition de l'état  $\Omega_0$  vers l'état  $\Omega_i$ , i.e. la probabilité par unité de temps qu'une particule initialement en  $x_0$  s'échappe de  $\Omega_0$  pour aller dans  $\Omega_i$  (cf. (1.3.23) et la discussion au-dessous dans la partie précédente), alors  $\sum_{i=1}^n k_{0i}$  est la probabilité par unité de temps qu'une particule initialement en  $x_0$  s'échappe de  $\Omega_0$ , ce qui signifie encore que  $\tau_{\Omega_0}$  suit une loi exponentielle de paramètre  $\sum_{i=1}^n k_{0i}$ . Le point iii) traduit quant à lui le fait que pour tout  $i \in \{1, \dots, n\}$ , la probabilité pour une particule de s'échapper vers  $\Omega_i$  est proportionnelle à  $k_{0i}$ . Enfin, d'après nos hypothèses sur  $\Omega_0$ , le point iv) signifie que les taux  $k_{0i}$  satisfont la formule d'Eyring-Kramers « exacte », i.e. sans terme d'erreur, déduite

de la formule (1.3.24) en dimension supérieure :

$$k_{0i} = \frac{\partial_n V(z_i)}{\sqrt{2\pi h}} \frac{\sqrt{\det \text{Hess } V(x_0)}}{\sqrt{\det \text{Hess } V|_{\partial\Omega_0}(z_i)}} e^{-\frac{V(z_i)-V(x_0)}{h}}. \quad (1.3.33)$$

On notera que ce taux correspond asymptotiquement en dimension 1 au double de celui donné par (1.3.24). Cette différence est naturelle puisque  $k_{0i}$  correspond en fait au taux de transition pour atteindre  $\partial\Omega_0 \cap \partial\Omega_i$  partant de  $\Omega_0$ , soit deux fois le taux de transition pour atteindre  $\Omega_i$ . En effet, une fois sur la crête  $\partial\Omega_0 \cap \partial\Omega_i$ , le processus  $(X_t)_{t \geq 0}$  a une chance sur deux de revenir dans  $\Omega_0$  et une chance sur deux d'atteindre  $\Omega_i$  (cf. figure 1.3 dans la partie précédente et la discussion à ce sujet dans la partie 5.3.1 du chapitre 5, où il convient de remplacer  $h$  par  $2h$  d'après la différente échelle en  $h$  considérée dans (5.1.1)).

Les premiers résultats rigoureux dans le sens d'une justification asymptotique de la loi d'Eyring-Kramers dans ce cadre remontent aussi à la théorie des grandes déviations de Freidlin-Wentzell. Rappelons en effet déjà la relation (1.3.30) ci-dessus. D'après [FW12, théorèmes 4.1 et 7.4 des chapitres 4 et 6], on a également sous nos hypothèses le résultat suivant :

$$\forall x \in \Omega_0, \quad \lim_{h \rightarrow 0^+} h \ln \mathbb{E}_x[\tau_{\Omega_0}] = \min_{\partial\Omega} V - V(x_0) = \lim_{h \rightarrow 0^+} h \ln \frac{1}{\lambda_{1,h}}, \quad (1.3.34)$$

où nous rappelons que  $\lambda_{1,h}$  est la valeur propre principale de  $L_{V,h}^{D,(0)}$  et, d'après la formule de Dynkin, la fonction  $x \in \Omega_0 \rightarrow \mathbb{E}_x[\tau_{\Omega_0}]$  est, du point de vue des équations aux dérivées partielles, la solution du problème de Dirichlet homogène (cf. (1.3.15))

$$\begin{cases} L_{V,h}^{(0)} u = 1 & \text{dans } \Omega \\ u = 0 & \text{sur } \partial\Omega. \end{cases}$$

Cette asymptotique a ensuite notamment été précisée par Day au début des années 80 dans [Day83] où il est montré que pour tout  $x \in \Omega_0$ <sup>18</sup>,

$$\lambda_{1,h} \mathbb{E}_x[\tau_{\Omega_0}] = 1 + o(1) \quad (\text{uniformément sur les compacts de } \Omega_0) \quad (1.3.35)$$

et que  $\tau_{\Omega_0}$  (lorsque  $X_0 = x$ ) suit asymptotiquement une loi exponentielle de paramètre  $\lambda_{1,h}$ , i.e.

$$\forall s > 0, \quad \mathbb{P}_x[\tau_{\Omega_0} > \frac{1}{\lambda_{1,h}} s] = e^{-s} + o(1) \quad (\text{uniformément sur les compacts de } \Omega_0).$$

Comme nous l'avons déjà mentionné ci-dessus, ces résultats obtenus par la théorie des grandes déviations s'appliquent pour des opérateurs très généraux, i.e. de la forme  $-h\Delta - b \cdot \nabla$  où  $b$  est un champ vectoriel tel que  $\Omega_0$  soit confinant pour la dynamique  $\dot{x} = b(x)$  (cf. définition ci-dessus). Cependant, ils ne permettent pas d'obtenir des formules de type Eyring-Kramers pour les taux de transitions  $k_{0i}$  (cf. (1.3.33)) mais seulement d'obtenir leurs taux d'Arrhenius (cf. (1.3.34) et (1.3.30)).

18. Nous renvoyons aussi à [Sug01, Nec19] pour des généralisations de ce résultat à des domaines  $\Omega_0$  plus généraux. En particulier, le tout récent travail [Nec19] établit à notre connaissance les premiers résultats rigoureux de ce type lorsque le potentiel  $V$  admet des points critiques sur  $\partial\Omega_0$ .

Signalons aussi ici que le calcul précis, i.e. avec préfacteur, de  $\lambda_{1,h}$  dans notre cadre est donné par les travaux [HN06, DLLN19b] (cf. proposition 5.2.3 dans le chapitre 5, où il convient de remplacer  $h$  par  $2h$  d'après la différente échelle en  $h$  considérée dans (5.1.1)) :

$$\lambda_{1,h} = \sum_{j \in \{1, \dots, n\}} k_{0j} (1 + o(1)) = \sum_{j \in \{1, \dots, n\} : V(z_j) = \min_{\partial\Omega_0} V} k_{0j} (1 + o(1)), \quad (1.3.36)$$

où les  $k_{0i}$ ,  $i \in \{1, \dots, n\}$ , sont définis par (1.3.33).

Supposons maintenant que  $X_0$  est distribué selon la distribution quasi-stationnaire  $\nu_h$ . D'après les deux premiers points de la proposition 1.3.5, en définissant, pour tout  $i \in \{1, \dots, n\}$ ,

$$\tilde{k}_{0i} := \mathbb{P}_{\nu_h} (X_{\tau_{\Omega_0}} \in \partial\Omega_0 \cap \partial\Omega_i) \lambda_{1,h},$$

alors les trois premiers points de la définition 1.3.6 sont automatiquement satisfaits pour les taux  $(\tilde{k}_{0i})_{i \in \{1, \dots, n\}}$ . Enfin, d'après la définition des  $\tilde{k}_{0i}$  ci-dessus et le troisième point de la proposition 1.3.5, on a, pour tout  $i \in \{1, \dots, n\}$ ,

$$\tilde{k}_{0i} = -h \frac{\int_{\partial\Omega_0 \cap \partial\Omega_i} \partial_n u_h e^{-\frac{V}{h}} d\mu_{\partial\Omega}}{\int_{\Omega_0} u_h e^{-\frac{V}{h}} d\mu}. \quad (1.3.37)$$

Pour montrer que l'évènement de sortie de  $\Omega_0$  suit asymptotiquement la loi d'Eyring-Kramers lorsque  $X_0$  est distribué selon  $\nu_h$ , il nous suffit donc de montrer que pour tout  $i \in \{1, \dots, n\}$ , le quotient intégral de la relation (1.3.37) est de la forme  $k_{0i} (1 + o(1))$ , où  $k_{0i}$  est défini par la formule d'Eyring-Kramers (1.3.33) ! Cela signifie une étude fine du comportement asymptotique de la première fonction propre de  $L_{V,h}^{D,(0)}$  (ou, de façon équivalente, de celle du laplacien de Witten  $\Delta_{\frac{V}{2},h}^{D,(0)}$  avec conditions au bord de type Dirichlet) et en particulier de sa dérivée normale le long du  $\partial\Omega_0$ . Les estimées asymptotiques les plus délicates à démontrer concernent sans surprise les  $\tilde{k}_{0i}$  où  $i \in \{1, \dots, n\}$  est tel que  $V(z_i) > \min_{\partial\Omega_0} V$ .

Dans le cas d'un puits confinant comme considéré dans [DLLN17b] et donc dans le chapitre 5, cela conduit bien aux formules  $\tilde{k}_{0i} = k_{0i} (1 + o(1))$  pour tout  $i \in \{1, \dots, n\}$ , où les  $k_{0i}$  sont définis par la formule (1.3.33) (cf. corollaire 5.2.8, où il convient de remplacer  $h$  par  $2h$  d'après la différente échelle en  $h$  considérée dans (5.1.1)). Dans les algorithmes utilisés en pratique (cf. [HTB90, Vot97, Vot98, SV00, Vot05]), le domaine  $\Omega_0$  est supposé être le bassin d'attraction d'un minimum de  $V$  pour la dynamique  $\dot{x} = -\nabla V(x)$ , auquel cas  $\partial\Omega_0$  contient de véritables points selles, et les taux de transition considérés sont de la forme

$$k_{0i} = \frac{|\lambda(z_i)|}{2\pi} \frac{\sqrt{|\det \text{Hess } V(x_0)|}}{\sqrt{|\det \text{Hess } V(z_i)|}} e^{-\frac{V(z_i) - V(x_0)}{h}}, \quad (1.3.38)$$

où  $\lambda(z_i)$  est la valeur propre négative de  $\text{Hess } V(z_i)$ . Tout cela est expliqué plus précisément dans le chapitre 5 (cf. sections 5.1 et 5.3.1).

# Chapter 2

## Brascamp-Lieb's type inequalities

We present in this chapter the main results of our work [Lep17].

### 2.1 The case without boundary

Let  $V \in \mathcal{C}^2(\mathbb{R}^d, \mathbb{R})$  be a strictly convex function such that  $e^{-V} \in L^1(\mathbb{R}^d)$  and let  $\nu$  be the probability measure defined by  $d\nu := \frac{e^{-V}}{\int_{\mathbb{R}^d} e^{-V} d\mu} d\mu$  (where  $\mu$  denotes the Lebesgue measure on  $\mathbb{R}^d$ ). The classical Brascamp-Lieb's inequality proven in [BL76] states that every smooth compactly supported function  $\omega$  satisfies the estimate

$$\int_{\mathbb{R}^d} |\omega - (\int_{\mathbb{R}^d} \omega d\nu)|^2 d\nu \leq \int_{\mathbb{R}^d} (\text{Hess } V)^{-1} (\nabla \omega, \nabla \omega) d\nu. \quad (2.1.1)$$

This inequality and suitable variants have since been e.g. used in works such as [HS94, Sjö96, NS97, Hel98, BJS00, BM03, BM04] studying correlation asymptotics in statistical mechanics. The latter works exploit in particular crucially some relations of the following type and which at least go back to the work of Helffer and Sjöstrand [HS94]:

$$\left\| \eta - \langle \eta, \frac{e^{-\frac{V}{2}}}{\|e^{-\frac{V}{2}}\|} \rangle \frac{e^{-\frac{V}{2}}}{\|e^{-\frac{V}{2}}\|} \right\|^2 = \langle (\Delta_{\frac{V}{2}}^{(1)})^{-1} (d_{\frac{V}{2}} \eta), d_{\frac{V}{2}} \eta \rangle, \quad (2.1.2)$$

where  $\eta \in \mathcal{C}_c^\infty(\mathbb{R}^d)$ ,  $\langle \cdot, \cdot \rangle$  and  $\| \cdot \|$  stand for the usual  $L^2(\mathbb{R}^d, d\mu)$  inner product and norm,  $d_{\frac{V}{2}} := d + d\frac{V}{2}$  and  $\Delta_{\frac{V}{2}}^{(1)}$  is the Witten Laplacian acting on 1-forms (or equivalently on vector fields) which is given by (cf. (1.1.1)–(1.1.4) in the introductory chapter)

$$\Delta_{\frac{V}{2}}^{(1)} := \Delta_{\frac{V}{2}}^{(0)} \otimes \text{Id} + \text{Hess } V = (-\Delta + |\nabla \frac{V}{2}|^2 - \Delta \frac{V}{2}) \otimes \text{Id} + \text{Hess } V. \quad (2.1.3)$$

In the last relation,

$$\Delta_{\frac{V}{2}}^{(0)} := -\Delta + |\nabla \frac{V}{2}|^2 - \Delta \frac{V}{2} = (-\text{div} + \nabla \frac{V}{2})(\nabla + \nabla \frac{V}{2}) = d_{\frac{V}{2}}^* d_{\frac{V}{2}} \quad (2.1.4)$$

denotes the Witten Laplacian acting on functions (or equivalently on 0-forms). We recall from the introductory chapter that the Witten Laplacian is more generally defined on the full algebra of differential forms, that it is nonnegative and essentially self-adjoint (when acting on smooth compactly supported forms) on the space

of  $L^2(\mathbb{R}^d, d\mu)$  differential forms, and that it is moreover supersymmetric, which essentially amounts, when restricting our attention to the interplay between  $\Delta_{\frac{V}{2}}^{(0)}$  and  $\Delta_{\frac{V}{2}}^{(1)}$ , to the intertwining relation

$$\forall \eta \in \mathcal{C}_c^\infty(\mathbb{R}^d), \quad d_{\frac{V}{2}} \Delta_{\frac{V}{2}}^{(0)} \eta = \Delta_{\frac{V}{2}}^{(1)} d_{\frac{V}{2}} \eta,$$

which enables to prove relations of the type (2.1.2) (when  $\Delta_{\frac{V}{2}}^{(1)}$  is invertible). The nonnegativity of  $\Delta_{\frac{V}{2}}^{(0)}$  together with the relations (2.1.2) and (2.1.3) then easily leads to (2.1.1) when  $V$  is strictly convex (at least formally) taking finally  $\omega := e^{\frac{V}{2}} \eta$ . To connect to some spectral properties of  $\Delta_{\frac{V}{2}}^{(0)}$ , the relation (2.1.2) together with the lower bound  $\Delta_{\frac{V}{2}}^{(1)} \geq c$  for some  $c > 0$  – which is in particular satisfied if  $\text{Hess } V \geq c$  – implies, according to formula (2.1.4), a spectral gap greater than or equal to  $c$  for  $\Delta_{\frac{V}{2}}^{(0)}$  (its kernel being  $\text{Span}\{e^{-\frac{V}{2}}\}$  as it can be seen from (2.1.4), or equivalently from (1.3.8)). In addition to the already mentioned [Sjö96, Hel98] making extra assumptions on  $V$ , we refer especially to the very complete [Joh00] for precise statements and proofs in relation with the above discussion. See also the above Section 1.3.1 in this connection.

More generally, in the case of a Riemannian manifold without boundary  $\Omega$ , it is also well known that an inequality of the type (2.1.1) holds if one replaces  $\text{Hess } V$  (and the condition  $\text{Hess } V > 0$  everywhere) by the following quadratic form, sometimes called the Bakry-Émery (-Ricci) tensor,

$$\text{Ric} + \text{Hess } V \quad (\text{and if we assume its strict positivity everywhere}),$$

$\text{Ric}$  denoting the Ricci tensor. We refer for example to [BGL14, Theorem 4.9.3] for a precise statement whose proof relies on the supersymmetry of the counterpart of the Witten Laplacian in the weighted space  $L^2(\Omega, e^{-V} d\text{Vol}_\Omega)$ , sometimes called the weighted Laplacian and more precisely defined when acting on functions by (see (1.3.2), (1.3.6), and (1.3.7) in Section 1.3.1)

$$L_V^{(0)} := e^{\frac{V}{2}} \left( -\Delta + |\nabla \frac{V}{2}|^2 - \Delta \frac{V}{2} \right) e^{-\frac{V}{2}} = -\Delta + \nabla V \cdot \nabla.$$

This operator, unitarily equivalent to  $\Delta_{\frac{V}{2}}^{(0)}$ , is an important model of the Bakry-Émery theory of diffusion processes and we refer especially in this direction to the pioneering work of Bakry and Émery [BE85] or to the book [BGL14] for an overview of the concerned literature. On its side, the Bakry-Émery tensor  $\text{Ric} + \text{Hess } V$  – named after [BE85] but first introduced by Lichnerowicz in [Lic70] – is the natural counterpart of the Ricci tensor  $\text{Ric}$  in the weighted Riemannian manifold  $(\Omega, e^{-V} d\text{Vol}_\Omega)$  and we refer for example to [Lic70, Lot03] for some of its geometric properties. Let us also mention e.g. [LV09] extending this notion to metric measure spaces.

In the work [Lep17], we derive from the supersymmetry of the Witten Laplacian Brascamp-Lieb's type inequalities for general differential forms on a Riemannian manifold with a boundary. In addition to the supersymmetry, our results essentially follow from suitable decompositions of the quadratic forms associated with

the self-adjoint Neumann and Dirichlet realizations of the Witten Laplacian (see Section 1.2.3 in the introductory chapter) stated in Theorem 2.4.1 below. When restricting to the interplay between 0- and 1-forms, they imply in particular the already mentioned results in the case of  $\mathbb{R}^d$  or of a compact manifold with empty boundary as well as some results recently obtained by Kolesnikov and Milman in [KM17] in the case of a compact manifold with a boundary (see indeed Corollaries 2.4.3 and 2.4.4, and the corresponding remarks).

## 2.2 Notions of Riemannian geometry

We now introduce the concepts of Riemannian geometry which will be needed to state properly our further hypotheses and results. This part is rather long since we made the choice to define these classical notions quite precisely in order to stay comprehensible for readers not familiar with Riemannian geometry. The following objects are essentially defined according to the PDE framework developed in [Sch95] and we refer especially to Sections 1.1 and 1.2 there for further details and references, the notation adopted being nevertheless slightly different.

We work with a smooth  $d$ -dimensional oriented connected and compact Riemannian manifold  $(\Omega, g = \langle \cdot, \cdot \rangle)$  with boundary  $\partial\Omega$  and we recall the notation introduced in Section 1.1:

The cotangent (resp. tangent) bundle of  $\Omega$  is denoted by  $T^*\Omega$  (resp.  $T\Omega$ ) and the exterior fiber bundle by  $\Lambda T^*\Omega = \bigoplus_{p=0}^n \Lambda^p T^*\Omega$ . The fiber bundles  $T^*\partial\Omega$ ,  $T\partial\Omega$ , and  $\Lambda T^*\partial\Omega = \bigoplus_{p=0}^{n-1} \Lambda^p T^*\partial\Omega$  are defined similarly. The (bundle) scalar product on  $\Lambda^p T^*\Omega$  inherited from  $g$  is denoted by  $\langle \cdot, \cdot \rangle_{\Lambda^p}$ . Let us recall that  $\langle \cdot, \cdot \rangle_{\Lambda^1}$  is defined by

$$\langle \omega, \eta \rangle_{\Lambda^1} := \langle \omega^\sharp, \eta^\sharp \rangle,$$

where, for any  $\xi \in T^*\Omega$ ,  $\xi^\sharp$  is the element of  $T\Omega$  satisfying, for any  $X \in T\Omega$ ,

$$\langle \xi^\sharp, X \rangle := \xi(X). \quad (2.2.1)$$

The map  $\xi \mapsto \xi^\sharp$  is an isomorphism from  $T^*\Omega$  into  $T\Omega$  and we denote by  $T\Omega \ni X \mapsto X^\flat \in T^*\Omega$  its inverse isomorphism. The inner product  $\langle \cdot, \cdot \rangle_{\Lambda^p}$  is then defined as the bilinear form satisfying the following relation on decomposable  $p$ -forms:

$$\langle \omega_1 \wedge \cdots \wedge \omega_p, \eta_1 \wedge \cdots \wedge \eta_p \rangle_{\Lambda^p} := \det \left( \langle \omega_i, \eta_j \rangle_{\Lambda^1} \right)_{1 \leq i, j \leq p}.$$

The space of  $\mathcal{C}^\infty$ ,  $L^2$ , etc. sections of any of the above fiber bundles  $E$ , over  $O = \Omega$  or  $O = \partial\Omega$ , are respectively denoted by  $\mathcal{C}^\infty(O, E)$ ,  $L^2(O, E)$ , etc.. The more compact notation  $\Lambda^p \mathcal{C}^\infty(\Omega)$ ,  $\Lambda^p L^2(\Omega)$ , etc. will also be used instead of  $\mathcal{C}^\infty(\Omega, \Lambda^p T^*\Omega)$ ,  $L^2(\Omega, \Lambda^p T^*\Omega)$ , etc. and we will denote by  $\mathcal{L}(\Lambda^p T^*\Omega)$  the space of smooth bundle endomorphisms of  $\Lambda^p T^*\Omega$ . The  $L^2$  spaces are those associated with the respective unit volume forms  $\mu$  and  $\mu_{\partial\Omega}$  for the Riemannian structures on  $\Omega$  and on  $\partial\Omega$ .

The notion of *local orthonormal frame* (on  $\Omega$  or  $\partial\Omega$ ) will be frequently used in this chapter. By local orthonormal frame on (say)  $\Omega$ , we mean a family  $(E_1, \dots, E_n)$  of smooth sections of  $T\Omega$  defined on an open set  $U \subset \Omega$  such that

$$\forall i, j \in \{1, \dots, n\}, \forall x \in U, \quad \langle E_i, E_j \rangle_x = \delta_{i,j}.$$

According for example to [Sch95, Definition 1.1.6] and to the related remarks, it is always possible to cover  $\Omega$  with a finite family (since  $\Omega$  is compact) of opens sets  $U$ 's such that there exists a local orthonormal frame  $(E_1, \dots, E_n)$  on each  $U$ . Such a covering is called a nice cover of  $\Omega$ .

The outgoing normal vector field will be denoted by  $\vec{n}$  and the orientation is chosen such that

$$\mu_{\partial\Omega} = \mathbf{i}_{\vec{n}} \mu,$$

where  $\mathbf{i}$  denotes the interior product. Owing to the Collar Theorem stated in [Sch95, Theorem 1.1.7], the vector field  $\vec{n} \in \mathcal{C}^\infty(\partial\Omega, T\Omega|_{\partial\Omega})$  can be extended to a smooth vector field on a neighborhood of the boundary  $\partial\Omega$ . Moreover, taking maybe a finite refinement of a nice cover of  $\Omega$  as defined previously, one can always assume that the local orthonormal frame  $(E_1, \dots, E_n)$  corresponding to any of its elements  $U$  meeting  $\partial\Omega$  is such that  $E_n|_{\partial\Omega} = \vec{n}$ . In particular, the vector fields  $E_1, \dots, E_{n-1}$  are such that

$$\forall j \in \{1, \dots, n-1\}, \quad E_j|_{\partial\Omega} \in (T\Omega|_{\partial\Omega})^T = T\partial\Omega.$$

Here, with a slight abuse of notation, we have made the identification between the space of tangential vector fields

$$(T\Omega|_{\partial\Omega})^T := \{X \in T\Omega|_{\partial\Omega} \text{ such that } \langle X, \vec{n} \rangle = 0\}$$

and the tangent bundle of  $\partial\Omega$  (see [Sch95, pp. 15–16] for more details).

We denote by  $d : \mathcal{D}'(\Omega) \rightarrow \mathcal{D}'(\Omega)$  the exterior differential, where we recall that  $\mathcal{D}'(\Omega) = \bigoplus_{p=0}^d \mathcal{D}'^{(p)}(\Omega)$  is the space of currents on  $\Omega$ , and by  $d^*$  its formal adjoint with respect to the  $L^2$  scalar product inherited from the Riemannian structure (see Section 1.1). We recall that they satisfy the relation  $d^2 = (d^*)^2 = 0$  and that the Hodge Laplacian  $\Delta_{\mathbb{H}} : \mathcal{D}'(\Omega) \rightarrow \mathcal{D}'(\Omega)$  is then defined by

$$\Delta_{\mathbb{H}} := d^*d + dd^* = (d + d^*)^2.$$

For a (real) smooth function  $f$  and a smooth vector field  $X$ , we will use the notation

$$\nabla_X f := X \cdot f = df(X),$$

the normal derivative of  $f$  along the boundary being in particular defined by

$$\partial_n f := \langle \nabla f, \vec{n} \rangle = \nabla_{\vec{n}} f.$$

We will also denote by  $\nabla : \mathcal{C}^\infty(\Omega, T\Omega) \times \mathcal{C}^\infty(\Omega, T\Omega) \rightarrow \mathcal{C}^\infty(\Omega, T\Omega)$  the Levi-Civita connection on  $\Omega$  and by  $\nabla_X(\cdot)$  the covariant derivative (in the direction of  $X$ ) of vector fields as well as the induced covariant derivative on  $\Lambda^p T^* \Omega$ .

The second covariant derivative (acting for example on  $T\Omega$  and on  $\Lambda^p T^* \Omega$ ) is then the bilinear mapping on  $T\Omega$  defined, for  $X, Y \in \mathcal{C}^\infty(\Omega, T\Omega)$  by

$$\nabla_{X,Y}^2 := \nabla_X \nabla_Y - \nabla_{\nabla_X Y}.$$

When  $f$  is a smooth function,  $\nabla_{X,Y}^2 f$  is simply the Hessian of  $f$ . It is in this case a symmetric bilinear form and has the simpler writing

$$\text{Hess } f(X, Y) := \nabla_{X,Y}^2 f = (\nabla_X df)(Y) = \langle \nabla_X \nabla f, Y \rangle. \quad (2.2.2)$$

The Bochner Laplacian  $\Delta_B : \mathcal{D}'(\Omega) \rightarrow \mathcal{D}'(\Omega)$  is defined as minus the trace of the bilinear mapping  $(X, Y) \mapsto \nabla_{X,Y}^2$ . More precisely, we have for any  $\omega \in \mathcal{D}'(\Omega)$ :

$$\Delta_B \omega := -\text{Tr} \left( (X, Y) \mapsto \nabla_{X,Y}^2 \omega \right), \quad (2.2.3)$$

which implies that for any local orthonormal frame  $(E_1, \dots, E_n)$  on  $U \subset \Omega$ ,  $\Delta_B$  is given on  $U$  by

$$\Delta_B = -\sum_{i=1}^n (\nabla_{E_i} \nabla_{E_i} - \nabla_{\nabla_{E_i} E_i}). \quad (2.2.4)$$

The Hodge and Bochner Laplacians  $\Delta_H^{(p)}$  and  $\Delta_B^{(p)}$  (the superscript  $(p)$  means that we are considering their action on differential  $p$ -forms) are related by the Weitzenböck formula: there exists a smooth bundle symmetric endomorphism  $\text{Ric}^{(p)} \in \mathcal{L}(\Lambda^p T^* \Omega)$  such that (see [Sch95, p. 26] where the opposite convention of sign is adopted)

$$\Delta_B^{(p)} = \Delta_H^{(p)} - \text{Ric}^{(p)}. \quad (2.2.5)$$

This operator vanishes on 0-forms (i.e. on functions) and  $\text{Ric}^{(1)}$  is the element of  $\mathcal{L}(\Lambda^1 T^* \Omega)$  canonically identified with the Ricci tensor  $\text{Ric}$  (see below for the precise definition of this identification). We recall that  $\text{Ric}$  is the symmetric  $(0, 2)$ -tensor defined, for  $X, Y \in T\Omega$ , by

$$\text{Ric}(X, Y) := \text{Tr} \left( Z \mapsto R(Z, X)Y \right), \quad (2.2.6)$$

where  $R$  denotes the Riemannian curvature tensor which is defined, for every  $X, Y, Z$  in  $T\Omega$ , by

$$R(X, Y)Z := (\nabla_{X,Y}^2 - \nabla_{Y,X}^2)Z = \nabla_X \nabla_Y Z - \nabla_Y \nabla_X Z - \nabla_{[X,Y]}Z. \quad (2.2.7)$$

The tensor  $\text{Ric}$  hence satisfies on any open set  $U \subset \Omega$  where is given a local orthonormal frame  $(E_1, \dots, E_n)$ :

$$\text{Ric}(X, Y) = \sum_{i=1}^n \langle R(E_i, X)Y, E_i \rangle = -\sum_{i=1}^n \langle R(E_i, X)E_i, Y \rangle, \quad (2.2.8)$$

the last line following from the relation  $\langle R(X, Y)Z, T \rangle = -\langle R(X, Y)T, Z \rangle$  for any  $X, Y, Z, T \in T\Omega$ . It is then canonically identified with a symmetric bilinear form acting on  $T^* \Omega$  (i.e. a symmetric  $(2, 0)$ -tensor), still denoted by  $\text{Ric}$  and defined by (see (2.2.1) for the meaning of  $T^* \Omega \ni \omega \mapsto \omega^\sharp \in T\Omega$ )

$$\text{Ric}(\omega, \eta) := \text{Ric}(\omega^\sharp, \eta^\sharp).$$

The latter symmetric bilinear form is then itself identified via  $\langle \cdot, \cdot \rangle_{\Lambda^1}$  with the element of  $\mathcal{L}(\Lambda^1 T^* \Omega)$  denoted by  $\text{Ric}^{(1)}$ . More precisely, we have for any  $\omega$  and  $\eta$  in  $T^* \Omega$ :

$$\langle \text{Ric}^{(1)} \omega, \eta \rangle_{\Lambda^1} := \text{Ric}(\omega, \eta).$$

**Remark 2.2.1.** Denoting also by  $\text{Ric}$  the bundle symmetric endomorphism of  $T\Omega$  defined by  $\langle \text{Ric}X, Y \rangle := \text{Ric}(X, Y)$  (i.e. by  $\text{Ric}X := -\sum_{i=1}^n R(E_i, X)E_i$  according to (2.2.8)), we have for any  $\omega, \eta$  in  $T^* \Omega$  and  $X$  in  $T\Omega$ ,

$$\begin{aligned} \text{Ric}^{(1)} \omega(X) &= \langle \text{Ric}^{(1)} \omega, X^\flat \rangle_{\Lambda^1} = \text{Ric}(\omega, X^\flat) \\ &= \text{Ric}(\omega^\sharp, X) \\ &= \langle \omega^\sharp, \text{Ric}X \rangle = \omega(\text{Ric}X). \end{aligned} \quad (2.2.9)$$



More generally, for any local orthonormal frame  $(E_1, \dots, E_n)$  on  $U \subset \Omega$ ,  $\text{Ric}^{(p)}$  is defined on  $U$  for any  $p \in \{1, \dots, n\}$  by

$$\begin{aligned} & (\text{Ric}^{(p)}\omega)(X_1, \dots, X_p) \\ & := - \sum_{i=1}^n \sum_{j=1}^k \left( (R(E_i, X_j))^{(p)}\omega \right)(X_1, \dots, X_{j-1}, E_i, X_{j+1}, \dots, X_k), \end{aligned} \quad (2.2.10)$$

where  $(R(E_i, X_j))^{(1)} \in \mathcal{L}(\Lambda^1 T^* \Omega)$  is canonically identified with  $R(E_i, X_j)$  via

$$\left( (R(E_i, X_j))^{(1)}\omega \right)(X) = \omega(R(E_i, X_j)X)$$

and

$$(R(E_i, X_j))^{(p)} = \left( (R(E_i, X_j))^{(1)} \right)^{(p)},$$

where for any  $A \in \mathcal{L}(\Lambda^1 T^* \Omega)$ ,  $(A)^{(p)}$  is the element of  $\mathcal{L}(\Lambda^p T^* \Omega)$  satisfying the following relation on decomposable  $p$ -forms:

$$(A)^{(p)}(\omega_1 \wedge \dots \wedge \omega_p) = \sum_{i=1}^p \omega_1 \wedge \dots \wedge A\omega_i \wedge \dots \wedge \omega_p. \quad (2.2.11)$$

We end up this part by recalling the definition of the second fundamental form of  $\partial\Omega \subset \Omega$  and of related concepts. The second fundamental form  $\mathcal{K}_2$  of  $\partial\Omega \subset \Omega$  is the bilinear mapping defined by

$$\mathcal{K}_2 : \begin{array}{ccc} T\partial\Omega \times T\partial\Omega & \longrightarrow & T\Omega|_{\partial\Omega} \\ (U, V) & \longmapsto & (\nabla_U V)^\perp := \langle \nabla_U V, \vec{n} \rangle \vec{n} \end{array} \quad (2.2.12)$$

It is symmetric and the value of  $\mathcal{K}_2(U, V)|_\sigma$  at  $\sigma \in \partial\Omega$  only depends on the values of the tangential fields  $U_\sigma$  and  $V_\sigma$  at that point. The shape operator of  $\partial\Omega \subset \Omega$  is the bundle endomorphism  $\mathcal{K}_1 \in \mathcal{L}(T\partial\Omega)$  defined by

$$\forall U \in T\partial\Omega, \quad \mathcal{K}_1(U) := -\nabla_U \vec{n}. \quad (2.2.13)$$

It is then completely determined by  $\mathcal{K}_2$  since it satisfies

$$\forall (U, V) \in T\partial\Omega \times T\partial\Omega, \quad \langle \mathcal{K}_1(U), V \rangle \vec{n} = \mathcal{K}_2(U, V).$$

The mean curvature of  $\partial\Omega \subset \Omega$  is defined as the trace of the bilinear mapping  $(U, V) \mapsto \langle \mathcal{K}_2(U, V), \vec{n} \rangle$  or equivalently as the trace of the shape operator  $\mathcal{K}_1$ . We recall lastly that with our choice of orientation for  $\vec{n}$ ,  $\Omega$  is locally convex iff  $\langle \mathcal{K}_2(\cdot, \cdot), \vec{n} \rangle$  is nonpositive.

## 2.3 Witten and weighted Laplacians

We recall from Section 1.1 that for a (real) smooth function  $f$ , the distorted differential operators  $d_f : \mathcal{D}'(\Omega) \rightarrow \mathcal{D}'(\Omega)$  and  $d_f^* : \mathcal{D}'(\Omega) \rightarrow \mathcal{D}'(\Omega)$  are defined by

$$d_f := e^{-f} d e^f \quad \text{and} \quad d_f^* := e^f d^* e^{-f},$$

and that the Witten Laplacian  $\Delta_f : \mathcal{D}'(\Omega) \rightarrow \mathcal{D}'(\Omega)$  is then defined by

$$\Delta_f := d_f^* d_f + d_f d_f^* = (d_f + d_f^*)^2.$$

According moreover to Section 1.2.3, the Dirichlet and Neumann realizations  $\Delta_f^{\mathbf{t}}$  and  $\Delta_f^{\mathbf{n}}$  of the Witten Laplacian, whose domains are respectively defined by

$$D(\Delta_f^{\mathbf{t}}) = \{\omega \in \Lambda H^2(\Omega), \mathbf{t}\omega = 0 \text{ and } \mathbf{t}d_f^*\omega = 0 \text{ on } \partial\Omega\} \quad (2.3.1)$$

and

$$D(\Delta_f^{\mathbf{n}}) = \{\omega \in \Lambda H^2(\Omega), \mathbf{n}\omega = 0 \text{ and } \mathbf{n}d_f\omega = 0 \text{ on } \partial\Omega\}, \quad (2.3.2)$$

are self-adjoint and nonnegative on (the flat space)  $\Lambda L^2(\Omega)$ . Here, for  $\omega \in \Lambda H^1(\Omega)$ ,

$$\mathbf{t}\omega = \mathbf{i}_{\vec{n}}(\vec{n}^\flat \wedge \omega) \in H^{\frac{1}{2}}(\partial\Omega, \Lambda T^*\Omega|_{\partial\Omega}) \text{ and } \mathbf{n}\omega = \vec{n}^\flat \wedge (\mathbf{i}_{\vec{n}}\omega) \in H^{\frac{1}{2}}(\partial\Omega, \Lambda T^*\Omega|_{\partial\Omega})$$

denote respectively the tangential and normal components of the differential form  $\omega$  (see Section 1.2.3 for more details).

Furthermore, for  $\mathbf{b} \in \{\mathbf{t}, \mathbf{n}\}$ , the quadratic form associated with  $\Delta_f^{\mathbf{b}}$ , that we will denote by  $\mathcal{D}_f^{\mathbf{b}}$ , has for domain

$$\Lambda H_{\mathbf{b}}^1(\Omega) := \{\omega \in \Lambda^p H^1(\Omega), \mathbf{b}\omega = 0 \text{ on } \partial\Omega\} \quad (2.3.3)$$

and we have, for every  $\omega \in \Lambda^p H_{\mathbf{b}}^1(\Omega)$  (again, see Section 1.2.3 for more details),

$$\mathcal{D}_f^{\mathbf{b},(p)}(\omega) := \mathcal{D}_f^{\mathbf{b},(p)}(\omega, \omega) = \langle d_f\omega, d_f\omega \rangle_{\Lambda^{p+1}L^2} + \langle d_f^*\omega, d_f^*\omega \rangle_{\Lambda^{p-1}L^2}. \quad (2.3.4)$$

Let us also recall from Section 1.3.1 that the Witten Laplacian  $\Delta_f$  is unitarily equivalent to the weighted (or Bakry-Émery) Laplacian

$$L_V := \Delta_{\mathbf{H}} + \mathcal{L}_{\nabla V}, \text{ where } V := 2f,$$

acting on the weighted space  $\Lambda L^2(\Omega, e^{-V}d\mu)$  according to the relation (1.3.7) that we recall here:

$$L_V = e^f \Delta_f e^{-f} \text{ where } V := 2f. \quad (2.3.5)$$

We denote moreover by  $L_V^{\mathbf{t}}$  and  $L_V^{\mathbf{n}}$  the nonnegative self-adjoint unbounded operators on  $\Lambda L^2(\Omega, e^{-V}d\mu)$  associated with  $\Delta_f^{\mathbf{t}}$  and  $\Delta_f^{\mathbf{n}}$  via (2.3.5). For  $\mathbf{b} \in \{\mathbf{n}, \mathbf{t}\}$ , the domain of  $L_V^{\mathbf{b}}$  is easily deduced from the one of  $\Delta_f^{\mathbf{b}}$  thanks to the relation (2.3.5). Note moreover that according to (2.3.3) and (2.3.5), the domain of the quadratic form associated with  $L_V^{\mathbf{b}}$  is simply the weighted Sobolev space

$$\Lambda H_{\mathbf{b}}^1(\Omega, e^{-V}d\mu) := \{\omega \in \Lambda H^1(\Omega, e^{-V}d\mu), \mathbf{b}\omega = 0 \text{ on } \partial\Omega\}, \quad (2.3.6)$$

which is actually nothing but  $\Lambda^p H_{\mathbf{b}}^1(\Omega)$  (algebraically and topologically) since  $\Omega$  is compact.

Coming back to the Witten Laplacian, we have the following formula (see (1.1.4)):

$$\forall p \in \{0, \dots, d\}, \quad \Delta_f^{(p)} = \Delta_{\mathbf{H}}^{(p)} + |\nabla f|^2 + 2 \text{Hess}^{(p)}f + \Delta_{\mathbf{H}}f. \quad (2.3.7)$$

This relation is not very common in the literature dealing with semiclassical Witten Laplacians – i.e. where one studies  $h^2\Delta_{\frac{f}{h}}$  at the limit  $h \rightarrow 0^+$  – which motivated the work [Lep17], at least when  $\Omega$  is not flat. We refer for example to [Jam12] or to [Lep17] for a proof. Let us incidentally specify the sense of (2.3.7). There,  $\text{Hess}^{(0)}f = 0$  and  $\text{Hess}^{(1)}f$  is the element of  $\mathcal{L}(\Lambda^1 T^*\Omega)$  canonically identified with  $\text{Hess} f$  (see the lines below (2.2.8) for more details). More precisely, we have for any  $\omega$  and  $\eta$  in  $T^*\Omega$ ,

$$\langle \text{Hess}^{(1)}f \omega, \eta \rangle_{\Lambda^1} = \text{Hess} f(\omega, \eta) = \text{Hess} f(\omega^\sharp, \eta^\sharp),$$

and  $\text{Hess}^{(p)}f$  is the bundle symmetric endomorphism of  $\Lambda^p T^*\Omega$  defined by

$$\text{Hess}^{(p)}f := (\text{Hess}^{(1)}f)^{(p)} \quad (\text{see (2.2.11) for the meaning of } (A)^{(p)}). \quad (2.3.8)$$

## 2.4 Results in the case with boundary

### 2.4.1 An integration by parts formula

We consider here  $f$  a smooth (real) function,  $V := 2f$ , and the probability measure  $\nu$  associated with  $V$  defined by

$$d\nu := \frac{e^{-V}}{\int_{\Omega} e^{-V} d\mu} d\mu = \frac{e^{-2f}}{\|e^{-f}\|_{L^2}^2} d\mu.$$

We denote, for any  $p \in \{0, \dots, d\}$ , by  $\Lambda^p L^2(\Omega, d\nu)$ ,  $\Lambda^p H^1(\Omega, d\nu)$ ,  $\langle \cdot, \cdot \rangle_{\Lambda^p L^2(d\nu)}$  and  $\|\cdot\|_{\Lambda^p L^2(d\nu)}$  the associated Lebesgue and Sobolev spaces,  $L^2$  scalar product and  $L^2$  norm. For  $\mathbf{b} \in \{\mathbf{n}, \mathbf{t}\}$ , we also denote by  $\Lambda^p H_{\mathbf{b}}^1(\Omega, d\nu)$  the subspace of  $\Lambda^p H^1(\Omega, d\nu)$  made of the differential forms  $\omega$  such that  $\mathbf{b}\omega = 0$  on  $\partial\Omega$ . Note in particular that, for  $\mathbf{b} \in \{\mathbf{n}, \mathbf{t}\}$ ,  $\Lambda^p H_{\mathbf{b}}^1(\Omega, d\nu)$  is simply the space  $\Lambda^p H_{\mathbf{b}}^1(\Omega, e^{-V} d\mu)$  defined in (2.3.6).

In addition to the material of Riemannian geometry already recalled in Section 2.2, the following statements involve a smooth bundle endomorphism  $\mathcal{K}_{\mathbf{b}}^{(p)} \in \mathcal{L}(\Lambda^p T^*\Omega|_{\partial\Omega})$ , where  $\mathbf{b} \in \{\mathbf{n}, \mathbf{t}\}$ , determined by the second fundamental form  $\mathcal{K}_2$  of  $\partial\Omega \subset \Omega$  defined in (2.2.12):

1. For any  $p \in \{0, \dots, d\}$ ,  $\mathcal{K}_{\mathbf{n}}^{(p)} \in \mathcal{L}(\Lambda^p T^*\Omega|_{\partial\Omega})$  vanishes on 0-forms and:
  - i) for any  $\omega \in \Lambda^1 T^*\Omega$ ,  $\mathcal{K}_{\mathbf{n}}^{(1)}\omega$  is tangential and

$$(\mathcal{K}_{\mathbf{n}}^{(1)}\omega)(X^T + x^\perp \vec{n}) = -\omega(\mathcal{K}_1(X^T)) = \omega(\nabla_{X^T} \vec{n}), \quad (2.4.1)$$

where  $\mathcal{K}_1$  is the shape operator defined in (2.2.13),

- ii) for any  $p \in \{1, \dots, n\}$  and  $\omega \in \Lambda^p T^*\Omega$ ,  $\mathcal{K}_{\mathbf{n}}^{(p)}\omega$  is tangential and for any  $X_1^T, \dots, X_p^T \in T\partial\Omega$ ,

$$(\mathcal{K}_{\mathbf{n}}^{(p)}\omega)(X_1^T, \dots, X_p^T) = ((\mathcal{K}_{\mathbf{n}}^{(1)})^{(p)}\omega)(X_1^T, \dots, X_p^T), \quad (2.4.2)$$

where the notation  $(A)^{(p)}$  has been defined in (2.2.11).

2. For any  $p \in \{0, \dots, d\}$ ,  $\mathcal{K}_{\mathbf{t}}^{(p)} \in \mathcal{L}(\Lambda^p T^*\Omega|_{\partial\Omega})$  vanishes on 0-forms and:
  - i) for any  $\omega \in \Lambda^1 T^*\Omega$ ,  $\mathcal{K}_{\mathbf{t}}^{(1)}\omega$  is normal and

$$(\mathcal{K}_{\mathbf{t}}^{(1)}\omega)(X^T + x^\perp \vec{n}) = -x^\perp \text{Tr}(\mathcal{K}_1)\omega(\vec{n}), \quad (2.4.3)$$

- ii) for any  $p \in \{1, \dots, n\}$  and  $\omega \in \Lambda^p T^* \Omega$ ,  $\mathcal{K}_{\mathbf{t}}^{(p)} \omega$  is normal and for any local orthonormal frame  $(E_1, \dots, E_n)$  on  $U \subset \Omega$  such that  $E_n|_{\partial\Omega} = \vec{n}$  (with  $U \cap \partial\Omega \neq \emptyset$ ) and  $X_1^T, \dots, X_p^T \in T\partial\Omega$ , we have on  $U \cap \partial\Omega$ :

$$\begin{aligned} & (\mathcal{K}_{\mathbf{t}}^{(p)} \omega)(\vec{n}, X_1^T, \dots, X_{p-1}^T) \\ & := - \sum_{i=1}^{n-1} \left( (\mathcal{K}_2(E_i, \cdot))^{(p)} \omega \right) (E_i, X_1^T, \dots, X_{p-1}^T), \end{aligned} \quad (2.4.4)$$

where  $(\mathcal{K}_2(E_i, \cdot))^{(p)} = \left( (\mathcal{K}_2(E_i, \cdot))^{(1)} \right)^{(p)}$  and

$$\left( (\mathcal{K}_2(E_i, \cdot))^{(1)} \omega \right) (X) = \omega(\mathcal{K}_2(E_i, X)).$$

Note that the point 2.ii) is nothing but the statement of 2.i) when  $p = 1$ .

The different Brascamp-Lieb's type inequalities stated in [Lep17] arise from the following integration by parts formulas relating the quadratic forms  $\mathcal{D}_f^{\mathbf{t},(p)}$  and  $\mathcal{D}_f^{\mathbf{n},(p)}$  (see (2.3.4)) with the geometry of  $\Omega$ .

**Theorem 2.4.1.** *Let  $\omega \in \Lambda^p H_{\mathbf{b}}^1$  with  $\mathbf{b} \in \{\mathbf{n}, \mathbf{t}\}$  and  $p \in \{0, \dots, d\}$ . It holds*

$$\begin{aligned} \mathcal{D}_f^{\mathbf{b},(p)}(\omega) &= \|e^f \omega\|_{\dot{H}^1(e^{-2f} d\mu)}^2 + \langle (\text{Ric}^{(p)} + 2 \text{Hess}^{(p)} f) \omega, \omega \rangle_{L^2} \\ &+ \int_{\partial\Omega} \langle \mathcal{K}_{\mathbf{b}}^{(p)} \omega, \omega \rangle_{\Lambda^p} d\mu_{\partial\Omega} - 2 \mathbf{1}_{\mathbf{t}}(\mathbf{b}) \int_{\partial\Omega} \langle \omega, \omega \rangle_{\Lambda^p} \partial_n f d\mu_{\partial\Omega}, \end{aligned} \quad (2.4.5)$$

where  $\text{Ric}^{(p)}$ ,  $\text{Hess}^{(p)} f$ , and  $\mathcal{K}_{\mathbf{b}}^{(p)}$  have been respectively defined in (2.2.10), (2.3.8), and (2.4.1)–(2.4.4),  $\mathbf{1}_{\mathbf{t}}(\mathbf{b}) = 1$  if  $\mathbf{b} = \mathbf{t}$  and 0 if not, and

$$\| \cdot \|_{\dot{H}^1(e^{-2f} d\mu)}^2 := \| \cdot \|_{H^1(e^{-2f} d\mu)}^2 - \| \cdot \|_{L^2(e^{-2f} d\mu)}^2.$$

When  $f = 0$ , we recover Theorems 2.1.5 and 2.1.7 of [Sch95] which were generalizing results in the boundaryless case due to Bochner for  $p = 1$  and to Gallot and Meyer for general  $p$ 's (see [Boc48, GM75]). These results allow in particular to draw topological conclusions on the cohomology of  $\Omega$  from its geometry. When the boundary  $\partial\Omega$  is not empty, the relative and absolute cohomologies of  $\Omega$  (corresponding respectively to the Dirichlet and Neumann boundary conditions) have to be considered (see [Sch95, Section 2.6]). To be more precise, note from Theorem 2.4.1 that for any  $p \in \{0, \dots, d\}$ , the (everywhere) positivity of the quadratic form  $\text{Ric}^{(p)} + 2 \text{Hess}^{(p)} f$  together with the nonnegativity of  $\mathcal{K}_{\mathbf{n}}^{(p)}$  (resp. of  $\mathcal{K}_{\mathbf{t}}^{(p)} - 2 \partial_n f$ ) implies the lower bounds (in the sense of quadratic forms)

$$\Delta_f^{\mathbf{b},(p)} \geq \text{Ric}^{(p)} + 2 \text{Hess}^{(p)} f > 0 \quad (\mathbf{b} \in \{\mathbf{t}, \mathbf{n}\})$$

for the Witten Laplacian and hence the triviality of its kernel which is isomorphic to the  $p$ -th absolute (resp. relative) cohomology group of  $\Omega$  (see indeed Section 1.2.3 in this connection).

### 2.4.2 Consequences: Brascamp-Lieb's type inequalities

Playing with the supersymmetry, we easily get from Theorem 2.4.1 the following Brascamp-Lieb's type inequalities for differential forms, where for any  $\mathbf{b} \in \{\mathbf{n}, \mathbf{t}\}$  and  $p \in \{0, \dots, d\}$ ,  $\pi_{\mathbf{b}} = \pi_{\mathbf{b}}^{(p)}$  denotes the orthogonal projection on  $\text{Ker}(L_V^{\mathbf{b},(p)})$ .

**Theorem 2.4.2** (Brascamp-Lieb's inequalities for differential forms).

1. Let  $p \in \{0, \dots, d\}$  and let us assume that  $\mathcal{K}_{\mathbf{n}}^{(p)} \geq 0$  everywhere on  $\partial\Omega$  and that  $\text{Ric}_V^{(p)} := \text{Ric}^{(p)} + \text{Hess}^{(p)}V > 0$  everywhere on  $\Omega$  (in the sense of quadratic forms). It then holds:

i) if  $p > 0$ , we have for every  $\omega \in \Lambda^{p-1}H_{\mathbf{n}}^1(\Omega, d\nu)$  such that  $d_V^*\omega = 0$ :

$$\|\omega - \pi_{\mathbf{n}}\omega\|_{L^2(d\nu)}^2 \leq \int_{\Omega} \langle (\text{Ric}_V^{(p)})^{-1}d\omega, d\omega \rangle_{\Lambda^p} d\nu,$$

ii) if  $p < n$ , we have for every  $\omega \in \Lambda^{p+1}H_{\mathbf{n}}^1(\Omega, d\nu)$  such that  $d\omega = 0$ :

$$\|\omega - \pi_{\mathbf{n}}\omega\|_{L^2(d\nu)}^2 \leq \int_{\Omega} \langle (\text{Ric}_V^{(p)})^{-1}d_V^*\omega, d_V^*\omega \rangle_{\Lambda^p} d\nu.$$

2. Assume similarly that  $\mathcal{K}_{\mathbf{t}}^{(p)} - \partial_n V \geq 0$  everywhere on  $\partial\Omega$  and that  $\text{Ric}_V^{(p)} > 0$  everywhere on  $\Omega$ . It then holds:

i) if  $p > 0$ , we have for every  $\omega \in \Lambda^{p-1}H_{\mathbf{t}}^1(\Omega, d\nu)$  such that  $d_V^*\omega = 0$ :

$$\|\omega - \pi_{\mathbf{t}}\omega\|_{L^2(d\nu)}^2 \leq \int_{\Omega} \langle (\text{Ric}_V^{(p)})^{-1}d\omega, d\omega \rangle_{\Lambda^p} d\nu,$$

ii) if  $p < n$ , we have for every  $\omega \in \Lambda^{p+1}H_{\mathbf{t}}^1(\Omega, d\nu)$  such that  $d\omega = 0$ :

$$\|\omega - \pi_{\mathbf{t}}\omega\|_{L^2(d\nu)}^2 \leq \int_{\Omega} \langle (\text{Ric}_V^{(p)})^{-1}d_V^*\omega, d_V^*\omega \rangle_{\Lambda^p} d\nu.$$

In the case  $p = 1$ , the points 1.i) and 2.i) of Theorem 2.4.2 take a simpler form. Every  $\omega \in \Lambda^0 H^1(\Omega, d\nu)$  satisfies indeed  $d_V^*\omega = 0$ . Moreover, we have simply

$$\Lambda^0 H_{\mathbf{n}}^1(\Omega, d\nu) = H^1(\Omega, d\nu) \quad \text{and} \quad \text{Ker}(L_V^{\mathbf{n},(0)}) = \text{Span}\{1\}$$

as well as (when  $\partial\Omega$  is not empty)

$$\Lambda^0 H_{\mathbf{t}}^1(\Omega, d\nu) = H_0^1(\Omega, d\nu) \quad \text{and} \quad \text{Ker}(L_V^{\mathbf{t},(0)}) = \{0\}.$$

Defining the mean of  $u \in L^2(\Omega, d\nu)$  by  $\langle u \rangle_{\nu} := \langle u, 1 \rangle_{L^2(d\nu)}$ , we then immediately get from Theorem 2.4.2 (together with (2.4.1) and (2.4.3)) the following (where  $\mathcal{K}_1$  denotes the shape operator defined in (2.2.13)):

**Corollary 2.4.3.** i) Assume that the shape operator  $\mathcal{K}_1$  is nonpositive everywhere on  $\partial\Omega$  and that  $\text{Ric} + \text{Hess}V > 0$  everywhere on  $\Omega$ . It then holds: for every  $\omega \in H^1(\Omega, d\nu)$ ,

$$\|\omega - \langle \omega \rangle_{\nu}\|_{L^2(d\nu)}^2 \leq \int_{\Omega} (\text{Ric} + \text{Hess}V)^{-1}(\nabla\omega, \nabla\omega) d\nu. \quad (2.4.6)$$

ii) Assume similarly that  $-\text{Tr}(\mathcal{K}_1) - \partial_n V \geq 0$  everywhere on  $\partial\Omega$  and that  $\text{Ric} + \text{Hess} V > 0$  everywhere on  $\Omega$ . It then holds: for every  $\omega \in H_0^1(\Omega, d\nu)$ ,

$$\|\omega\|_{L^2(d\nu)}^2 \leq \int_{\Omega} (\text{Ric} + \text{Hess} V)^{-1}(\nabla\omega, \nabla\omega) d\nu. \quad (2.4.7)$$

When  $\Omega \setminus \partial\Omega$  appears to be a smooth open subset of  $\mathbb{R}^d$ ,  $\text{Ric}$  and  $\text{Ric}^{(p)}$  vanish and the latter corollary as well as Theorem 2.4.2 then write in a simpler way just relying on a control from below of  $\text{Hess} V$  or  $\text{Hess}^{(p)}V$  instead of  $\text{Ric}_V^{(p)} = \text{Ric}^{(p)} + \text{Hess}^{(p)}V$ . One recovers in particular the usual Brascamp-Lieb's inequality when  $\Omega = \mathbb{R}^d$ : even if  $\Omega$  has been assumed compact here, we recover the estimate (2.1.1) for a probability measure  $d\nu$  on  $\mathbb{R}^d$  using the first point of Corollary 2.4.3 for the family of measures  $\left(\frac{1}{\nu(B(0,N))} d\nu|_{B(0,N)}\right)_{N \in \mathbb{N}}$  and letting  $N \rightarrow +\infty$  since  $B(0, N)$  is convex; see also [Joh00].

The above results can be useful for semiclassical problems involving the low spectrum of semiclassical Witten Laplacians (or equivalently of semiclassical weighted Laplacians) in large dimension, such as problems dealing with correlation asymptotics, under some suitable (and uniform in the dimension) estimates on the eigenvalues of  $\text{Hess} V$  (and then of  $\text{Hess}^{(p)}V$ ) on some parts of  $\Omega$ . We refer for example to [HS94, BJS00, BM03, BM04] or to our work [DL17] (see Section 3.4 concerning the latter article) for some works exploiting this kind of estimates. Let us recall that we consider in this setting, for a small parameter  $h > 0$ ,  $\frac{f}{h}$  and  $\frac{V}{h}$  instead of  $f$  and  $V$ , and  $h^2 \Delta_f^{(p)}$  instead of  $\Delta_f^{(p)}$  for the usual semiclassical Schrödinger operator form. Note then from  $\text{Ric}_{\frac{V}{h}}^{(p)} = h^{-1}(h \text{Ric}^{(p)} + \text{Hess}^{(p)}V)$  that the curvature effects due to  $\text{Ric}^{(p)}$  become negligible at the semiclassical limit  $h \rightarrow 0^+$  under the condition  $\text{Hess}^{(p)}V > 0$  everywhere on  $\Omega$ . To apply Theorem 2.4.2 for any small  $h > 0$  in the Neumann case under this condition then only requires the additional  $h$ -independent condition  $\mathcal{K}_n^{(p)} \geq 0$  everywhere on  $\partial\Omega$ . In the Dirichlet case, the required additional condition becomes  $h \mathcal{K}_t^{(p)} - \partial_n V \geq 0$ , which requires in particular  $\partial_n V \leq 0$  everywhere on  $\partial\Omega$ . The point ii) of Corollary 2.4.3 is thus irrelevant in this case.

Let us lastly underline that to prove Theorem 2.4.2 (and then Corollary 2.4.3), we only use the supersymmetric structure and the relation

$$\Delta_f^{\mathbf{b},(p)} \geq \text{Ric}^{(p)} + 2 \text{Hess}^{(p)} f > 0$$

implied by Theorem 2.4.1 together with the hypotheses of Theorem 2.4.2. However, a control from below of the restriction  $\Delta_f^{\mathbf{b},(p)}|_{\text{Ran } d_f}$  for the points 1.i) and 2.i) (resp. of  $\Delta_f^{\mathbf{b},(p)}|_{\text{Ran } d_f^*}$  for the points 1.ii) and 2.ii)) would actually be sufficient as it can be understood by looking for example at the relation (2.1.2).

The specific form of the nonnegative first term in the r.h.s. of the integration by parts formula (2.4.5) stated in Theorem 2.4.1 is moreover not used, i.e. only its nonnegativity comes into play. When  $p = 1$ , we can easily slightly improve Corollary 2.4.3 by taking advantage of this nonnegative term which allows to compare  $\Delta_f^{\mathbf{b},(1)}|_{\text{Ran } d_f}$  (or equivalently  $L_V^{\mathbf{b},(1)}|_{\text{Ran } d}$ ) with the so-called  $N$ -dimensional Bakry-Émery tensor

$$\text{Ric}_{V,N} := \text{Ric} + \text{Hess} V - \frac{1}{N-n} dV \otimes dV, \quad (2.4.8)$$

where  $N \in (-\infty, +\infty]$  and, when  $N = n$ ,  $\text{Ric}_{V,n}$  is defined iff  $V$  is constant. The hypotheses of Corollary 2.4.3 require in particular the (everywhere) positivity of  $\text{Ric}_{V,+\infty}$  and we have more generally the

**Corollary 2.4.4.** *In the following, we assume that  $N \in (-\infty, 0] \cup [n, +\infty)$ .*

*i) Assume that  $\mathcal{K}_1 \leq 0$  everywhere on  $\partial\Omega$  and that  $\text{Ric}_{V,N} > 0$  everywhere on  $\Omega$ . It then holds: for every  $\omega \in H^1(\Omega, d\nu)$ ,*

$$\|\omega - \langle \omega \rangle_\nu\|_{L^2(d\nu)}^2 \leq \frac{N-1}{N} \int_{\Omega} (\text{Ric}_{V,N})^{-1}(\nabla\omega, \nabla\omega) d\nu.$$

*ii) Assume similarly that  $-\text{Tr}(\mathcal{K}_1) - \partial_n V \geq 0$  everywhere on  $\partial\Omega$  (here assumed non empty) and that  $\text{Ric}_{V,N} > 0$  on  $\Omega$ . It then holds: for every  $\omega \in H_0^1(\Omega, d\nu)$ ,*

$$\|\omega\|_{L^2(d\nu)}^2 \leq \frac{N-1}{N} \int_{\Omega} (\text{Ric}_{V,N})^{-1}(\nabla\omega, \nabla\omega) d\nu.$$

Note that  $\frac{1}{N}$  appears here as a natural parameter and that  $N \in (-\infty, 0] \cup [n, +\infty)$  is equivalent to  $\frac{1}{N} \in [-\infty, \frac{1}{n}]$  with the convention  $\frac{1}{0} = -\infty$ . When  $N = 1$ , that is  $n = N = 1$  and  $V$  is constant, the statement is empty since in that case  $\text{Ric}_{V,N} = 0$ . This statement does moreover not say anything when  $N = 0$  since in this case  $\frac{N-1}{N} = +\infty$  (and  $\nabla\omega = 0$  iff  $\omega$  is constant).

To the best of our knowledge, the statement of Corollary 2.4.4 has, apart from our work [Lep17], only been obtained at this level of generality in the slightly earlier article [KM17] of Kolesnikov-Milman, and it corresponds to the cases (1) and (2) of Theorem 1.2 in their work. The authors derive these formulas from the so-called generalized Reilly formula stated in Theorem 1.1 there, which somehow generalizes, in the weighted space setting, the statement given by Theorem 2.4.1 when  $p = 1$  and  $\omega$  has the form  $d_f\eta$ , to arbitrary  $\omega = d_f\eta$  which are not assumed tangential nor normal. The statement of Corollary 2.4.4 unifies and generalizes different inequalities obtained in the weighted and non-weighted (i.e when  $V = 0$ ) setting, when  $\partial\Omega$  is empty or not. We are more specific just below.

Apart from [KM17], the first item of Corollary 2.4.4 seems in particular new when  $\partial\Omega \neq \emptyset$  and the space is not Euclidean, even when  $N = +\infty$  in which case it boils down to the first item of Corollary 2.4.3. It moreover generalizes inequalities obtained in the Euclidean setting when  $N \leq 0$  in [BL09, Ngu14]. Besides, the second item of Corollary 2.4.4 seems completely new.

When applied to get informations on the second eigenvalue of  $L_V^{\mathbf{n},(0)}$  (remember that  $\text{Ker}(L_V^{\mathbf{n},(0)}) = \text{Span}\{1\}$ ) or on the first eigenvalue of  $L_V^{\mathbf{t},(0)}$  (when  $\partial\Omega \neq \emptyset$ ), Corollary 2.4.4 leads to the following: assume that  $\text{Ric}_{V,N} \geq \kappa g$ ,  $\kappa > 0$ , and that either the hypotheses of the first item of Corollary 2.4.4 hold, in which case we denote by  $\lambda$  the second eigenvalue of  $L_V^{\mathbf{n},(0)}$ , or that the hypotheses of the second item of Corollary 2.4.4 hold, in which case we denote by  $\lambda$  the first eigenvalue of  $L_V^{\mathbf{t},(0)}$ . It then holds

$$\lambda \geq \frac{N}{N-1} \kappa.$$

This generalizes different Lichnerowicz type estimates obtained in the non-weighted setting (i.e. when  $V = 0$  and  $N = n$ ) by Lichnerowicz in [Lic58] when  $\partial\Omega = \emptyset$  and

in [Esc90, Xia91, Rei77] when  $\partial\Omega \neq \emptyset^1$ , in the weighted setting in [MD10, LW15] when  $N \in [n, +\infty]$  and in [Oht16] when  $N < 0$  and  $\partial\Omega = \emptyset$ .

We refer in particular to [KM17], where the optimality of these inequalities is also proven when  $N \in (-\infty, -1] \cup [n, +\infty]$ , for more details and references concerning these estimates and concerning the  $N$ -dimensional Bakry-Émery tensor (2.4.8) and its connections with the Bakry-Émery operators  $\Gamma$  and  $\Gamma_2$  (see (1.3.8) and (1.3.9) in Section 1.3.1, and also [BGL14]).

Note lastly that for  $N > n$ , Corollary 2.4.4 does not provide any improvement in comparison with Corollary 2.4.3 in the semiclassical setting, that is when  $V$  is replaced by  $\frac{V}{h}$  where  $h \rightarrow 0^+$ , because of the term  $-\frac{1}{(N-n)h^2} dV \otimes dV$  involved in  $\text{Ric}_{\frac{V}{h}, N}$  (see indeed (2.4.8)).

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1. In this case, it thus means a lower bound on the second (or first) eigenvalue of the Hodge Laplacian, with Neumann (or Dirichlet) boundary conditions when  $\partial\Omega \neq \emptyset$ .





# Chapter 3

## Low spectrum of the Witten Laplacian

In Sections 3.1 to 3.3 of this chapter, we give an overview of the known results – and some elements of proof – on the precise study of the low spectrum of the Witten Laplacian  $\Delta_{f,h}^{(0)}$  acting on functions in the case of a Morse type potential  $f$ . We refer to the work [DLLN19b]<sup>1</sup> for our results obtained in this context.

We also present in these sections the main results of our work [LNV13], and of [Lep11] in the two-dimensional case, concerning the case of the low spectrum of the Witten Laplacian  $\Delta_{f,h}^{(p)}$  acting on  $p$ -forms. The major differences with the study of  $\Delta_{f,h}^{(0)}$  are presented as well.

Then, in Section 3.4, we present the main results of our work [DL17] dealing with the low spectrum of  $\Delta_{f,h}^{(0)}$  in large dimension when  $f$  is an explicit double-well potential naturally associated with the stochastically perturbed one-dimensional Allen-Cahn equation (see (3.4.2)).

### 3.1 Landscape of the sublevel sets of a Morse function

In this section, we will assume unless otherwise stated that  $f : \Omega \rightarrow \mathbb{R}^d$  is a smooth Morse function, where  $\Omega$  is either  $\mathbb{R}^d$  or a smooth compact and connected  $d$ -dimensional Riemannian manifold without boundary. In the case  $\Omega = \mathbb{R}^d$ , we will moreover assume that  $f(x) \rightarrow +\infty$  when  $|x| \rightarrow +\infty$  and that  $f$  has a finite number of critical points.

We then denote, for  $p \in \{0, \dots, d\}$ , the set of critical points with index  $p$  of  $f$  by  $\mathcal{U}_\Omega^{(p)}$  (see (1.2.19)) and we define  $\mathbf{m}_p := \text{Card} \mathcal{U}_\Omega^{(p)}$ . According to the introductory chapter, we know that  $\Delta_{f,h}^{(p)}$  has, for some  $c > 0$  small enough and for every  $h > 0$  small enough, exactly  $\mathbf{m}_p$  eigenvalues counted with multiplicity in the interval  $[0, ch]$ , these eigenvalues being moreover bounded by  $e^{-\frac{c}{h}^2}$ .

To precisely estimate these small eigenvalues, we first need to understand the energetic barriers in play that will *in fine* give the Arrhenius rates of these eigen-

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1. This work corresponds to the first part of the preprint [DLLN19a].

2. In the case  $\Omega = \mathbb{R}^d$ , we also assume that for some constant  $C > 0$ ,  $|\nabla f| \geq \frac{1}{C}$  and  $|\text{Hess } f| \leq C|\nabla f|^2$  outside some compact set  $K$ , which ensures that the essential spectrum of  $\Delta_{f,h}^{(p)}$  is bounded from below by some positive constant.

values, i.e. the  $\lim_{h \rightarrow 0^+} -h \ln \lambda_{j,h}^{(p)}$ 's for  $j \in \{1, \dots, \mathbf{m}_p\}$  (see (1.2.6), (1.2.7) and the discussion in between in Section 1.2.2).

In the case of functions, i.e. when  $p = 0$ , the analysis of these activation energies has motivated various mathematical studies within the probabilistic approach and simulated annealing techniques in the 80's. These quantities were first understood in this setting and under weaker hypotheses on the function  $f$ , neither assumed to be Morse nor  $\mathcal{C}^\infty$ , and we refer in particular to [FW12, HKS89, Mic95] in this direction. Let us note, however, that under these weak hypotheses, we are generally not able to compute the prefactors, that is precisely what we are interested in here.

Moreover, as it will be made more precise below in the case of a smooth Morse potential  $f$ , understanding these activation energies in the case  $p = 0$  actually amounts to studying how the number of connected components of the sublevel set  $\{f < \lambda\}$  evolves when  $\lambda$  crosses a critical value. In what follows, when  $f$  is a Morse potential, this study will lead to the construction of an injective map (defined in Section 3.1.2)

$$\mathbf{j} : \mathcal{U}_\Omega^{(0)} \setminus \{m_1\} \rightarrow \mathcal{P}(\mathcal{U}_\Omega^{(1)}) \cap \cup_{C \in \mathbb{R}} \{f = C\},$$

where  $m_1$  is some arbitrary global minimum of  $f$  in  $\Omega$  and  $\mathcal{P}(\mathcal{U}_\Omega^{(1)}) = \{\omega, \omega \subset \mathcal{U}_\Omega^{(1)}\}$ , such that the Arrhenius rates of the small eigenvalues of  $\Delta_{f,h}^{(0)}$  are precisely given by the  $2(f(\mathbf{j}(m)) - f(m))$ 's for  $m \in \mathcal{U}_\Omega^{(0)} \setminus \{m_1\}$  and  $+\infty$  (corresponding to the eigenvalue 0). Let us also mention that, generically, the map  $\mathbf{j}$  actually sends  $\mathcal{U}_\Omega^{(0)} \setminus \{m_1\}$  into  $\mathcal{U}_\Omega^{(1)}$  and we refer in this connection to (1.3.22) and the discussion around in Section 1.3.2.

In the case of general  $p$ -forms considered in [Lep11, LNV13], such a simple picture is no more relevant as it already appears in the case of surfaces treated in [Lep11]. Understanding the Arrhenius rates in this case requires, as we shall see in Section 3.1.4, the introduction of more sophisticated topological constructions.

### 3.1.1 Separating saddle points

The concept of separating saddle point enables to precisely understand the energetic barriers in play in the case of 0-forms. These barriers depend on the energies of the local minima of the Morse function  $f$  (in same number as the eigenvalues searched for!) and of some threshold energies to be crossed to reach, starting from one of these minima, a minimum of lower energy.

This notion already implicitly appeared in the article [HKN04] but it was only clearly defined in the work [HHS11] dealing with the more general Kramers-Fokker-Planck operators. Before defining a separating saddle point for a Morse function, we recall the following property:

**Proposition 3.1.1.** *Let  $z \in \Omega$  and  $f : \Omega \rightarrow \mathbb{R}$  be a Morse function. Then, for every  $r > 0$  small enough,  $B(z, r) \cap \{f < f(z)\}$  has at least two connected components (in  $\Omega$ ) if and only if  $z \in \mathcal{U}_\Omega^{(1)}$ , in which case  $B(z, r) \cap \{f < f(z)\}$  has two connected components.*

In other words, when  $\lambda$  decreases, the number of connected components of the sublevel set  $\{f < \lambda\}$  can only increase when  $\lambda$  crosses a critical value of  $f$  belonging to  $f(\mathcal{U}_\Omega^{(1)})$ . A separating saddle point is then defined as follows:

**Definition 3.1.2.** *i) A saddle point  $z \in \mathcal{U}_\Omega^{(1)}$  is said to be a separating saddle point if the two connected components of  $B(z, r) \cap \{f < f(z)\}$  (where  $r > 0$  is as in the previous proposition) are contained in (two) different connected components of  $\{f < f(z)\}$ . We denote by SSP the set made of these points.*

*ii) We call critical component of  $\Omega$  any connected component of  $\{f < f(z)\}$ , where  $z \in \Omega$ , whose boundary meets SSP. Such a component is thus necessarily a connected component of  $\{f < f(z)\}$  for some  $z \in \text{SSP}$ .*

### 3.1.2 Association between local minima and separating saddle points

We will omit details when associating local minima and separating saddle points below, but the following proposition (cf. [DLLN19b, Proposition 18]) will be useful to well understand the reasoning.

**Proposition 3.1.3.** *Let  $\lambda \in \mathbb{R}$  and  $\mathcal{C}$  be a connected component of  $\{f < \lambda\}$ . Then,*

$$\mathcal{C} \cap \text{SSP} \neq \emptyset \text{ iff } \text{Card}(\mathcal{C} \cap \mathcal{U}_\Omega^{(0)}) \geq 2.$$

Let us also define

$$\sigma := \max_{\mathcal{C} \cap \text{SSP}} f$$

with the convention  $\sigma := \min_{\mathcal{C}} f$  when  $\mathcal{C} \cap \text{SSP} = \emptyset$ . It then holds:

- i) For every  $\mu \in (\sigma, \lambda]$ , the set  $\mathcal{C} \cap \{f < \mu\}$  is a connected component of  $\{f < \mu\}$ .*
- ii) If  $\mathcal{C} \cap \text{SSP} \neq \emptyset$ , then  $\mathcal{C} \cap \mathcal{U}_\Omega^{(0)} \subset \{f < \sigma\}$  and all the connected components of  $\mathcal{C} \cap \{f < \sigma\}$  are critical.*

We now assume that  $\mathbf{m}_0 \geq 2^3$ , so that  $\text{SSP} \neq \emptyset$  by the preceding proposition, and we note  $f(\text{SSP}) = \{\sigma_2, \dots, \sigma_N\}$ , where  $N \geq 2$  and  $\sigma_2 > \dots > \sigma_N$ . Let  $N_1 := 1$ ,  $m_{1,1}$  be a global minimum of  $f$  (arbitrarily chosen if there are more than one), and  $E_{1,1} := \Omega$ . We now proceed in the following way:

1. Let us denote, for some  $N_2 \geq 1$ , by  $E_{2,1}, \dots, E_{2,N_2}$  the connected components of  $\{f < \sigma_2\}$  which do not contain  $m_{1,1}$ . They are all critical by the preceding proposition and we associate to each  $E_{2,j}$ , where  $j \in \{1, \dots, N_2\}$ , some global minimum  $m_{2,j}$  of  $f|_{E_{2,j}}$  (arbitrarily chosen if there are more than one).
2. Let us then consider, for some  $N_3 \geq 1$ , the connected components  $E_{3,1}, \dots, E_{3,N_3}$  of  $\{f < \sigma_3\}$  which do not contain the local minima of  $f$  previously labelled. These components are also critical and included in the  $E_{2,j} \cap \{f < \sigma_3\}$ 's,  $j \in \{1, \dots, N_2\}$ , such that  $E_{2,j} \cap \{f = \sigma_3\} \cap \text{SSP} \neq \emptyset$  (and  $\sigma_3 = \max_{E_{2,j} \cap \text{SSP}} f$  for such a  $j$ ). We then again associate to each  $E_{3,j}$ ,  $j \in \{1, \dots, N_3\}$ , some global minimum  $m_{3,j}$  of  $f|_{E_{3,j}}$ .
3. We continue this process until having considered the connected components of  $\{f < \sigma_N\}$  after which all the local minima of  $f$  have been labelled (see Figure 3.1 below).

---

3. When  $\mathbf{m}_0 = 1$ , the analysis of the exponentially small eigenvalues of  $\Delta_{f,h}^{(0)}$  is trivial : 0 is the only exponentially small eigenvalue, it has multiplicity one, and  $\text{Ker } \Delta_{f,h}^{(0)} = \text{Span}\{e^{-\frac{f}{h}}\}$ .

Next, we define two mappings  $\tilde{\mathbf{j}} : \mathcal{U}_\Omega^{(0)} \rightarrow \mathcal{P}(\Omega)$  and  $\mathbf{j} : \mathcal{U}_\Omega^{(0)} \rightarrow \mathcal{P}(\text{SSP})$  by

$$\forall i \in \{1, \dots, N\}, \forall j \in \{1, \dots, N_i\}, \tilde{\mathbf{j}}(m_{i,j}) := E_{i,j} \quad (3.1.1)$$

and

$$\forall i \in \{1, \dots, N\}, \forall j \in \{1, \dots, N_i\}, \mathbf{j}(m_{i,j}) := \partial E_{i,j} \cap \text{SSP}. \quad (3.1.2)$$

It then holds in particular  $\tilde{\mathbf{j}}(m_{1,1}) = \Omega$ ,  $\mathbf{j}(m_{1,1}) = \emptyset$ , and

$$\forall i \in \{2, \dots, N\}, \forall j \in \{1, \dots, N_i\}, \emptyset \neq \mathbf{j}(m_{i,j}) \subset \{f = \sigma_i\}.$$

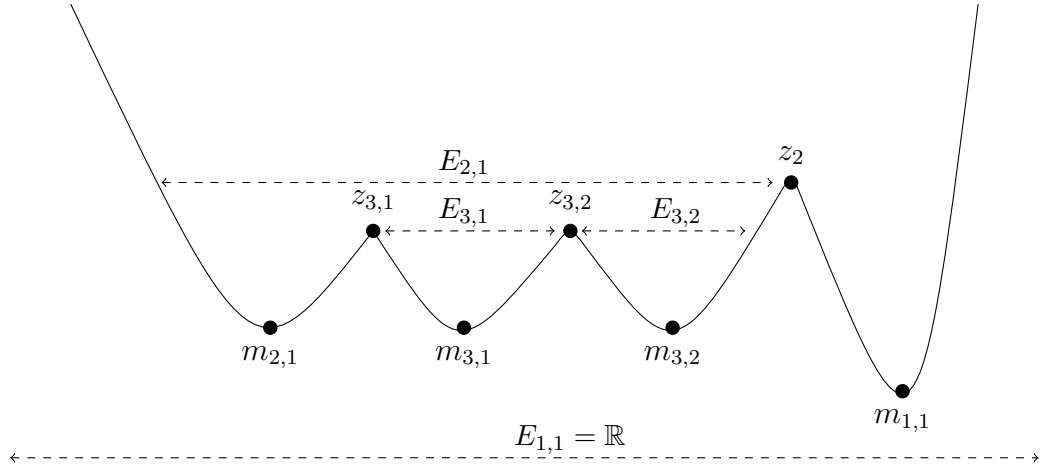


Figure 3.1 – An example of the preceding association when  $\Omega = \mathbb{R}$  and  $f$  admits four local minima. On this example,  $f(m_{1,1}) < f(m_{2,1}) = f(m_{3,1}) = f(m_{3,2})$ ,  $\mathbf{j}(m_{2,1}) = \{z_2\}$ ,  $\mathbf{j}(m_{3,1}) = \{z_{3,1}, z_{3,2}\}$ , and  $\mathbf{j}(m_{3,2}) = \{z_{3,2}\}$ . Note that in this example, other choices of construction of the maps  $\mathbf{j}$  and  $\tilde{\mathbf{j}}$  are possible since  $\arg \min_{E_{2,1}} f = \{m_{2,1}, m_{3,1}, m_{3,2}\}$ .

### 3.1.3 The case with boundary

In the case of a compact and connected manifold  $\Omega$  with boundary  $\partial\Omega$ , we can generalize this construction. Let us however keep in mind that we want *in fine* to obtain precise estimates on the first eigenvalues of the Witten Laplacian and that the construction in the case with boundary has therefore to be adapted according to the corresponding homology: absolute homology in the case of Neumann type conditions and relative homology in the case of Dirichlet type conditions (see Section 1.2.3 for more details in this connection).

We are more precise below and we will assume, to bring us back to the works already mentioned in this context [HN06, Lep10, DLLN19b, LN19a] that

$$f : \Omega \rightarrow \mathbb{R} \text{ and } f|_{\partial\Omega} \text{ are Morse functions and } \nabla f \neq 0 \text{ on } \partial\Omega.$$

### Neumann type boundary conditions

In this case, we proceed exactly as in the preceding part after having respectively replaced, for  $p \in \{0, 1\}$ ,  $\mathcal{U}_\Omega^{(p)}$  and  $\mathbf{m}_p = \text{Card}\mathcal{U}_\Omega^{(p)}$  by

$$\mathcal{U}_\Omega^{N,(p)} := \mathcal{U}_\Omega^{(p)} \cup \mathcal{U}_{\partial\Omega}^{N,(p)} \quad \text{and} \quad \mathbf{m}_p^N := \text{Card}\mathcal{U}_\Omega^{N,(p)},$$

where we recall that (see (1.2.20))

$$\mathcal{U}_{\partial\Omega}^{N,(p)} = \{\text{critical points } z \text{ with index } p \text{ of } f|_{\partial\Omega} \text{ s.t. } \partial_n f(z) < 0\}. \quad (3.1.3)$$

According to the terminology of [HN06, Lep10], the elements of  $\mathcal{U}_\Omega^{N,(1)}$  are called generalized saddle points of  $f$  in the Neumann setting (corresponding to absolute homology). Note indeed that the following property is well satisfied (see Proposition 3.1.1): for every  $z \in \Omega$  and every  $r > 0$  small enough,  $B(z, r) \cap \{f < f(z)\}$  has at least two connected components (in  $\Omega$ ) if and only if  $z \in \mathcal{U}_\Omega^{N,(1)}$ , in which case  $B(z, r) \cap \{f < f(z)\}$  has two connected components.

We then define the separating saddle points in  $\Omega$ , and then the mappings  $\tilde{\mathbf{j}}$  and  $\mathbf{j}$ , as previously.

### Dirichlet type boundary conditions

In this case, we define, for  $p \in \{0, 1\}$ ,

$$\mathcal{U}_\Omega^{D,(p)} := \mathcal{U}_\Omega^{(p)} \cup \mathcal{U}_{\partial\Omega}^{D,(p)} \quad \text{and} \quad \mathbf{m}_p^D := \text{Card}\mathcal{U}_\Omega^{D,(p)}, \quad (3.1.4)$$

where we recall that (see (1.2.21))

$$\mathcal{U}_{\partial\Omega}^{D,(p)} = \{\text{critical points } z \text{ with index } p - 1 \text{ of } f|_{\partial\Omega} \text{ s.t. } \partial_n f(z) > 0\}. \quad (3.1.5)$$

According to the terminology of [HN06, Lep10], the elements of  $\mathcal{U}_\Omega^{D,(1)}$  are now called generalized saddle points of  $f$  in the Dirichlet setting. Here, we have to be more careful than in the Neumann case because the corresponding homology is the relative homology, for which  $\partial\Omega$  is somehow assumed to be a point. This is also consistent with the physical interpretation consisting in extending the potential function  $f$  by  $-\infty$  outside  $\Omega$ . Let us make this clearer with the following definition.

**Definition 3.1.4.** *Let  $\omega$  be a nonempty set, disjoint from  $\Omega$ . We define the topological space  $X = \Omega \cup \omega$  whose topology is the topology generated by the elements of*

$$\{\omega \cup \mathcal{O}; \mathcal{O} \text{ open in } \Omega \text{ meeting } \partial\Omega\} \cup \{\mathcal{O}; \mathcal{O} \text{ open in the interior of } \Omega\}.$$

With this topology, one can easily check that  $\omega$  is connected and that  $\partial\omega = \partial\Omega$ . Let us moreover extend  $f$  to  $X$  by setting  $f|_\omega = -\infty$  and let us define, for  $x \in \Omega$  and  $r > 0$ ,  $B_X(x, r) = B(x, r)$  if  $B(x, r) \cap \partial\Omega = \emptyset$  and  $B_X(x, r) = B(x, r) \cup \omega$  else.

It then well holds (compare with Proposition 3.1.1): for every  $z \in \Omega$  and every  $r > 0$  small enough,  $B(z, r) \cap \{f < f(z)\}$  has at least two connected components in  $X$  if and only if  $z \in \mathcal{U}_\Omega^{D,(1)}$ , in which case  $B(z, r) \cap \{f < f(z)\}$  has precisely two connected components.

Another way to understand that the elements of  $\mathcal{U}_{\partial\Omega}^{D,(1)}$  geometrically play the role of saddle points in this setting is the following: when  $z \in \mathcal{U}_{\partial\Omega}^{D,(1)} \subset \partial\Omega = \partial\omega$ ,  $z$

is a local minimum of  $f|_{\partial\Omega}$  and a local maximum of  $f|_{D_i}$ , where  $D_i$  is the “straight line” passing through  $z$  and orthogonal to  $\partial\Omega$  at  $z$ .

Next, we define the separating saddle points of  $\Omega$  as the elements  $z$  of  $\mathcal{U}_\Omega^{D,(1)}$  such that the two connected components of  $B(z,r) \cap \{f < f(z)\}$  are included in (two) different connected components of  $\{f < f(z)\}$  in  $X$ . In this case, at least one of these components is included in  $\Omega \setminus \partial\Omega$ .

We can then define the mappings  $\tilde{\mathbf{j}}$  and  $\mathbf{j}$  roughly the same way as previously. We have nevertheless to “separate” the elements of  $\mathcal{U}_\Omega^{D,(0)} = \mathcal{U}_\Omega^{(0)}$ , that is the local minima of  $f$  in the interior  $\Omega$ , from the boundary. Let us explain this fact ; it is then easy to define the mappings  $\tilde{\mathbf{j}}$  and  $\mathbf{j}$ .

We first note, with our new definition of SSP,  $f(\text{SSP}) = \{\sigma_1, \dots, \sigma_N\}$ , where  $N \geq 1$  (this is the case as soon as  $\mathcal{U}_\Omega^{(0)} \neq \emptyset$ ) and  $\sigma_1 > \dots > \sigma_N$ , and we proceed as follows:

1. We denote, for some  $N_1 \geq 1$ , by  $E_{1,1}, \dots, E_{1,N_1}$  the connected components of  $\{f < \sigma_1\}$  **included in**  $\Omega \setminus \partial\Omega$  (they are all critical) and we associate to each  $E_{1,j}$  an arbitrary global minimum  $m_{1,j}$  of  $f|_{E_{1,j}}$ .
2. We then consider, for some  $N_2 \geq 1$ , the connected components  $E_{2,1}, \dots, E_{2,N_2}$  of  $\{f < \sigma_2\}$  **included in**  $\Omega \setminus \partial\Omega$  which do not contain the local minima previously labelled (they are critical). Then, we associate to each  $E_{2,j}$  some global minimum  $m_{2,j}$  of  $f|_{E_{2,j}}$ .
3. We continue this process until having considered the connected components of  $\{f < \sigma_N\}$  after which all the local minima of  $f$  have been labelled.

We refer to [DLLN19b, Section 2] for more details on this topic.

### 3.1.4 A finer analysis of the landscape of the sublevel sets

We assume in this part that  $\Omega$  is a smooth compact and connected  $d$ -dimensional Riemannian manifold without boundary and that  $f$  is a smooth Morse function whose critical points have **distinct** critical values.

Under these assumptions, note that the injective map  $\mathbf{j}$  constructed in Section 3.1.2 (see (3.1.2)) has actually the form

$$\mathbf{j} : \mathcal{U}_\Omega^{(0)} \setminus \{m_1\} \rightarrow \mathcal{U}_\Omega^{(1)}$$

and satisfies  $\mathbf{j}(\mathcal{U}_\Omega^{(0)} \setminus \{m_1\}) = \text{SSP} \subset \mathcal{U}_\Omega^{(1)}$  (according to Proposition 3.1.3). Moreover, as we shall see below in Section 3.2.1, the Arrhenius rates of the small eigenvalues of  $\Delta_{f,h}^{(0)}$  are given by the  $2(f(\mathbf{j}(m)) - f(m))$ 's, where  $m \in \mathcal{U}_\Omega^{(0)} \setminus \{m_1\}$ , and  $+\infty$ , corresponding to the eigenvalue 0, of multiplicity  $\mathbf{b}_0(\Omega) = 1$  (see (1.2.3)).

Let us now look at the evolution of the number of connected components of  $\{f < \lambda\}$ , i.e. of the 0-th Betti number  $\mathbf{b}_0(\{f < \lambda\})$  (for the absolute homology), when  $\lambda$  increases in  $\mathbb{R} \setminus f(\cup_{p \in \{0, \dots, d\}} \mathcal{U}_\Omega^{(p)})$ <sup>4</sup>. From the above, the function  $\lambda \mapsto \mathbf{b}_0(\{f < \lambda\})$  is a step function such that  $\mathbf{b}_0(\{f < \lambda\}) = \mathbf{b}_0(\Omega) = 1$  for every  $\lambda$  large enough, with values in  $\mathbb{N}$ , which only increases, by 1, when  $\lambda$  crosses a critical

4. This domain of definition ensures that  $\{f < \lambda\}$  is a manifold with (possibly empty) boundary  $\{f = \lambda\}$ .

value in  $f(\mathcal{U}_\Omega^{(0)})$ , and which only decreases, by 1, when  $\lambda$  crosses a critical value in  $f(\text{SSP}) \subset f(\mathcal{U}_\Omega^{(1)})$ . More precisely, following the terminology of the survey [EH08] on persistent homology, for each  $m \in \mathcal{U}_\Omega^{(0)}$ , a new 0-th homology class is born when  $\lambda$  crosses the value  $f(m)$ , and, when  $m \neq m_1$ , this 0-th homology class dies when  $\lambda$  crosses the value  $f(\mathbf{j}(m))$ . This value is indeed the minimal value  $\lambda$  such that the connected component of  $\{f \leq \lambda\}$  containing  $m \neq m_1$  contains at least one local minimum of  $f$  lower in energy than  $m$ , and then such that  $m$  is in the same connected component – i.e. in the same 0-th homology class – as some local minimum lower in energy and then associated to a prior 0-th homology class.

With in mind the close relation between the low spectrum of  $\Delta_{f,h}$  and the singular homology of  $\Omega$  given by the Morse inequalities (see Theorem 1.2.4), let us try to adapt the preceding point of view to some general  $p \in \{0, \dots, d\}$ . From Morse theory (see in particular [Mil63]), there are two mutually exclusive possibilities for how homology might change when  $\lambda$  crosses a critical value in  $f(\mathcal{U}_\Omega^{(p)})$ : either  $\mathbf{b}_p(\{f < \lambda\})$  increases by 1 and  $\mathbf{b}_k(\{f < \lambda\})$  does not change for  $k \neq p$ , or  $\mathbf{b}_{p-1}(\{f < \lambda\})$  decreases by 1 and  $\mathbf{b}_k(\{f < \lambda\})$  does not change for  $k \neq p-1$ . Following the terminology adopted in our work [LNV13], whose topological part was inspired by Barannikov’s presentation of Morse theory in [Bar94], we call the elements  $z \in \mathcal{U}_\Omega^{(p)}$  such that the second possibility occurs, i.e. such that  $\mathbf{b}_{p-1}(\{f < \lambda\})$  decreases by 1 when  $\lambda$  crosses  $f(z)$ , the upper critical values of  $f$  with index  $p$ . We denote by  $\mathcal{U}_U^{(p)}$  the set made of these  $z$ ’s and by

$$\mathcal{U}_U = \cup_{p \in \{0, \dots, d\}} \mathcal{U}_U^{(p)} \subset \mathcal{U}_\Omega = \cup_{p \in \{0, \dots, d\}} \mathcal{U}_\Omega^{(p)}$$

the sets made of all the upper critical points of  $f$ . Note that  $\mathcal{U}_U^{(0)} = \emptyset$  (since  $\mathbf{b}_{-1}(\{f < \lambda\}) = 0$  for every  $\lambda$ ) and that in the case  $p = 1$ , the set  $\mathcal{U}_U^{(1)}$  is precisely the set SSP defined in Definition 3.1.2.

We moreover say that an element  $z \in \mathcal{U}_\Omega^{(p)}$  is a lower critical point of  $f$  with index  $p$  when  $\mathbf{b}_p(\{f < \lambda\})$  increases by 1 when  $\lambda$  crosses  $f(z)$ , that is when some new  $p$ -th homology class is born when  $\lambda$  crosses the value  $f(z)$ , and when this  $p$ -th homology class eventually dies. We denote by  $\mathcal{U}_L^{(p)}$  the set made of these  $z$ ’s and by

$$\mathcal{U}_L = \cup_{p \in \{0, \dots, d\}} \mathcal{U}_L^{(p)} \subset \mathcal{U}_\Omega.$$

Note that when  $p = 0$ ,  $\mathcal{U}_L^{(0)}$  equals  $\mathcal{U}_\Omega^{(0)} \setminus \{m_1\}$ .

The (possibly) remaining critical points with order  $p$  are called homological critical points and we note  $\mathcal{U}_H^{(p)}$  the set made of these points, as well as

$$\mathcal{U}_H = \cup_{p \in \{0, \dots, d\}} \mathcal{U}_H^{(p)} \subset \mathcal{U}_\Omega.$$

Note that when  $p = 0$ , it holds  $\text{Card}(\mathcal{U}_H^{(0)}) = 1 = \mathbf{b}_0(\Omega)$  and it actually holds more generally:

$$\forall p \in \{0, \dots, d\}, \quad \text{Card}(\mathcal{U}_H^{(p)}) = \mathbf{b}_p(\Omega).$$

This property follows from the observation that  $\text{Card}(\mathcal{U}_H^{(p)})$  is precisely the number of  $p$ -th homology classes born which do not die when  $\lambda \rightarrow +\infty$ .



Lastly, let us define, for any  $z \in \mathcal{U}_L^{(p)}$ ,

$\lambda(z) := \inf\{\lambda \in (f(z), +\infty) \setminus f(\mathcal{U}_\Omega), \text{ the homology class born at } f(z) \text{ died at } f(\lambda)\}$ .

One then clearly has  $\lambda(z) > f(z)$  and one can show that there exists some (necessarily unique)  $z' \in \mathcal{U}_U^{(p+1)}$  such that  $f(z') = \lambda(z)$ . One then defines  $\mathbf{j}_B : \mathcal{U}_L \rightarrow \mathcal{U}_U$  by<sup>5</sup>

$$\forall p \in \{0, \dots, d\}, \forall z \in \mathcal{U}_L^{(p)}, \quad \mathbf{j}_B(z) := \{f = \lambda(z)\} \cap \mathcal{U}_U^{(p+1)}, \quad (3.1.6)$$

where, with a slight abuse of notation, we identify  $\mathbf{j}_B(z)$  with the singleton  $\{f = \lambda(z)\} \cap \mathcal{U}_U^{(p+1)}$ . The map  $\mathbf{j}_B : \mathcal{U}_L \rightarrow \mathcal{U}_U$  is moreover bijective and, as we shall see in Section 3.2.2, the Arrhenius rates of the small eigenvalues of  $\Delta_{f,h}^{(p)}$  counted with multiplicity are given by  $+\infty$ , corresponding to the eigenvalue 0, with multiplicity  $\mathbf{b}_p(\Omega)$  (see (1.2.3)), and by the

$2(f(\mathbf{j}_B(z)) - f(z))$ 's, where  $z \in \mathcal{U}_L^{(p)}$ , and the  $2(f(z) - f(\mathbf{j}_B^{-1}(z)))$ 's, where  $z \in \mathcal{U}_U^{(p)}$ .

Note in passing that according to the supersymmetric structure of the Witten Laplacian exhibited in (1.2.5), proving this fact actually amounts to proving that the Arrhenius rates of the non zero small eigenvalues of  $\Delta_{f,h}|_{\text{Ker } d_{f,h}^*}$  counted with multiplicity are precisely given by the  $f(\mathbf{j}_B(z)) - f(z)$ 's, where  $z \in \mathcal{U}_L$ .

We refer to [LNV13, Section 2] for details on the above discussion. Let us also stress here that in the context of persistent homology, the pairs  $(f(z), +\infty)$ 's, where  $z \in \mathcal{U}_H$ , and  $(f(z), f(\mathbf{j}_B(z)))$ 's, where  $z \in \mathcal{U}_L$ , give the persistent diagram of  $f$  on the manifold  $\Omega$ , which thus consists in the knowledge of the Arrhenius rates of the small eigenvalues of  $\Delta_{f,h}$ . We refer in particular to the survey article [EH08] and references therein on the subject of persistent homology.

## 3.2 Sharp bounds on the small eigenvalues and prefactors

### 3.2.1 The case of the Witten Laplacian acting on functions

Let us now state some results that can be obtained once the construction of Sections 3.1.2 and 3.1.3 is done. Some elements of proof, and especially the construction of adapted quasimodes, will be given in the following section. We will also try to gather the results obtained in the case without boundary and in the case with boundary, whether Neumann or Dirichlet type conditions are considered. We refer to Section 1.2.3 for precise definitions concerning these conditions.

We therefore assume here that  $\Omega$  is  $\mathbb{R}^d$  or a smooth compact and connected  $d$ -dimensional Riemannian manifold with possibly empty boundary  $\partial\Omega$ . We assume moreover that  $f : \Omega \rightarrow \mathbb{R}$  is a smooth Morse function such that, when  $\partial\Omega \neq \emptyset$ ,

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5. We adopt here the dual convention from the one used in [LNV13] where one actually defined a boundary operator map  $\partial_B$  such that  $\partial_B|_{\mathcal{U}_U} : \mathcal{U}_U \rightarrow \mathcal{U}_L$ . The subscript  $_B$  refers to Barannikov's presentation of Morse theory in [Bar94].

$\nabla f \neq 0$  on  $\partial\Omega$  and  $f|_{\partial\Omega}$  is Morse. Finally, when  $\Omega = \mathbb{R}^d$ , we also assume that there exists some constant  $C > 0$  such that outside some compact set  $K$ ,

$$|\nabla f| \geq \frac{1}{C} \quad \text{and} \quad |\text{Hess } f| \leq C |\nabla f|^2,$$

and that  $f(x) \rightarrow +\infty$  when  $|x| \rightarrow +\infty$ <sup>6</sup>. These hypotheses, in the case  $\Omega = \mathbb{R}^d$ , ensure that the essential spectrum of  $\Delta_{f,h}^{(p)}$ ,  $p \in \{0, \dots, d\}$ , is bounded from below by some positive constant when  $h > 0$  is small enough and that  $e^{-\frac{f}{h}}$  belongs to  $L^2(\mathbb{R}^d)$ , i.e. that  $0 \in \text{Sp}(\Delta_{f,h}^{(0)})$  (see [HKN04] for more details).

We can then state the following results that we prefer to write in a rather vague way for more simplicity. They follow from the results of the works [HHS11, Mic19] generalizing the work [HKN04] in the case without boundary and from our work [DLLN19b]<sup>7</sup> generalizing in particular the main results of [HN06] in the case of Dirichlet type boundary conditions. In the case of Neumann type boundary conditions, the first result also generalizes [Lep10] and is to our knowledge new at this level of generality.

**Theorem 3.2.1** (Case without boundary or with Neumann type conditions). *Let  $\Omega$  and  $f$  be as previously. We denote by  $\Delta_{f,h}^{N,(0)}$  the associated self-adjoint realization of the Witten Laplacian, with Neumann type boundary conditions when  $\partial\Omega \neq \emptyset$  (see Section 1.2.3). Let us also define  $\mathbf{m}_0^N = \text{Card}(\mathcal{U}_\Omega^{N,(0)})$  ( $= \text{Card}(\mathcal{U}_\Omega^{(0)})$  when  $\partial\Omega = \emptyset$ ), and  $\mathbf{j}$  the associated mapping defined in the preceding section.*

*Then, there exists  $c > 0$  such that for every  $h > 0$  small enough, the spectrum of  $\Delta_{f,h}^{N,(0)}$  satisfies*

$$\text{Sp}(\Delta_{f,h}^{N,(0)}) \cap [0, ch] = \text{Sp}(\Delta_{f,h}^{N,(0)}) \cap [0, e^{-\frac{c}{h}}],$$

*and the latter set consists in the eigenvalues  $\lambda_{1,h} = 0 < \lambda_{2,h} \leq \dots \leq \lambda_{\mathbf{m}_0^N,h}$  counted with multiplicity.*

*Let us moreover order the local minima  $m_1, \dots, m_{\mathbf{m}_0^N}$  of  $f$  so that  $\mathbf{j}(m_1) = \emptyset$  ( $m_1$  is thus a global minimum of  $f$ ) and  $S : \{2, \dots, \mathbf{m}_0^N\} \rightarrow \mathbb{R}, k \mapsto f(\mathbf{j}(m_k)) - f(m_k)$  is decreasing. Then, there exists  $C > 0$  such that for every  $h > 0$  small enough:*

$$\forall k \in \{2, \dots, \mathbf{m}_0^N\}, \exists p_k \text{ independent of } h, \quad \frac{1}{C} h^{p_k} e^{-2\frac{S(k)}{h}} \leq \lambda_{k,h} \leq C h^{p_k} e^{-2\frac{S(k)}{h}},$$

*where  $p_k$  only depends from the fact that  $m_k$  belongs to  $\Omega$  or to  $\partial\Omega$  and that  $\mathbf{j}(m_k)$  meets  $\partial\Omega$  or not.*

*Let us lastly assume that  $S(2) > S(3)$ ,  $f(m_2) > f(m_1)$ , and that  $\mathbf{j}(m_k) \cap \mathbf{j}(m_2) = \emptyset$  for every  $k \in \{3, \dots, \mathbf{m}_0^N\}$ . It then holds for every  $h > 0$  small enough the following Eyring-Kramers type formula:*

$$\lambda_{2,h} = A_2 h^{p_2} e^{-2\frac{S(2)}{h}} (1 + \mathcal{O}(h^{\frac{1}{2}})),$$

*where  $A_2$  is an explicit constant only depending on the partial derivatives of  $f$  (of order  $\leq 2$ ) on  $\mathbf{j}(m_2)$  and on  $\arg \min_{\mathbf{j}(m_2)} f$ . Moreover, the term  $\mathcal{O}(h^{\frac{1}{2}})$  admits a full*

6. One can show that when  $|\nabla f| \geq \frac{1}{C}$  outside a compact set, the a priori weaker assumption  $f \geq M$  for some  $M \in \mathbb{R}$  implies that  $f(x) \rightarrow +\infty$  when  $|x| \rightarrow +\infty$

7. See also our more recent work [LN19b] which generalizes the results of [HN06, DLLN19b] to the case where  $f$  admits critical points on  $\partial\Omega$ .

asymptotic expansion in  $h^{\frac{1}{2}}$  which, when  $\mathbf{j}(m_2) \subset \partial\Omega$  or  $\mathbf{j}(m_2) \subset \Omega$ , is a  $\mathcal{O}(h)$  with a full asymptotic expansion in  $h$ .

**Theorem 3.2.2** (Case with Dirichlet type conditions). *Let  $\Omega$  and  $f$  be as previously, and assume that  $\partial\Omega \neq \emptyset$ . We denote by  $\Delta_{f,h}^{D,(0)}$  the associated self-adjoint realization of the Witten Laplacian with Dirichlet type boundary conditions (see Section 1.2.3). We also define  $\mathbf{m}_0 = \text{Card}(\mathcal{U}_\Omega^{(0)}) = \text{Card}(\mathcal{U}_\Omega^{D,(0)})$  and  $\mathbf{j}$  the associated mapping defined in the previous section (in the case of Dirichlet type boundary conditions).*

*Then, there exists  $c > 0$  such that the spectrum of  $\Delta_{f,h}^{D,(0)}$  satisfies*

$$\text{Sp}(\Delta_{f,h}^{D,(0)}) \cap [0, ch] = \text{Sp}(\Delta_{f,h}^{D,(0)}) \cap [0, e^{-\frac{c}{h}}],$$

*and the latter set consists in the eigenvalues  $0 < \lambda_{1,h} < \lambda_{2,h} \leq \dots \leq \lambda_{\mathbf{m}_0,h}$  counted with multiplicity. Let us moreover order the local minima  $m_1, \dots, m_{\mathbf{m}_0}$  of  $f$  so that  $S : \{1, \dots, \mathbf{m}_0\} \rightarrow \mathbb{R}, k \mapsto f(\mathbf{j}(m_k)) - f(m_k)$  is decreasing. Then, there exists  $C > 0$  such that for every  $h > 0$  small enough:*

$$\forall k \in \{1, \dots, \mathbf{m}_0\}, \exists p_k \text{ independent of } h, \frac{1}{C} h^{p_k} e^{-2\frac{S(k)}{h}} \leq \lambda_{k,h} \leq C h^{p_k} e^{-2\frac{S(k)}{h}},$$

*where  $p_k$  only depends from the fact that  $\mathbf{j}(m_k)$  meets  $\partial\Omega$  or not.*

*Let us lastly assume that  $S(1) > S(2)$  and that  $\mathbf{j}(m_k) \cap \mathbf{j}(m_1) = \emptyset$  for every  $k \in \{2, \dots, \mathbf{m}_0\}$  or that  $\mathbf{j}(m_1) \cap \partial\Omega \neq \emptyset$ . It then holds for every  $h > 0$  small enough the following Eyring-Kramers type formula:*

$$\lambda_{1,h} = A_1 h^{p_1} e^{-2\frac{S(1)}{h}} (1 + \mathcal{O}(h^{\frac{1}{2}})),$$

*where  $A_1$  is an explicit constant only depending on the partial derivatives of  $f$  (of order  $\leq 2$ ) on  $\mathbf{j}(m_1)$  and on  $\arg \min_{\mathbf{j}(m_1)} f$ . Moreover, the term  $\mathcal{O}(h^{\frac{1}{2}})$  admits a full asymptotic expansion in  $h^{\frac{1}{2}}$  when  $\mathbf{j}(m_k) \cap \mathbf{j}(m_1) = \emptyset$  for every  $k \in \{2, \dots, \mathbf{m}_0\}$ , which is actually an expansion in  $h$  when  $\mathbf{j}(m_1) \subset \partial\Omega$  or  $\mathbf{j}(m_1) \subset \Omega$ .*

The above results can be specified or improved in various situations. Let us mention in particular the article [Mic19] in the case without boundary where Michel proves the existence of a full asymptotic expansion of the small eigenvalues of the Witten Laplacian in the general case. In general, a phenomenon of tunneling effect appears: the prefactors depend on the values of the derivatives of  $f$  in several wells. It should moreover be possible to adapt the study led in [Mic19] to the cases of Neumann or Dirichlet type boundary conditions considered in [HN06, Lep10, DLLN19b].

Let us conclude this section by pointing out that the constants  $A_1$  and  $A_2$  of the previous theorems arise from the Laplace method.

Assume for example, in one of the theorems stated above, that for the  $i \in \{1, 2\}$  in question:  $\arg \min_{\mathbf{j}(m_i)} f = \{m_i\} \subset \Omega$  and  $\mathbf{j}(m_i) = \{z\} \subset \Omega$ . It then precisely holds

$$\lambda_{i,h} = \frac{|\lambda(z)| \sqrt{|\det \text{Hess } f(m_i)|}}{\sqrt{|\det \text{Hess } f(z)|}} \frac{h}{\pi} e^{-2\frac{S(i)}{h}} (1 + \mathcal{O}(h)),$$

where  $\lambda(z)$  is the negative eigenvalue of  $\text{Hess } f(z)$ . It then corresponds to  $h$  times the formula (1.3.22) stated in Section 1.3.2 once the potential  $V$  there has been

replaced by  $2f^8$ . Moreover, if one only assumes  $\arg \min_{\mathbf{j}(m_i)} f \subset \Omega$  and  $\mathbf{j}(m_i) \subset \Omega$ , we have to consider barycentric sums depending on the Hessian matrix of  $f$  at the elements of  $\arg \min_{\mathbf{j}(m_i)} f$  and of  $\mathbf{j}(m_i)$ .

Similarly, if we assume to be under the hypotheses of Theorem 3.2.2 with for example  $\mathbf{j}(m_1) = \{z_1, \dots, z_{n_0}\} \subset \partial\Omega$ , it precisely holds

$$\lambda_{1,h} = 2 \sqrt{\frac{h}{\pi}} \sqrt{\det \text{Hess } f(m_1)} \sum_{i=1}^{n_0} \frac{\partial_n f(z_i)}{\sqrt{\det \text{Hess } f|_{\partial\Omega}(z_i)}} e^{-2\frac{S(1)}{h}} (1 + \mathcal{O}(h)), \quad (3.2.1)$$

which leads in particular to the statement of Proposition 5.2.3 in Chapter 5<sup>9</sup> (see also in this connection (1.3.33) and (1.3.36) in Section 1.3.3).

### 3.2.2 The case of the Witten Laplacian acting on forms

As in Section 3.1.4, we assume in this part that  $\Omega$  is a smooth compact and connected  $d$ -dimensional Riemannian manifold without boundary and that  $f$  is a smooth Morse function whose critical points have distinct critical values.

We then recall from Section 3.1.4 that the set of critical points of  $f$  in  $\Omega$  admits the following partition into upper, lower and homological critical points:

$$\mathcal{U}_\Omega = \mathcal{U}_U \cup \mathcal{U}_L \cup \mathcal{U}_H \quad \text{where, for } A \in \{U, L, H\}, \quad \mathcal{U}_A = \cup_{p \in \{0, \dots, d\}} \mathcal{U}_A^{(p)}.$$

The main result of [LNV13] is the following.

**Theorem 3.2.3.** *Let  $\Omega$  and  $f$  be as previously. For  $p \in \{0, \dots, d\}$ , we denote by  $\Delta_{f,h}^{(p)}$  the self-adjoint realization of the Witten Laplacian, and by  $\mathbf{j}_B : \mathcal{U}_L \rightarrow \mathcal{U}_U$  the bijective map defined by (3.1.6).*

*Then, for any  $p \in \{0, \dots, d\}$ , there exists  $c > 0$  such that for every  $h > 0$  small enough, the spectrum of  $\Delta_{f,h}^{(p)}$  satisfies*

$$\text{Sp}(\Delta_{f,h}^{(p)}) \cap [0, ch] = \text{Sp}(\Delta_{f,h}^{(p)}) \cap [0, e^{-\frac{c}{h}}],$$

*and the latter set consists in  $\mathbf{m}_p$  eigenvalues counted with multiplicity.*

*For every  $h > 0$  small enough, there exists moreover a bijection  $j : \mathcal{U}_\Omega^{(p)} \rightarrow \text{Sp}(\Delta_{f,h}^{(p)}) \cap [0, ch]$ , where the latter set is counted with multiplicity, such that:*

1. *For every  $z$  in  $\mathcal{U}_H^{(p)}$ , it holds*

$$j(U^{(p)}) = 0.$$

2. *For every  $z$  in  $\mathcal{U}_L^{(p)}$ , there exists a homological rational constant  $\kappa_z > 0$  such that, defining  $z' := \mathbf{j}_B(z)$ , the following Eyring-Kramers type formula holds:*

$$j(z) = \kappa_z \frac{h}{\pi} \frac{|\lambda_1(z') \cdots \lambda_{p+1}(z')| |\det \text{Hess } f(z)|^{\frac{1}{2}}}{|\lambda_1(z) \cdots \lambda_p(z)| |\det \text{Hess } f(z')|^{\frac{1}{2}}} e^{-2\frac{f(z')-f(z)}{h}} (1 + \mathcal{O}(h)),$$

*where, for any critical point  $s$  of  $f$  with index  $\ell$ ,  $\lambda_1(s), \dots, \lambda_\ell(s)$  denote the negative eigenvalues of  $\text{Hess } f(s)$ .*

8. We recall that this multiplicative factor  $h$  arises from the relation (1.3.17) :  $\Delta_{f,h}^{(0)} = e^{-\frac{V}{2h}} h L_{V,h}^{(0)} e^{\frac{V}{2h}}$ , where  $V = 2f$ .

9. The asymptotic of  $\lambda_{1,h}$  is  $2h$  times the one of  $\lambda_h$  in Proposition 5.2.3 since the weighted Laplacian considered in Chapter 5 is actually  $L_{f,\frac{h}{2}}^{(0)}$  and  $\Delta_{f,h}^{(0)} = 4\Delta_{\frac{f}{2},\frac{h}{2}}^{(0)} = 2h e^{-\frac{f}{h}} L_{f,\frac{h}{2}}^{(0)} e^{\frac{f}{h}}$ .

3. Finally, for every  $z$  in  $\mathcal{U}_U^{(p)}$ , there exists a homological rational constant  $\kappa_z > 0$  such that, defining  $z' := \mathbf{j}_B^{-1}(z)$ , the following Eyring-Kramers type formula holds:

$$j(z) = \kappa_z \frac{h}{\pi} \frac{|\lambda_1(z) \cdots \lambda_p(z)|}{|\lambda_1(z') \cdots \lambda_{p-1}(z')|} \frac{|\det \text{Hess } f(z')|^{\frac{1}{2}}}{|\det \text{Hess } f(z)|^{\frac{1}{2}}} e^{-2\frac{f(z)-f(z')}{h}} (1 + \mathcal{O}(h)),$$

where, for any critical point  $s$  of  $f$  with index  $\ell$ ,  $\lambda_1(s), \dots, \lambda_\ell(s)$  denote the negative eigenvalues of  $\text{Hess } f(s)$ .

The corresponding theorem in [LNV13] is actually stated under the following additional assumption:

the values  $f(\mathbf{j}_B(z)) - f(z)$ 's, where  $z \in \mathcal{U}_L$ , are all distinct.

Note that this assumption precisely means that for any  $p \in \{0, \dots, d\}$ , the non zero eigenvalues of  $\Delta_{f,h}^{(p)}$  associated with the elements of  $\mathcal{U}_L^{(p)}$  have distinct Arrhenius rates, and then ensures that these non zero eigenvalues are distinct in the limit  $h \rightarrow 0^+$ . Nevertheless, this assumption is actually not used in the analysis made in [LNV13].

Let us conclude this part with a few words about the rational constants  $\kappa_z$ 's,  $z \in \mathcal{U}_L \cup \mathcal{U}_U$  involved in Theorem 3.2.3. These constants arise from the analysis of the homology of  $\Omega$  with real (or with rational) coefficients near the elements of  $\mathcal{U}_U$  (see [LNV13, Proposition 2.12]). They are more precisely determined by the structure of the homology groups of the sublevel sets  $\{f < \lambda\}$ ,  $\lambda \in \mathbb{R}$  and do neither depend on  $h$ , nor on the Riemannian metric  $g$  and on the Morse function  $f$  (as long as our generic assumptions are fulfilled), contrary to the other factors. This is why we use the attribute ‘‘homological’’ for these constants.

Note also that by supersymmetry, it is clear that for any  $z \in \mathcal{U}_L$ , it holds  $\kappa_z = \kappa_{\mathbf{j}_B(z)}$  (see (1.2.5)). Moreover, as shown in [HKN04, HN06, Lep10], these homological constants  $\kappa_z$  equal 1 when  $p = 0$ , and also when  $p = d$  by duality. In the case of surfaces treated in [Lep11], a combination of these results together with simple duality and chain complex arguments then implies that these constants equal 1 for any  $p \in \{0, 1, 2\}$ . Nevertheless, contrary to this indication that it could be true in general, which was moreover our intuition when we wrote [LNV13], it appears from recent discussions with Claude Viterbo that this actually fails to be true in general as soon as  $d \geq 3$ .

### 3.3 Adapted quasimodes to the computation of the small singular values

We give in this section some elements permitting to understand the reasoning leading to the statement of the above Theorems 3.2.1 to 3.2.3 once the mappings  $\mathbf{j}$  (see Sections 3.1.2 and 3.1.3) and  $\mathbf{j}_B$  (see (3.1.6) in Section 3.1.4) have been constructed.

When trying to compute the small eigenvalues of  $\Delta_{f,h}$ , the basic strategy is to construct, for every  $p \in \{0, \dots, d\}$ , good ‘‘global’’ quasimodes for  $p$ -forms and coarser

local quasimodes for  $(p+1)$ -forms. Thanks to the supersymmetric structure, we will then be able to reduce the problem to the study of the small singular values of  $d_{f,h}|_{\text{Ker } d_{f,h}^*}$ , whose squares are precisely the eigenvalues we are looking for.

Let us stress here that working simultaneously with quasimodes for  $p$ -forms and for  $(p+1)$ -forms brings more flexibility than only considering quasimodes for  $p$ -forms. In the case  $p=0$ , the analysis of the low spectrum of  $\Delta_{f,h}^{(0)}$  can however be handled, at least partially, only using quasimodes for functions and we will come back to this point of view which has several interests in Sections 3.4.2 and 3.5. This nevertheless requires to construct the quasimodes for functions much more precisely and the subsequent analysis does moreover not lead so easily to the existence of a full asymptotic expansion of the low spectrum of  $\Delta_{f,h}^{(0)}$ .

In Sections 3.3.1 to 3.3.3, we focus on the case  $p=0$ . Since we will return at length to the case of Dirichlet type boundary conditions in the last two chapters, we will only consider this case there. This requires a little more general study than in the case without boundary (cf. [HKN04, HHS11, Mic19]) because two types of saddle points have to be considered: the saddle points in  $\Omega \setminus \partial\Omega$ , in the neighborhood of which everything happens as in the case without boundary, and those in  $\partial\Omega$ , in the neighborhood of which the analysis is noticeably different.

Then, in Section 3.3.4, we briefly explain how the analysis for 0-forms can be adapted to the case of  $p$ -forms.

### 3.3.1 “Global” quasimodes for functions

We construct the quasimodes for functions in the following way: to each local minimum of  $f$  having the form  $m_{i,j}$  defined in Section 3.1.3 in the case of Dirichlet type boundary conditions (i.e. to each local minimum in  $\Omega \setminus \partial\Omega$ ), we associate a smooth cut-off function  $\chi_{m_{i,j}}$  “closed to” the characteristic function of  $E_{i,j}$ . This type of construction appears for example in [HKN04, HN06, Lep10, HHS11, Mic19, DLLN19b, LN19a] and depends not much from the fact that the considered manifold has a boundary or not. It just requires to be conveniently adapted in the case with boundary.

Let us focus here on the construction made in [DLLN19b], which slightly differs from the other ones, and to which we refer for more details. The idea is to consider a family of cut-off functions  $\chi_{m_{i,j}} = \chi_{m_{i,j},\varepsilon}$  depending on a parameter  $\varepsilon > 0$ , small and arbitrarily small, such that

$$\chi_{m_{i,j}} = 1 \quad \text{on} \quad E_{i,j} \cap \{f < f(\mathbf{j}(m_{i,j})) - \varepsilon\}. \quad (3.3.1)$$

Notice that this set is connected when  $\varepsilon$  is small enough. We want moreover  $\chi_{m_{i,j}}$  to be equal to 0 or to 1 in some fixed (i.e. independent of the small parameter  $\varepsilon > 0$ ) neighborhood of each element of  $\mathcal{U}_\Omega^{D,(1)} \setminus \mathbf{j}(m_{i,j})$  and to be supported in the interior of  $\Omega$ .

When  $\partial\tilde{\mathbf{j}}(m_{i,j}) \cap \mathcal{U}_\Omega^{D,(1)} \subset \text{SSP}$ , this is automatically satisfied for every  $\varepsilon > 0$  small enough as soon as  $\chi_{m_{i,j}}$  satisfies (3.3.1) and

$$\text{supp } \chi_{m_{i,j}} \subset E_{i,j}.$$

Otherwise, we modify the preceding cut-off function so that  $\chi_{m_{i,j}} = 1$  in a small but fixed (that is independent of the small parameter  $\varepsilon > 0$ ) neighborhood of each

$z \in \mathcal{U}_\Omega^{D,(1)} \cap \partial\tilde{\mathbf{j}}(m_{i,j}) \setminus \text{SSP}$ . Notice that such a  $z$  necessarily belongs to  $\Omega \setminus \partial\Omega$  and that by definition, for every  $r > 0$  small enough, the two connected components of  $\{f < f(z)\} \cap B(z, r)$  are included in  $E_{i,j}$ . The function  $\chi_{m_{i,j}}$  constructed in this way is not supported in  $E_{i,j}$  but  $\text{supp } \chi_{m_{i,j}}$  only meets  $E_{i,j}^c$  in a small but fixed neighborhood of  $\mathcal{U}_\Omega^{D,(1)} \cap \partial\tilde{\mathbf{j}}(m_{i,j}) \setminus \text{SSP}$  (see Figures 3.2 and 3.3 below).

The latter neighborhoods and  $\varepsilon > 0$  can lastly be chosen small enough so that for every  $(i, j) \neq (i', j') : \text{supp } \chi_{m_{i,j}} \cap \text{supp } \chi_{m_{i',j'}} = \emptyset$  or, up to switching  $(i, j)$  and  $(i', j')$ ,  $\text{supp } \chi_{m_{i,j}} \subset \{\chi_{m_{i',j'}} = 1\}$ .

Once the  $\chi_{m_{i,j}}$  are defined, we define the following quasimodes:

$$\psi_{m_{i,j}}^{(0)} := \frac{\chi_{m_{i,j}} e^{-\frac{f}{h}}}{\|\chi_{m_{i,j}} e^{-\frac{f}{h}}\|_{L^2}}. \quad (3.3.2)$$

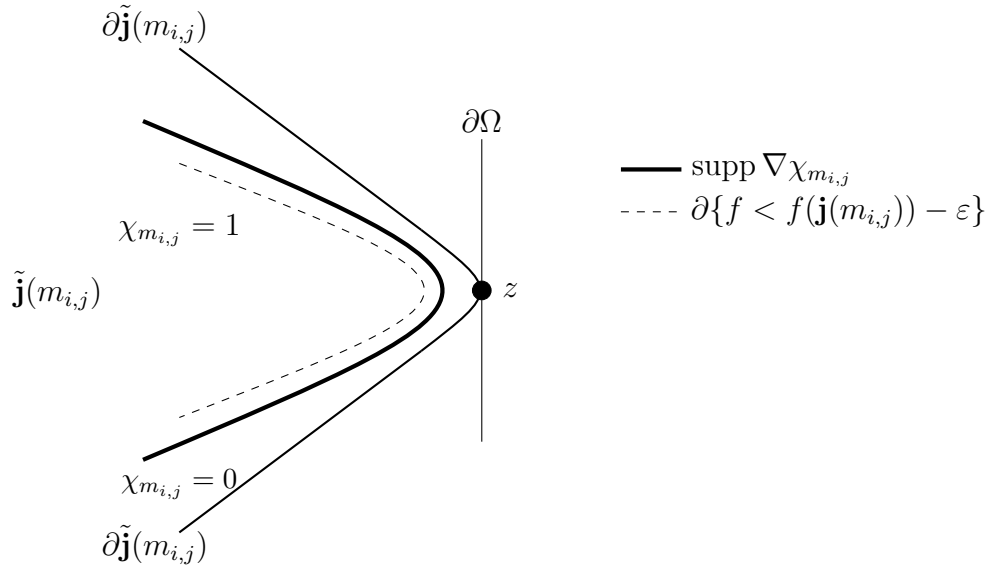


Figure 3.2 – Representation of  $\chi_{m_{i,j}}$  near some  $z \in \mathbf{j}(m_{i,j}) \cap \partial\Omega \subset \text{SSP}$ .

### 3.3.2 Local quasimodes for 1-forms

For the 1-forms, one first considers, in a small but fixed neighborhood  $\mathcal{V}_z$  of each element  $z$  in  $\mathcal{U}_\Omega^{(1)} \subset \Omega \setminus \partial\Omega$ , the principal unitary 1-form  $\psi_z$  associated with the operator  $\Delta_{f,h}^{(1)}$  with full Dirichlet conditions on the boundary of this neighborhood. From the work of Helffer-Sjöstrand [HS85c], this operator has, when  $h \rightarrow 0^+$ , one unique eigenvalue in  $[0, ch]$  for some small enough constant  $c > 0$ . This eigenvalue is moreover exponentially small, i.e. has the form  $\mathcal{O}(e^{-\frac{c}{h}})$  if one chooses  $c$  small enough. One has moreover Agmon type decay estimates on  $\psi_z$  as well as some very precise WKB approximation whose first term is explicit along the stable and unstable manifolds of  $z$  for the flow of  $-\nabla f$ .

In addition, there exists on  $\mathcal{V}_z$  (chosen small enough) a unique nonnegative solution to the eikonal equation

$$|\nabla f| = |\nabla \varphi| \quad \text{with initial value } \varphi(z) = 0$$

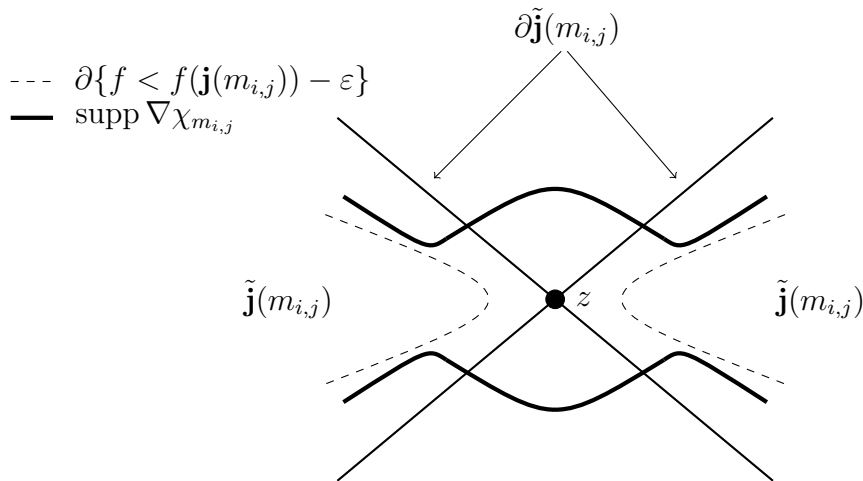


Figure 3.3 – Representation of  $\chi_{m_{i,j}}$  near some  $z \in \mathcal{U}_{\Omega}^{D,(1)} \cap \partial\tilde{\mathbf{j}}(m_{i,j}) \setminus \text{SSP}$ .

and one has  $\varphi(x) = d_{\text{Ag}}(x, z)$  on  $\mathcal{V}_z$ , where  $d_{\text{Ag}}$  is the Agmon distance associated with the metric  $|\nabla f|^2 dg$ , where  $dg$  denotes the Riemannian metric on  $\Omega$ .

We then define for every such  $z$  :

$$\psi_z^{(1)} := \frac{\theta \psi_z}{\|\theta \psi_z\|_{L^2}}, \quad (3.3.3)$$

where  $\theta$  is a smooth cut-off function such that  $\theta = 1$  near  $z$  and  $\text{supp } \theta \subset \mathcal{V}_z$ .

When  $z \in \mathcal{U}_{\partial\Omega}^{D,(1)} \subset \partial\Omega$ , we proceed similarly by using this time the study led around such a point in [HN06]. The boundary conditions for the local problem considered are in this case (tangential) Dirichlet type boundary conditions on  $\mathcal{V}_z \cap \partial\Omega$  and full Dirichlet ones on  $\partial\mathcal{V}_z$ . This problem admits again one unique exponentially small eigenvalue and one defines again

$$\psi_z^{(1)} := \frac{\theta \psi_z}{\|\theta \psi_z\|_{L^2}}, \quad (3.3.4)$$

where  $\psi_z$  is an eigen-1-form associated with this eigenvalue and  $\theta$  is a cut-off function such that  $\theta = 1$  near  $z$  and  $\text{supp } \theta \subset \mathcal{V}_z$ . Agmon estimates on  $\psi_z$  – and hence on  $\psi_z^{(1)}$  – and the existence of a precise WKB approximation are proven in [HN06]. Let us just mention here that the natural Agmon distance to  $z$  is here locally given by the unique solution  $\varphi$  to the eikonal equation

$$|\nabla f| = |\nabla \varphi| \quad \text{with boundary value } \partial_n \varphi = -\partial_n f \text{ and initial value } \varphi(z) = 0$$

(we recall that  $z$  is a local minimum of  $f|_{\partial\Omega}$  such that  $\partial_n f(z) > 0$ ).

### 3.3.3 Reduction of the problem to some interaction matrix

Let us now explain how the expression of the interaction matrix of  $d_{f,h}$  in convenient bases built from the previous quasimodes can be estimated accurately, which leads to spectral results of the type of Theorems 3.2.1 and 3.2.2. We begin by the following remarks (some of them are obvious by definition of our quasimodes) where we recall that we consider the case with Dirichlet type boundary conditions:



- The family  $(\psi_z^{(1)})_{z \in \mathcal{U}_\Omega^{D,(1)}}$  is orthonormal in  $\Lambda^1 L^2(\Omega)$ , included in  $\Lambda^1 H_{\mathfrak{t}}^1(\Omega)$  which is the domain of the closed quadratic form  $\mathcal{D}_{f,h}^{(1)}$  associated with  $\Delta_{f,h}^{D,(1)}$  (see (1.2.8) in Section 1.2.3), and satisfies:

$$\exists c > 0, \forall z \in \mathcal{U}_\Omega^{D,(1)}, \mathcal{D}_{f,h}^{(1)}(\psi_z, \psi_z) \leq e^{-\frac{c}{h}}. \quad (3.3.5)$$

The latter property follows from the Agmon estimates mentioned above.

- The family  $(\psi_m^{(0)})_{m \in \mathcal{U}_\Omega^{(0)}}$  is a family of smooth functions supported in  $\Omega$  and unitary in  $L^2(\Omega)$ . Moreover, from (3.3.1), for every  $\delta > 0$ , the parameter  $\varepsilon > 0$  appearing in the definition of  $\psi_m^{(0)}$  (cf. (3.3.1) and (3.3.2)) can be chosen small enough so that:

$$\forall m \in \mathcal{U}_\Omega^{(0)}, \mathcal{D}_{f,h}^{(0)}(\psi_m^{(0)}, \psi_m^{(0)}) = \|d_{f,h}\psi_m^{(0)}\|_{L^2}^2 \leq e^{-2\frac{f(\mathfrak{j}(m)) - f(m) - \delta}{h}}. \quad (3.3.6)$$

This family is not orthogonal in general but is however linearly independent, and this, uniformly in  $h$  (cf. [HHS11, DLLN19b]).

- For every  $m \in \mathcal{U}_\Omega^{(0)}$  and  $z \in \mathcal{U}_\Omega^{D,(1)}$ , either  $z \notin \mathfrak{j}(m)$ , in which case

$$\langle d_{f,h}\psi_m^{(0)}, \psi_z^{(1)} \rangle_{L^2} = 0,$$

or  $z \in \mathfrak{j}(m)$ , in which case

$$\langle d_{f,h}\psi_m^{(0)}, \psi_z^{(1)} \rangle_{L^2} = A(m, z)h^{p(z)}e^{-\frac{f(\mathfrak{j}(m)) - f(m)}{h}}(1 + \mathcal{O}(h)),$$

where  $p(z)$  is an explicit constant only depending from the fact that  $z \in \partial\Omega$  or not,  $A(m, z)$  is an explicit nonzero constant only depending on the derivatives of  $f$  (of order  $\leq 2$ ) at  $z$  and on  $\arg \min_{\mathfrak{j}(m_1)} f$ , and the term  $\mathcal{O}(h)$  admits a full asymptotic expansion in  $h$ . The delicate point in this computation is to precisely estimate the term

$$\langle d_{f,h}\chi_m e^{-\frac{f}{h}}, \psi_z^{(1)} \rangle_{L^2} = h \langle e^{-\frac{f}{h}} d\chi_m, \psi_z^{(1)} \rangle_{L^2},$$

since  $\|\chi_m e^{-\frac{f}{h}}\|_{L^2}$  (see (3.3.2)) is easily estimated by the Laplace method (and the prefactor of this estimate only depends on the derivatives of  $f$  of order  $\leq 2$  on  $\arg \min_{\mathfrak{j}(m_1)} f$ ). We are then reduced to a computation in the neighborhood of  $z$  which can be performed thanks to the precise WKB approximation of  $\psi_z$  – and thus of  $\psi_z^{(1)}$  – together with the Laplace method and a tricky use of the Stokes formula (see in particular [DLLN19b] where, contrary to the other references mentioned in this context, we do not require additional properties on the cut-off function  $\chi_m$  near  $z$ ).

Let us now consider, for  $i \in \{0, 1\}$ , the spectral projector

$$\pi_h^{(i)} := \pi_{[0, ch)}^{(i)}(\Delta_{f,h}^{D,(i)})$$

associated with the interval  $[0, ch)$ , where  $c > 0$  is chosen sufficiently small so that  $\dim \text{Ran}(\pi_h^{(i)}) = \mathbf{m}_i^D$  (see Theorem 1.2.5). Using (3.3.5), (3.3.6), and the Markov type estimate

$$\forall b, a > 0, \mathcal{D}_{f,h}^{(i)}(u, u) \leq b \text{ implies } \|u - \pi_{[0, a)}^{(i)}(\Delta_{f,h}^{D,(i)})u\|^2 \leq \frac{b}{a}, \quad (3.3.7)$$

we obtain the following relations:

- There exists  $c > 0$  such that for every  $z \in \mathcal{U}_\Omega^{D,(1)}$  and  $m \in \mathcal{U}_\Omega^{(0)}$ ,

$$\varphi_z^{(1)} := \pi_h^{(1)} \psi_z^{(1)} = \psi_z^{(1)} + \mathcal{O}(e^{-\frac{c}{h}}) \quad \text{and} \quad \varphi_m^{(0)} := \pi_h^{(0)} \psi_m^{(0)} = \psi_m^{(0)} + \mathcal{O}(e^{-\frac{c}{h}}).$$

It follows that the family  $(\varphi_z^{(1)})_{z \in \mathcal{U}_\Omega^{D,(1)}}$  defined above is quasi-orthonormal (i.e. that  $\langle \varphi_z^{(1)}, \varphi_{z'}^{(1)} \rangle_{L^2} = \delta_{z,z'} + \mathcal{O}(e^{-\frac{c}{h}})$  for every  $z, z'$ ) and that the family  $(\varphi_m^{(0)})_{m \in \mathcal{U}_\Omega^{(0)}}$  is uniformly linearly independent and satisfies  $\|\varphi_m^{(0)}\|_{L^2} = 1 + \mathcal{O}(e^{-\frac{c}{h}})$  for every  $m$ . These families are hence respective bases of  $\text{Ran}(\pi_h^{(1)})$  and of  $\text{Ran}(\pi_h^{(0)})$ .

- For every  $m \in \mathcal{U}_\Omega^{(0)}$  and  $z \in \mathcal{U}_\Omega^{D,(1)}$ , since  $d_{f,h} \pi_h^{(0)} = \pi_h^{(1)} d_{f,h}$  on  $\Lambda H_{\mathfrak{t}}^1(\Omega)$ , it holds

$$\begin{aligned} \langle d_{f,h} \varphi_m^{(0)}, \varphi_z^{(1)} \rangle_{L^2} &= \langle d_{f,h} \psi_m^{(0)}, \varphi_z^{(1)} \rangle_{L^2} \\ &= \langle d_{f,h} \psi_m^{(0)}, \psi_z^{(1)} \rangle_{L^2} + \langle d_{f,h} \psi_m^{(0)}, \varphi_z^{(1)} - \psi_z^{(1)} \rangle_{L^2} \\ &= \langle d_{f,h} \psi_m^{(0)}, \psi_z^{(1)} \rangle_{L^2} + \mathcal{O}(e^{-\frac{f(\mathbf{j}(m)) - f(m) - \delta}{h}}) \mathcal{O}(e^{-\frac{c}{h}}). \end{aligned}$$

Then, by choosing the parameter  $\varepsilon > 0$  appearing in the definition of  $\psi_m^{(0)}$  small enough so that  $\delta < \frac{\varepsilon}{3}$ :

$$\langle d_{f,h} \varphi_m^{(0)}, \varphi_z^{(1)} \rangle_{L^2} = \begin{cases} \mathcal{O}(e^{-\frac{f(\mathbf{j}(m)) - f(m) + \frac{\varepsilon}{2}}{h}}) & \text{if } z \notin \mathbf{j}(m) \\ \langle d_{f,h} \psi_m^{(0)}, \psi_z^{(1)} \rangle_{L^2} (1 + \mathcal{O}(e^{-\frac{c}{2h}})) & \text{if } z \in \mathbf{j}(m), \end{cases}$$

where we recall that

$$\langle d_{f,h} \psi_m^{(0)}, \psi_z^{(1)} \rangle_{L^2} = A(m, z) h^{p(z)} e^{-\frac{f(\mathbf{j}(m)) - f(m)}{h}} (1 + \mathcal{O}(h)).$$

Let us conclude this section by showing how, from the previous analysis, we can get results of the type of Theorems 3.2.1 and 3.2.2. To simplify the presentation, we assume that the potential  $f$  is such that:

- the family  $(\psi_m^{(0)})_{m \in \mathcal{U}_\Omega^{(0)}}$  is quasi-orthonormal, and thus so is  $(\varphi_m^{(0)})_{m \in \mathcal{U}_\Omega^{(0)}}$ ,
- for every  $m \neq m'$ , it holds  $\mathbf{j}(m) \cap \mathbf{j}(m') = \emptyset$ .

These hypotheses are not general but nevertheless generic. They are moreover implied by the more restrictive generic hypotheses considered in [HN06]. We also refer to [HHS11, Mic19] in the case without boundary and to [DLLN19b]<sup>10</sup> in the case of Dirichlet type boundary conditions for more involved arguments of this type.

Let  $\mathcal{B}_0$  be an orthonormal basis of  $\text{Ran}(\pi_h^{(0)})$  and  $\mathcal{B}_1$  be an orthonormal basis of  $\text{Ran}(\pi_h^{(1)})$ . We define the matrix<sup>11</sup>

$$M := \text{Mat}_{\mathcal{B}_0, \mathcal{B}_1}(d_{f,h} : \text{Ran}(\pi_h^{(0)}) \rightarrow \text{Ran}(\pi_h^{(1)})).$$

10. See also our more recent work [LN19b] which generalizes the results of [HN06, DLLN19b] to the case where  $f$  admits critical points on  $\partial\Omega$ .

11. The fact that  $d_{f,h}|_{\text{Ran}(\pi_h^{(0)})}$  takes its values in  $\text{Ran}(\pi_h^{(1)})$  follows for example from (1.2.2).

The small eigenvalues of  $\Delta_{f,h}^{D,(0)}$  are hence precisely the squares of the singular values of  $M$ . Let us additionally arbitrarily order the local minima  $m$ 's and the saddle points  $z$ 's and let us define the matrices

$$S = (\langle d_{f,h}\varphi_m^{(0)}, \varphi_z^{(1)} \rangle_{L^2})_{z,m} \quad \text{and} \quad S' = (S'_{zm})_{z,m} \quad \text{where} \quad S'_{zm} = \begin{cases} 0 & \text{if } z \notin \mathbf{j}(m) \\ S_{zm} & \text{if } z \in \mathbf{j}(m) \end{cases}.$$

Let us lastly define the matrices

$$D = \text{Diag} \left( h^{p(m)} e^{-\frac{f(\mathbf{j}(m)) - f(m)}{h}} \right) \quad \text{and} \quad C' = S' D^{-1},$$

where  $p(m) = \min_{z \in \mathbf{j}(m)} p(z)$ .

Since the bases  $(\varphi_m^{(0)})_{m \in \mathcal{U}_\Omega^{(0)}}$  and  $(\varphi_z^{(1)})_{z \in \mathcal{U}_\Omega^{D,(1)}}$  are quasi-orthonormal, it holds

$$\|\text{Mat}_{(\varphi_m^{(0)})_{m \in \mathcal{U}_\Omega^{(0)}}} \mathcal{B}^{(0)}\| = 1 + \mathcal{O}(e^{-\frac{c}{h}}) \quad \text{and} \quad \|\text{Mat}_{(\varphi_z^{(1)})_{z \in \mathcal{U}_\Omega^{D,(1)}}} \mathcal{B}^{(1)}\| = 1 + \mathcal{O}(e^{-\frac{c}{h}})$$

for some  $c > 0$ . According to the Fan inequalities (in their simpler form arising from the Min-Max theorem), the singular values of  $M$  are consequently, up to a multiplicative error term of order  $1 + \mathcal{O}(e^{-\frac{c}{h}})$ , the singular values of the matrix  $S$ , according to the relation

$$M = \left( \text{Mat}_{(\varphi_z^{(1)})_{z \in \mathcal{U}_\Omega^{D,(1)}}} \mathcal{B}^{(1)} \right)^* S \text{Mat}_{(\varphi_m^{(0)})_{m \in \mathcal{U}_\Omega^{(0)}}} \mathcal{B}^{(0)}.$$

In addition, up to choosing  $c > 0$  smaller, it holds

$$S = S' + \left( \mathcal{O}(e^{-\frac{f(\mathbf{j}(m)) - f(m) + c}{h}}) \right)_{z,m} = (C' + \mathcal{O}(e^{-\frac{c}{2h}}))D.$$

Notice here that by definition, the matrix  $C'$  satisfies  $C' = \mathcal{O}(1)$ . Moreover, the hypothesis  $\mathbf{j}(m) \cap \mathbf{j}(m') = \emptyset$  when  $m \neq m'$  easily leads to the relation

$$\exists d > 0, \forall X \in \mathbb{R}^{\mathbf{m}_0}, \quad \|C'X\| \geq d\|X\|.$$

Indeed, for every  $m \in \mathcal{U}_\Omega^{(0)}$ , there exists by definition of  $D$  and of  $C'$  at least one element  $z \in \mathcal{U}_\Omega^{D,(1)}$  such that  $C'_{zm} = A(m, z)(1 + \mathcal{O}(h))$  with  $A(m, z) \neq 0$  and one has, since  $\mathbf{j}(m) \cap \mathbf{j}(m') = \emptyset$  when  $m \neq m'$ ,  $C'_{zm'} = 0$  for every  $m' \neq m$ . It follows that the matrix  $C'$  is injective and admits a left inverse, denoted by  $(C')^{-1}$ , satisfying  $(C')^{-1} = \mathcal{O}(1)$ . Hence, there exists a constant  $c > 0$  such that:

$$S = (C' + \mathcal{O}(e^{-\frac{c}{h}}))D = (I + \mathcal{O}(e^{-\frac{c}{h}}))(C')^{-1}C'D = (I + \mathcal{O}(e^{-\frac{c}{h}}))C'D.$$

Using again the Fan inequalities, we deduce that up to a multiplicative error term of order  $1 + \mathcal{O}(e^{-\frac{c}{h}})$ , the singular values of  $S$  – and hence those of  $M$  – are the singular values of  $C'D$ :

$$\forall k \in \{1, \dots, \mathbf{m}_0\}, \quad \mu_k(M) = \mu_k(S)(1 + \mathcal{O}(e^{-\frac{c}{h}})) = \mu_k(C'D)(1 + \mathcal{O}(e^{-\frac{c}{h}})).$$

It is then straightforward to conclude: the eigenvalues of  $M$  are, up to a multiplicative error term of order  $1 + \mathcal{O}(e^{-\frac{c}{h}})$ , those of the matrix  $D^*C'^*C'D$  which is, since  $\mathbf{j}(m) \cap \mathbf{j}(m') = \emptyset$  when  $m \neq m'$ , the diagonal matrix

$$\begin{aligned} D^*C'^*C'D &= \text{Diag} \left( \sum_{z \in \mathbf{j}(m)} \langle d_{f,h}\varphi_m^{(0)}, \varphi_z^{(1)} \rangle_{L^2}^2, m \in \mathcal{U}_\Omega^{(0)} \right) \\ &= \text{Diag} \left( \sum_{z \in \mathbf{j}(m)} A^2(m, z) h^{2p(z)} e^{-2\frac{f(\mathbf{j}(m)) - f(m)}{h}} (1 + \mathcal{O}(h)), m \in \mathcal{U}_\Omega^{(0)} \right). \end{aligned}$$

In this case, we always have the existence of a full asymptotic expansion of the eigenvalue associated with  $m$ , but this expansion is not in general in  $h$  since  $p : z \mapsto p(z)$  is in general not constant on  $\mathbf{j}(m)$ . More precisely, with the boundary conditions considered here,  $p(z) = \frac{1}{2}$  when  $z \in \Omega$  and  $p(z) = \frac{1}{4}$  when  $z \in \partial\Omega$ , which leads in general to an asymptotic expansion in  $\sqrt{h}$ . This difference arises from different Laplace methods whether  $z \in \Omega$ , in which case  $\nabla f(z) = 0$ , or  $z \in \partial\Omega$ , in which case  $\nabla f|_{\partial\Omega}(z) = 0$  and  $\partial_n f(z) > 0$ .

### 3.3.4 About the case of forms

As in Sections 3.1.4 and 3.2.2, we assume here that  $\Omega$  is a smooth compact and connected  $d$ -dimensional Riemannian manifold without boundary and that  $f$  is a smooth Morse function whose critical points have distinct critical values. We then recall the partition of  $\mathcal{U}_\Omega$  into upper, lower and homological critical points obtained in Section 3.1.4,

$$\mathcal{U}_\Omega = \mathcal{U}_U \cup \mathcal{U}_L \cup \mathcal{U}_H \quad \text{where, for } A \in \{U, L, H\}, \quad \mathcal{U}_A = \cup_{p \in \{0, \dots, d\}} \mathcal{U}_A^{(p)},$$

and the existence of a natural bijective map  $\mathbf{j}_B : \mathcal{U}_L \rightarrow \mathcal{U}_U$  from which we expect *in fine* to obtain the Arrhenius rates of the non zero small eigenvalues of the Witten Laplacian by considering the values  $f(\mathbf{j}_B(z)) - f(z)$ 's, where  $z \in \mathcal{U}_L$ .

We want to adapt the strategy adopted in Sections 3.3.1 to 3.3.3 when  $p = 0$  but using now the mapping  $\mathbf{j}_B : \mathcal{U}_L \rightarrow \mathcal{U}_U$  instead of  $\mathbf{j}$  (which simply becomes  $\mathbf{j}_B|_{\mathcal{U}_L^{(0)}}$  under our current assumptions). To this end, the main remaining difficulty is to define, for any  $p \in \{1, \dots, d\}$  the counterparts of the ‘‘global’’ quasimodes  $\psi_m^{(0)} = \frac{\chi_m e^{-\frac{f}{h}}}{\|\chi_m e^{-\frac{f}{h}}\|_{L^2}}$ 's,  $m \in \mathcal{U}_\Omega^{(0)} \setminus \{m_1\}$ , associated with the  $z \in \mathcal{U}_L^{(p)}$ . When  $p = 0$ , we recall that the latter quasimodes  $\psi_m^{(0)}$ 's enable in particular to only focus on the  $\mathbf{m}_0 - 1$  characteristic wells for  $\Delta_{f,h}^{(0)}$  and on their interactions with the relevant weakly resonant wells (see [HS85b, HS85a] on this topic), associated with the elements of SSP. Moreover, their construction crucially relies on the explicit knowledge of the kernel of  $\Delta_{f,h}^{(0)}$ , namely  $\text{Span}\{e^{-\frac{f}{h}}\}$ .

In the general case of  $p$ -forms, this information is missing and we thus want to adapt the analysis done for  $p = 0$  by constructing, for each  $z \in \mathcal{U}_L$ , a ‘‘global’’, but now non explicit, quasimode  $\psi_z$  as an element of the kernel of some suitable Witten Laplacian. This construction closely relies on the topological construction presented in Section 3.1.4. We are a little more specific below and give the main ideas leading to this construction.

First, the analysis presented in Section 3.1.4 is also valid if for example one considers, instead of the homology of  $\Omega$ , the absolute homology of the manifold with (in general non empty) boundary  $\{f \leq \lambda\}$  for  $\lambda \in \mathbb{R} \setminus f(\mathcal{U}_\Omega)$ . In this case, everything happens as if we were considering  $\Omega$  after having removed the critical points of  $f$  in  $\{f > \lambda\}$ , and we have thus again a partition of the critical points of  $f$  in  $\{f \leq \lambda\}$  into upper, lower, and homological points. More precisely, as it can be guessed from Section 3.1.4, the pairs of lower and upper critical points of  $f$  in  $\{f \leq \lambda\}$  are precisely the pairs  $(z, \mathbf{j}_B(z))$ 's such that  $z \in \mathcal{U}_L$  and both  $z$  and  $\mathbf{j}_B(z)$  belong to  $\{f \leq \lambda\}$ . We recall in passing that the corresponding Witten Laplacian

in this case is the Witten Laplacian  $\Delta_{f,h,\lambda}^N$  with Neumann boundary type conditions on  $\{f = \lambda\}$ .

Moreover, when  $z$  is a homological critical point in the manifold  $\{f \leq \lambda\}$  for some  $\lambda \in \mathbb{R} \setminus f(\mathcal{U}_\Omega)$ , the analysis led in [LNV13] permits to construct a unitary “global” quasimode  $\tilde{\psi}_z$  concentrated near  $z$  and belonging to  $\text{Ker } \Delta_{f,h,\lambda}^N$ . One has moreover Agmon type decay estimates on  $\tilde{\psi}_z$  as well as some very precise WKB approximation near  $z$ , whose first term is explicit along the stable and unstable manifolds of  $z$  for the flow of  $-\nabla f$ . This construction relies on semiclassical arguments adapted from [HS85b, HS85c] together with the Hodge decomposition of  $\Delta_{f,h,\lambda}^N$  (see Theorem 1.2.2) and the properties of the lower, upper, and homological critical points of  $f$ .

Then, when  $z$  belongs to  $\mathcal{U}_L$ , we consider, for  $\varepsilon > 0$  small but fixed, the manifold with boundary  $\{f \leq \lambda\}$ , where  $\lambda = f(\mathbf{j}_B(z)) - \varepsilon$ . In this manifold,  $z$  becomes a homological critical point. Hence, we can define  $\tilde{\psi}_z \in \text{Ker } \Delta_{f,h,\lambda}^N$  as above and

$$\psi_z := \chi_z \tilde{\psi}_z \in D(\Delta_{f,h}),$$

where the cut-off function  $\chi_z$  satisfies  $\text{supp } \chi_z \subset \{f < f(\mathbf{j}_B(z)) - \varepsilon\}$  and  $\chi_z = 1$  in  $\{f < f(\mathbf{j}_B(z)) - 2\varepsilon\}$ .

By a similar analysis as done in Section 3.3.3 in the case  $p = 0$ , the crucial point then becomes the accurate computation of the terms

$$\langle d_{f,h}\psi_z, \psi_{\mathbf{j}_B(z)} \rangle_{L^2} = h \langle (d\chi_z) \tilde{\psi}_z, \psi_{\mathbf{j}_B(z)} \rangle_{L^2},$$

where  $z \in \mathcal{U}_L$  and  $\psi_{\mathbf{j}_B(z)}$  is a suitable local quasimode associated with  $\mathbf{j}_B(z) \in \mathcal{U}_U$ . But, contrary to the analysis performed when  $p = 0$ ,  $\tilde{\psi}_z$  is not explicit and thus, we do not know how it behaves near  $d\chi_z$ , but only how it behaves near  $z$ . An answer to this problem is given by a side result of the homological analysis briefly explained in Section 3.1.4 (see more precisely [LNV13, Proposition 2.12]) which permits, by a subtle repeated use of Stokes’ theorem, to reduce the computation of the part of the quantity  $\langle (d\chi_z) \tilde{\psi}_z, \psi_{\mathbf{j}_B(z)} \rangle_{L^2}$  arising from  $(d\chi_z) \tilde{\psi}_z$  to a computation in a neighborhood of  $z$ , where  $\tilde{\psi}_z$  is explicitly known. To be a little more specific, this side result says that, for every  $a > 0$  small enough and some  $\kappa \in \mathbb{Q}^*$ , the boundary of the unstable manifold of  $\mathbf{j}_B(z)$  (for the flow of  $-\nabla f$ ) relatively to  $\{f < f(\mathbf{j}_B(z)) - a\}$  is homologous, for the homology of  $\{f < f(\mathbf{j}_B(z)) - a\}$  relatively to  $\{f < f(z) - a\}$ , to  $\kappa$  times the unstable manifold of  $z$  relatively to  $\{f < f(z) - a\}$ . The homological constants  $\kappa_z = \kappa_{\mathbf{j}_B(z)}$  involved in Theorem 3.2.3 are then precisely given by  $\kappa^2$ .

## 3.4 Study of a double-well potential in large dimension

We present in this section the main results of [DL17].

### 3.4.1 Description of the model and results

The work [DL17] concerns the rate of convergence to equilibrium at low temperature of a stochastic interacting particle system, which may be described as follows.

There are  $N$  particles, at each time  $t \geq 0$  the state of the  $k$ -th particle is a real random number  $\xi_k(t)$ , and the trajectory  $\xi_k = (\xi_k(t))_{t \geq 0}$  satisfies for some fixed  $\mu > 1$  the overdamped Langevin equation (see (1.3.1) in Section 1.3)

$$d\xi_k = \left[ \mu \frac{\xi_{k+1} + \xi_{k-1} - 2\xi_k}{4 \sin^2 \frac{\pi}{N}} + \xi_k - \xi_k^3 \right] dt + \sqrt{2hN} dB_k . \quad (3.4.1)$$

Here  $B_1 = (B_1(t))_{t \geq 0}, \dots, B_N = (B_N(t))_{t \geq 0}$  are  $N$  independent standard Brownian motions,  $h$  is a positive constant, and  $\xi_{N+1} := \xi_1$ , i.e. periodic boundary conditions are assumed. When  $h > 0$  is kept fixed and  $N$  is large, the system (3.4.1) can be seen as a discrete space approximation of the stochastically perturbed Allen-Cahn equation on the interval  $(0, \frac{2\pi}{\sqrt{\mu}})$ :

$$du(x, t) = \left[ \partial_x^2 u(x, t) + u(x, t) - u^3(x, t) \right] dt + \sqrt{2\tilde{h}} dB(x, t) , \quad (3.4.2)$$

where now  $(x, t) \in (0, \frac{2\pi}{\sqrt{\mu}}) \times (0, \infty)$ , the boundary condition  $u(0, t) = u(\frac{2\pi}{\sqrt{\mu}}, t)$  has to be satisfied for every  $t \geq 0$ ,  $\tilde{h} = \frac{2\pi}{\sqrt{\mu}}h$ , and  $dB$  is a space-time white noise. Thus, for large  $N$ , one might think of  $\xi_k(t) \sim u(\frac{k}{N} \frac{2\pi}{\sqrt{\mu}}, t)$ , and of the chain  $\xi(t) = (\xi_1(t), \dots, \xi_N(t))$  as giving the position at time  $t$  of an elastic ring of length  $\frac{2\pi}{\sqrt{\mu}}$  moving in a highly viscous, noisy environment and subject to a simple bistable external force.

Equation (3.4.2) is a basic and widely studied stochastic partial differential equation, see e.g. [FJ82, Fun83, BDP95, GM01, KORV07, Hai09, BG13, OWW14, DZ14, Bar15] and references therein. For a more general background on the particle system (3.4.1) we refer to [BFG07a, BFG07b]. See also [BBM10] for aspects closely related to our work [DL17]. The convergence of (3.4.1) to (3.4.2) for  $N \rightarrow +\infty$  is discussed in [Bar15].

### Relaxation properties: heuristics and previous results

For each fixed  $h > 0$  and number of particles  $N$ , we recall from Sections 1.3.1 and 1.3.2 in the introductory chapter that the long time behaviour of (3.4.1) is described by its unique equilibrium distribution, explicitly given by the probability measure on  $\mathbb{R}^N$  (see (1.3.5) and (1.3.16))

$$m_{h,N}(d\mu) = m_{V,hN}(d\mu) := \frac{e^{-\frac{V}{hN}} d\mu}{\int_{\mathbb{R}^N} e^{-\frac{V}{hN}} d\mu} ,$$

where the energy function  $V : \mathbb{R}^N \rightarrow \mathbb{R}$  is defined as

$$V(x) = V_N(x) := \sum_{k=1}^N \left( \frac{1}{4} x_k^4 - \frac{1}{2} x_k^2 \right) + \mu \sum_{k=1}^N \frac{(x_k - x_{k+1})^2}{8 \sin^2(\frac{\pi}{N})} + \frac{N}{4} , \quad (3.4.3)$$

with  $x_{N+1} := x_1$ . This indeed follows from the observation that the drift term in (3.4.1) is  $-\nabla V(\xi)$ . Similarly, for any fixed  $h > 0$ , there exists a unique equilibrium distribution  $m_{h,\infty}$  for the infinite-dimensional system (3.4.2), see [DZ14, RV05]. One might say that at equilibrium, no “phase transition” occurs in the thermodynamic

limit  $N \rightarrow +\infty$ . On the contrary, since for each  $N$ , the energy  $V$  admits two local minima given by

$$I_{\pm} = I_{\pm}(N) := \pm \underbrace{(1, \dots, 1)}_{N \text{ entries}},$$

the deterministic dynamics  $d\xi = -\nabla V(\xi)dt$ , obtained from (3.4.1) by setting  $h = 0$ , admits two stable equilibrium points. Thus, when  $h$  is positive but small, the typical picture of a so-called metastable dynamics emerges (see Section 1.3.2 and the related [BBM10]): the system quickly reaches a local equilibrium in the basin of attraction of  $I_+$  or  $I_-$ , depending on its initial condition; this local equilibrium endures for a long time, since, in order to be able to explore the whole state space and distribute according to the global equilibrium  $m_{h,N}$ , the system has to wait for a sufficiently large stochastic fluctuation allowing to overcome the energetic barrier separating  $I_+$  and  $I_-$ . The critical time scale at which such transitions between minima typically occur is exponentially large in the parameter  $h$ . Thus, for  $h \rightarrow 0^+$ , one observes a significant slowdown in the relaxation towards  $m_{h,N}$ , see Section 1.3.2 for more details.

The aim of our work [DL17] is to quantify the mentioned slowdown in the approach to equilibrium of (3.4.1) when at the same time  $h$  is small and  $N$  is large. More specifically, we study there for  $h \rightarrow 0^+$  and  $N \rightarrow +\infty$  the behaviour of the Poincaré constant  $\lambda(h, N)$  and of the logarithmic Sobolev constant  $\rho(h, N)$  of (3.4.1), that is the largest constants satisfying respectively, for every  $\varphi \in H^1(\mathbb{R}^N, m_{h,N})$ , the weighted Poincaré inequality (see (1.3.10) and the discussion below)

$$\lambda(h, N) \text{Var}_{m_{h,N}}(\varphi) \leq hN \int |\nabla \varphi|^2 dm_{h,N}, \quad (3.4.4)$$

and the Gross inequality (or logarithmic Sobolev inequality)

$$\rho(h, N) \text{Ent}_{m_{h,N}}(\varphi^2) \leq 2hN \int |\nabla \varphi|^2 dm_{h,N}. \quad (3.4.5)$$

Here,  $\text{Var}_{m_{h,N}}$  and  $\text{Ent}_{m_{h,N}}$  denote the variance and entropy with respect to  $m_{h,N}$ , i.e.  $\text{Var}_{m_{h,N}}(\varphi) := \int \varphi^2 dm_{h,N} - (\int \varphi dm_{h,N})^2$  and, for  $\varphi \geq 0$ ,  $\text{Ent}_{m_{h,N}}(\varphi) := \int \varphi \log \varphi dm_{h,N} - \int \varphi dm_{h,N} \log (\int \varphi dm_{h,N})$ .

As highlighted in Section 1.3.1, the Poincaré constant gives the exponential rate of convergence to equilibrium in variance (see indeed (1.3.12)), and the logarithmic Sobolev constant gives similarly the exponential rate of convergence to equilibrium in entropy. We refer e.g. to Theorems 4.2.5 and 5.2.1 in [BGL14], which also gives a general overview of the interplay between functional inequalities and Markov processes. We stress that, from the point of view of spin systems in statistical mechanics, we are dealing here with the problem of relaxation to equilibrium in a case of continuous unbounded single-spin state space and nonconvex energy function (see e.g. [Led01, Zeg96, BH99, BH00] in this context). Concerning exponential convergence of stochastic equations in infinite dimensions with fixed noise parameter  $h$  we point e.g. to [GM01, Hai02, Hai09, DZ14].

If  $N$  is kept fixed, we recall from Section 1.3.2 and from the beginning of Chapter 3 above that the leading asymptotic behaviour of  $\lambda(h, N)$  in the limit  $h \rightarrow 0^+$

is given by an Eyring-Kramers type formula (see [BGK05, HKN04, Mic19], treating generic multiwell-diffusions in the small noise regime, and also [HHS11, MS14, Mic15, LM19]). More specifically, it follows for example from [HKN04] and some straightforward adaptations of their arguments, that

$$\lambda(h, N) = \frac{1}{\pi} \left| \frac{\det \text{Hess } V(I_-)}{\det \text{Hess } V(0)} \right|^{\frac{1}{2}} e^{-\frac{1}{4h}} (1 + \epsilon(h, N)), \quad (3.4.6)$$

where the error  $\epsilon(h, N)$  satisfies, for  $h > 0$  sufficiently small,  $|\epsilon(h, N)| \leq C_N h$ . Here  $C_N$  is some positive constant which may a priori explode in  $N$ . On the other hand, as was already observed in [Ste04], the prefactor in (3.4.6) is convergent in the limit  $N \rightarrow +\infty$ :

$$p(N) := \frac{1}{\pi} \left| \frac{\det \text{Hess } V(I_-)}{\det \text{Hess } V(0)} \right|^{\frac{1}{2}} \xrightarrow{N \rightarrow +\infty} \frac{\sinh(\pi \sqrt{2\mu^{-1}})}{\pi \sin(\pi \sqrt{\mu^{-1}})}. \quad (3.4.7)$$

Similarly, regarding the log-Sobolev constant  $\rho(h, N)$ , it follows again from general results (see [MS14]) that for fixed  $N$ , the leading term of  $\rho(h, N)$  is again given by  $p(N)e^{-\frac{1}{4h}}$ . We stress that also here, as for the error in (3.4.6), there is no control in  $N$  on the error term. Thus, no rigorous conclusion in the limit  $N \rightarrow +\infty$  can be directly inferred from these results.

On the other hand, rather strong results have been obtained in the analysis of the mean time needed for the system (3.4.1) to go from  $I_+$  to  $I_-$ : indeed, it has been shown that an Eyring-Kramers type formula holds for this transition time, with an error which is uniform in  $N$  (see in particular [BBM10] and [Bar15, BG13], which extend the results to the infinite-dimensional system (3.4.2) and even to more general situations). Nevertheless, while the asymptotic relation between stochastically defined mean transition times and analytic objects as  $\lambda(h, N)$  is well-established in very general situations for fixed  $N$  (see again [BGK05]), to the best of our knowledge there are no rigorous results on how it might behave in the regime of large  $N$ , even in the specific model we are considering in [DL17]. In this paper, we do not rely on the mentioned results on mean transition times and rather use purely analytical arguments, partly inspired by the arguments presented in the beginning of this chapter.

### Statement of the main results of [DL17]

The first main result of [DL17] below shows that the Eyring-Kramers formula (3.4.6) provides an upper bound on  $\lambda(h, N)$  with an error term which can indeed be uniformly controlled in the system size  $N$ . Moreover it provides a quantitative lower bound at logarithmic scale on  $\rho(h, N)$  which is independent of  $N$ . In particular it ensures that  $\rho(h, N)$  and  $\lambda(h, N)$  do not degenerate for any fixed  $h$ . One might say that no “dynamical phase transition” occurs in the thermodynamic limit  $N \rightarrow +\infty$  (see also [GM01]).

**Theorem 3.4.1.** *For every  $\delta > 0$  there exists a constant  $C_\delta > 0$  such that for every  $h > 0$  and every  $N \in \mathbb{N}$ ,*

$$C_\delta e^{-\frac{3+2\sqrt{2+\delta}}{24h}} e^{-\frac{1}{4h}} \leq \rho(h, N) \leq \lambda(h, N) \leq p(N) e^{-\frac{1}{4h}} (1 + \epsilon(h, N)),$$



where the prefactor  $p(N)$  is given by (3.4.7) and the error term  $\epsilon(h, N)$  satisfies

$$\exists C > 0 \text{ s.t. } \forall h \in (0, 1], \forall N \in \mathbb{N}, \quad |\epsilon(h, N)| \leq C h .$$

The exponential decay in  $h$  given by the lower bound in Theorem 3.4.1 appears to be rather rough, but unfortunately, when insisting to get bounds with uniform control in  $N$ , it is for the moment not clear how one could obtain a substantial improvement, even when focusing only on  $\lambda(h, N)$ . For the latter, one can exploit the spectral theory of self-adjoint operators: we recall from Section 1.3 that the generator of the Markovian semigroup giving the evolution of (3.4.1) is indeed the differential operator (see (1.3.15))

$$L_h = L_{V, hN}^{(0)} := -hN\Delta + \nabla V \cdot \nabla$$

and  $hL_h$  is here unitarily equivalent to the Witten Laplacian, acting in the flat space  $L^2(\mathbb{R}^N, d\mu)$  (see (1.3.17)),

$$\Delta_{f, h}^{(0)} := -h^2\Delta + |\nabla f|^2 - h\Delta f, \quad \text{where } f(x) := \frac{V(\sqrt{N}x)}{2N} .$$

We recall moreover from Sections 1.2.2 and 1.3.1 that the closure in  $L^2(m_{h, N})$  of  $L_h$  acting on  $\mathcal{C}_c^\infty(\mathbb{R}^N)$ , which we still denote by  $L_h$ , is self-adjoint and nonnegative, admits 0 as simple eigenvalue, and has purely discrete spectrum for each  $h, N$  fixed (it has indeed a compact resolvent). In addition, its spectral gap, defined as its first nonzero eigenvalue, coincides with  $\lambda(h, N)$  (see indeed (1.3.10) and (1.3.11)).

According to the second main result of [DL17] below, the problem of obtaining the Eyring-Kramers formula as lower bound for  $\lambda(h, N)$  can then be reduced to the problem of proving a suitable separation between  $\lambda(h, N)$  and the next eigenvalue of  $L_h$ . More precisely, the existence of a uniform lower bound on the “second spectral gap” in a certain regime in which  $N$  possibly grows to infinity, turns out to be sufficient for the validity of the Eyring-Kramers formula in the same regime:

**Theorem 3.4.2.** *Assume there exist constants  $h_0, \delta > 0$  and, for each  $h \in (0, h_0]$ , a set  $\mathcal{N}(h) \subset \mathbb{N}$  such that*

$$\forall h \in (0, h_0], \forall N \in \mathcal{N}(h), \quad \text{Sp}(L_h) \cap ]\lambda(h, N), \lambda(h, N) + \delta[ = \emptyset . \quad (3.4.8)$$

Then,

$$\lambda(h, N) = p(N) e^{-\frac{1}{4h}} (1 + \epsilon(h, N)),$$

where the prefactor  $p(N)$  is given by (3.4.7) and the error term  $\epsilon(h, N)$  satisfies

$$\exists C > 0 \text{ s.t. } \forall h \in (0, h_0], \forall N \in \mathcal{N}(h), \quad |\epsilon(h, N)| \leq C h .$$

Note here that when  $N$  is kept fixed, i.e. when the set  $\mathcal{N}(h)$  above does not depend on  $h$ , the hypothesis (3.4.8) – and then the statement of Theorem 3.4.2 – is a straightforward consequence of (1.3.19) and (1.3.20) in Section 1.3.2. However, nothing is said about a control of the second spectral gap with respect to  $N$  there, nor in the beginning of Chapter 3 above and in the references therein.

The last main theorem of [DL17] implies that there exist regimes with unbounded  $N$  under which the Eyring-Kramers formula (3.4.6) holds with bounded error  $\epsilon(h, N)$ . Indeed, in order to be in the situation of Theorem 3.4.2, it is enough that  $N$  grows slower than  $h^{-\frac{3}{4}}$ :

**Theorem 3.4.3.** *Let  $C > 0$  and  $\alpha \in (0, \frac{3}{4})$ . Then, there exist constants  $h_0, \delta > 0$  such that the condition (3.4.8) in Theorem 3.4.2 is fulfilled with*

$$\mathcal{N}(h) = \{ N \in \mathbb{N} : N \leq Ch^{-\alpha} \}.$$

### 3.4.2 Comments on the techniques used in this study

Though inspired by the supersymmetric approach of [HKN04], in the article [DL17] we do not make explicit use of  $\Delta_{f,h}^{(1)}$  as in the first part of Chapter 3 above. Indeed, a careful analysis of the energy  $V$  permits to construct a very efficient global quasimode passing through the bottleneck and connecting the two minima of  $V$ . This construction of an “almost optimal” quasimode, together with a precise analysis of Laplace integrals in large dimension, enables us to give the upper bound of Theorem 3.4.1.

We emphasize in particular here that semiclassical techniques as WKB expansions, Agmon estimates and harmonic approximation for Schrödinger operators, used e.g. in [HKN04], are generally not uniformly controlled in the limit  $N \rightarrow +\infty$  (see however [BM03, MM05] for previous works dealing with Witten Laplacians in large dimension and also [Sjö93a, Sjö93b, Hel95, Hel02] and references therein). Also for the specific model we consider here, the arguments of [HKN04] do not carry over with uniform bounds in  $N$ .

For the lower bound in Theorem 3.4.1, we depart from the semiclassical approach and rather exploit perturbation techniques for fixed  $h$ . These permit, even though for general  $\mu > 1$  the function  $V$  is not convex outside a compact set, to reduce to the case of a convex energy and then to apply the well-known Bakry-Émery criterion (see [BE85, BGL14]). We use here that the interaction part in the energy  $V$  is strong enough to ensure good relaxation properties for large  $N$ . Thus, roughly speaking, we regard the energy coming from the single particle double-well potential as a perturbation of the interaction part. This is opposed to the perturbative regime considered in previous works as [BH99, BH00]: in these references, the interaction constant  $\mu$  is tuned in a way that it is rather the interaction part to become a perturbation of the single particle potential.

The relevant quantity naturally appearing in the estimates leading to Theorem 3.4.2 is the quotient of quadratic forms defined, for any  $\varphi$  in the domain of  $L_h$ , by

$$\mathcal{E}(\varphi) := \frac{\int_{\mathbb{R}^N} |L_h \varphi|^2 dm_{h,N}}{hN \int_{\mathbb{R}^N} |\nabla \varphi|^2 dm_{h,N}}.$$

To connect with the introductory chapter of this dissertation, this quantity can be equivalently rewritten in the two forms

$$\mathcal{E}(\varphi) = \frac{\int_{\mathbb{R}^N} \Gamma_2(\varphi) dm_{h,N}}{\int_{\mathbb{R}^d} \Gamma(\varphi) dm_{h,N}} = \frac{\int_{\mathbb{R}^N} (L_h^{(1)} \nabla \varphi) \cdot \nabla \varphi dm_{h,N}}{\int_{\mathbb{R}^N} |\nabla \varphi|^2 dm_{h,N}}, \quad (3.4.9)$$

where  $\Gamma$  and  $\Gamma_2$  are respectively the carré du champ operator and its iteration (see (1.3.8) and (1.3.9) in Section 1.3.1 or for example [BGL14] for more details about this notion) and  $L_h^{(1)} := L_h \otimes \text{Id} + \text{Hess } V$  (see (1.3.7) and (1.3.14)).

We recall that the last expression in (3.4.9) can be generalized by allowing, instead of  $\nabla \varphi$ , more general non-gradient vector fields, which is one of the main

advantages of the supersymmetric approach and is crucially exploited in works as [HKN04, HN06, Lep10, HHS11, Dig13, BHM15, LN15, DLLN17b, Mic19, DLLN19b, LN19a]. In [DL17], we do not use this additional freedom and only work with the gradient of the “almost optimal” quasimode already exploited in the proof of Theorem 3.4.1. An important advantage of not explicitly using  $L_h^{(1)}$  (or equivalently  $\Delta_{f,h}^{(1)}$ ) there is to avoid the need of a relation similar to (3.4.8) for the first spectral gap of  $L_h^{(1)}$ . Indeed, we have only been able to prove such a relation for sets  $\mathcal{N}(h)$  where  $N$  grows slower than in the sets exhibited in Theorem 3.4.3. The proof of the latter result combines standard localization techniques for the analysis of semiclassical Schrödinger operators [CFKS87] and a two-scale analysis naturally adapted to the structure of the energy  $V$ .

## 3.5 Some perspectives

The preceding analysis has many possible interesting developments. We just mention below the ones we are now the most interested in.

### 3.5.1 Potentials with critical points on the boundary

We recall that in the case of a compact Riemannian manifold  $\Omega$  with a non-empty boundary  $\partial\Omega$ , the analysis of the low spectrum of the Witten Laplacian presented above was always made under the assumption that  $\nabla f \neq 0$  along  $\partial\Omega$  (see Theorem 1.2.5 in Section 1.2.3, Section 3.1.3 and Theorem 3.2.2 in Section 3.2.1). We stress moreover here that the general results relying on the large deviation theory mentioned in the introductory chapter (see more precisely Section 1.3.3) do not consider the case of critical points on the boundary.

Though this hypothesis is generic, the numerical methods relying on the fact that the exit event from a metastable state  $\Omega$  for the overdamped Langevin dynamics is well approximated by a Markov jump process whose transitions rates follow the Eyring-Kramers law (see Definition 1.3.6 in Section 1.3.3) assume in practice that  $\Omega$  is the basin of attraction of some local minimum of the potential function  $f$  for the dynamics  $\dot{x} = -\nabla f(x)$  (see (1.3.38) and the discussion around in Section 1.3.3, and Section 5.1). In this case, the boundary  $\partial\Omega$  thus contains critical points of  $f$ , and in particular saddle points.

With the aim of proving the asymptotic validity of the Eyring-Kramers law in this context (see Section 1.3.3 and Chapter 5), we then first need to generalize, in the Dirichlet setting, Theorem 1.2.5 and (at least a one-well version of) Theorem 3.2.2 when the potential  $f$  admits critical points on the boundary. Similar generalizations in the Neumann setting would also be interesting.

We expect that such generalizations, with the techniques presented in Sections 3.1 to 3.3 of this chapter, only hold for boundaries  $\partial\Omega$  satisfying suitable compatibility conditions around the critical points of  $f$  belonging to  $\partial\Omega$ . Concerning for example a generalization of Theorem 3.2.2 with these techniques when  $f$  admits saddle points on the boundary, we only expect to be able to show the existence of the prefactors of the small eigenvalues of  $\Delta_{f,h}^{D,(0)}$  when  $\partial\Omega$  is tangent, at any relevant saddle point  $z$ , to the stable manifold of  $z$  for the dynamics  $\dot{x} = -\nabla f(x)$ . Note in this respect that such an hypothesis is always satisfied when  $\Omega$  is the basin of attraction of some

local minimum (or of some family of local minima) of  $f$  for the flow of  $\dot{x} = -\nabla f(x)$ . Indeed,  $\partial\Omega$  coincides in this case, around each saddle point  $z$  of  $f$ , with the stable manifold of  $z$  for the dynamics  $\dot{x} = -\nabla f(x)$  (and is hence smooth near  $z$ ).

Nevertheless, even in the latter case, the presence of critical points on the boundary leads to substantial technical difficulties. For example, the “natural” WKB approximations of the quasimodes for 1-forms associated with the saddle points on the boundary (see Section 3.3.2 above in the case of generalized saddle points) do not satisfy in general the minimal boundary conditions required. This follows from the curvature of the boundary near these saddle points.

However, from our recent work [LN19b] with Boris Nectoux, working with “almost optimal” quasimodes, as mentioned in Section 3.4 about our work [DL17], permits to generalize Theorem 3.2.2 in this case without explicitly using  $\Delta_{f,h}^{D,(1)}$  (though our method does not give the existence of an asymptotic expansion of the error terms, see the last part of Theorem 3.2.2). This thus establishes the first step in the justification of the asymptotic validity of the Eyring-Kramers law in this context.

### 3.5.2 Non reversible overdamped Langevin dynamics

Another interesting continuation of the works presented in this chapter would be to generalize the precise computation of the small eigenvalues of the Witten Laplacian  $\Delta_{f,h}^{D,(0)}$ , or equivalently of the weighted Laplacian  $L_{V,h}^{D,(0)}$  where  $V = 2f$  (see (1.3.17)), to some non reversible (i.e. non-gradient) dynamics

$$dX_t = b(X_t)dt + \sqrt{2h} dB_t. \quad (3.5.1)$$

Let us recall here that  $L_{V,h}^{(0)} = -h\Delta + \nabla V \cdot \nabla$  while the infinitesimal generator of the above dynamics is given by  $L_{b,h} = -h\Delta - b \cdot \nabla$ .

Assume for example that the dynamics (3.5.1) is obtained from the reversible overdamped Langevin dynamics associated with the potential  $V : \mathbb{R}^d \rightarrow \mathbb{R}$  by adding the orthogonal vector field  $J(\nabla V)$ , where  $J$  is a constant skew-symmetric matrix of size  $d$ , i.e. that the vector field  $b$  has the form

$$b = -\nabla V - J(\nabla V).$$

In this case,  $L_{b,h}$  writes  $L_{b,h} = L_{V,h}^{(0)} + J(\nabla V) \cdot \nabla$  and, assuming that  $e^{-\frac{V}{h}} \in L^1(\mathbb{R}^d)$ , the probability measure

$$m_{V,h}(d\mu) = \left( \int_{\Omega} e^{-\frac{V}{h}} d\mu \right)^{-1} e^{-\frac{V}{h}} d\mu$$

is still an invariant measure for the process (3.5.1), i.e. it holds

$$L_{b,h}^\dagger e^{-\frac{V}{h}} = L_{V,h}^{\dagger,(0)} e^{-\frac{V}{h}} - \operatorname{div}(J(\nabla V) e^{-\frac{V}{h}}) = -\operatorname{div}(J(\nabla V) e^{-\frac{V}{h}}) = 0.$$

Note moreover that the term  $J(\nabla V) \cdot \nabla$  of  $L_{b,h}$  acting on  $\mathcal{C}_c^\infty(\mathbb{R}^d)$  is skew-symmetric in  $L^2(\Omega, m_{V,h})$ .

In this setting (and actually in a slightly more general one), we have recently proven, in the work [LM19] in collaboration with Laurent Michel, Eyring-Kramers

type formulas for the small eigenvalues of  $L_{b,h}$  when  $\partial\Omega = \emptyset$  and  $V$  is a multi-well Morse potential. This operator can be compared in some sense to  $L_{V,h}^{(0)}$  but is no more self-adjoint. Analyzing its low spectrum then requires in particular to adapt the arguments relying on the self-adjointness of  $L_{V,h}^{(0)}$ , such as the Max-Min principle, by proving suitable resolvent estimates for  $L_{b,h}$  (using some Grushin problems). The use of “almost optimal” quasimodes as mentioned in Sections 3.4 and 3.5.1 is moreover again a powerful tool to obtain the prefactors in this context.

Let us also mention that, up to our knowledge, this is the first result in this context in the literature. However, a generalization of [BEGK04] has recently been obtained in this setting in [LMS19] for a double-well potential  $V$  (see also [BR16] for a non rigorous proof). In particular, the results of [LM19] together with those of [LMS19] also provide, in the case of a double-well potential  $V$ , a connection between the first non zero eigenvalue of  $L_{b,h}$  and the mean exit time to go from one local minimum of  $V$  to the other one, precisely computed in [LMS19]. See in this spirit (1.3.21) and (1.3.22) (and [BGK05]) in the reversible setting.

We then plan to study the case  $\partial\Omega \neq \emptyset$  and then to look at more general vector fields  $b$ . In the case  $\partial\Omega \neq \emptyset$ , we expect, as in the reversible case, being only able to prove sharp asymptotic formulas when the boundary satisfies suitable “natural” compatibility conditions (see Section 3.5.1 above).

### 3.5.3 The case of non Morse potentials

Coming back to the self-adjoint case but concerning general  $p$ -forms, we plan, in future works in collaboration with Francis Nier and Claude Viterbo, to obtain a precise description, in terms of Arrhenius rates, of the low spectrum of the Witten Laplacian  $\Delta_{f,h}$  acting on forms when  $f$  is a rather general (non Morse) smooth function.

Our first objective is to consider the case of smooth functions with a finite number of critical values. Note that in this case, the number of critical points of  $f$  does not need to be finite or even countable. Nevertheless, the persistent diagram of  $f$  still consists in a finite number of barcodes (see Section 3.1.4 about this notion and the survey on persistent homology [EH08]).

In this context, we aim at proving that the Arrhenius rates of the exponentially small eigenvalues of the Witten Laplacian are still given by the lengths of the barcodes of the persistent diagram of  $f$ , where the number of infinite lengths of order  $p$  correspond to the  $p$ -th Betti number of the manifold.

A nice corollary would then be the stability of the Arrhenius rates of the exponentially small eigenvalues of  $\Delta_{f,h}$  with respect to small perturbations of  $f$  by admissible functions (that is, here, smooth functions with a finite number of critical values) for the  $\mathcal{C}^0$ -topology. Indeed, an important property of persistent homology is its stability under perturbations. More precisely, the so-called bottleneck distance between two persistent diagrams is bounded from above by the sup distance between the corresponding functions (see for example [EH08, Theorem 6.1]).

Notice moreover that in this setting, the critical points of  $f$  can be arbitrarily highly degenerate. One can hence not hope getting better in general than the Arrhenius rates of the exponentially small eigenvalues of  $\Delta_{f,h}$ .

However, the methods we plan to use for this analysis should lead to explicit formulas for these small eigenvalues in terms of interactions between suitable quasi-modes. It would then be interesting, in a second time, to see how they apply to specific situations.



# Chapter 4

## Exit from a metastable state: concentration of the first exit point distribution on the low energy saddle points

We present in this chapter the main results of [DLLN19a] and also briefly discuss the results of [LN19a]. We recall that the preprint [DLLN19a] has been divided into two parts for publication. The first part, [DLLN19b], focuses on the case where the initial condition is distributed according to the quasi-stationary distribution, while the second part deals with deterministic initial conditions. We also refer to the proceedings type work [LLN18] in this connection.

### 4.1 The case of a confining well

Let us consider a smooth open and connected set  $\Omega \subset \mathbb{R}^d$  and the associated exit event from  $\Omega$  for the overdamped Langevin dynamics<sup>1</sup>

$$dX_t = -\nabla f(X_t)dt + \sqrt{h} dB_t. \quad (4.1.1)$$

More precisely, let us introduce

$$\tau_\Omega := \inf\{t \geq 0 | X_t \notin \Omega\} \quad (4.1.2)$$

the first exit time from  $\Omega$ . The concentration of the law of first exit point  $X_{\tau_\Omega}$  on a subset of  $\partial\Omega$  is defined as follows.

**Definition 4.1.1.** *Let  $\mathcal{Y} \subset \partial\Omega$ . The law of  $X_{\tau_\Omega}$  concentrates on  $\mathcal{Y}$  in the limit  $h \rightarrow 0^+$  if for every neighborhood  $\mathcal{V}_\mathcal{Y}$  of  $\mathcal{Y}$  in  $\partial\Omega$ ,*

$$\lim_{h \rightarrow 0^+} \mathbb{P}[X_{\tau_\Omega} \in \mathcal{V}_\mathcal{Y}] = 1,$$

*and if for all  $x \in \mathcal{Y}$  and for all neighborhood  $\mathcal{V}_x$  of  $x$  in  $\partial\Omega$ ,*

$$\lim_{h \rightarrow 0^+} \mathbb{P}[X_{\tau_\Omega} \in \mathcal{V}_x] > 0.$$

*In other words,  $\mathcal{Y}$  is the support of the law of  $X_{\tau_\Omega}$  in the limit  $h \rightarrow 0^+$ .*

---

1. Note that the scaling in  $h$  considered here, which is the one considered in [DLLN19a], is different from the one considered in (1.3.1) in Section 1.3.



Let us moreover assume here that  $f : \bar{\Omega} \rightarrow \mathbb{R}$  is smooth and satisfies

$$\partial_n f > 0 \text{ on } \partial\Omega, \quad (4.1.3)$$

where  $\partial_n f$  is the outward normal derivative of  $f$  on  $\partial\Omega$ , and

$$\{x \in \Omega, |\nabla f(x)| = 0\} = \{x_0\} \text{ with } f(x_0) = \min_{\bar{\Omega}} f \text{ and } \det \text{Hess } f(x_0) > 0. \quad (4.1.4)$$

Note in passing that, under the assumption (4.1.3), the assumption (4.1.4) is equivalent to say that  $f$  admits one unique critical point  $x_0$  in  $\Omega$  ( $f$  then admits necessarily its global minimum on  $\bar{\Omega}$  at  $x_0$ ) and that  $x_0$  is non degenerate.

In this setting, using large deviation theory, when in addition  $f$  attains its minimum on  $\partial\Omega$  at one single point  $y_0$ , it is proved in [FW12, Theorem 2.1 in Chapter 4], which also covers the case of non reversible diffusions, that the law of  $X_{\tau_\Omega}$  in the limit  $h \rightarrow 0^+$  concentrates on  $y_0$  when  $X_0 = x \in \Omega$ . In [FW12, Theorem 5.1 in Chapter 6] (also covering the case of non reversible diffusions), under more general assumptions on  $f$ , for  $\Sigma \subset \partial\Omega$ , the limit of  $h \ln \mathbb{P}[X_{\tau_\Omega} \in \Sigma]$  when  $h \rightarrow 0^+$  is related to a minimization problem involving the quasipotential of the process (4.1.1) (see more precisely (1.3.30) in Section 1.3.3).

Let us mention two limitations when applying [FW12, Theorem 5.1 in Chapter 6] in order to obtain some information on the first exit point distribution. First, this theorem requires to be able to compute the quasipotential in order to get useful information: this is trivial under the assumptions (4.1.3) and (4.1.4) but more complicated under more general assumptions on  $f$  (in particular when  $f$  has several critical points in  $\Omega$ ). Second, even when the quasipotential is analytically known, this result only gives the subset of  $\partial\Omega$  where exit will not occur on an exponential scale in the limit  $h \rightarrow 0^+$ . It does not allow to exclude exit points with probability which goes to zero polynomially in  $h$  (this indeed occurs, see Section 4.2.4), and it does not give the relative probability to exit through exit points with non-zero probability in the limit  $h \rightarrow 0^+$ .

Using formal computations based on techniques developed for partial differential equations, the following formula was then derived in [MS77] when (4.1.3) and (4.1.4) hold: for any  $F \in \mathcal{C}^\infty(\partial\Omega, \mathbb{R})$  and  $x \in \Omega$ , one has when  $h \rightarrow 0^+$ :

$$\mathbb{E}_x[F(X_{\tau_\Omega})] = \frac{\int_{\partial\Omega} F \partial_n f e^{-\frac{2}{h}f} d\mu_{\partial\Omega}}{\int_{\partial\Omega} \partial_n f e^{-\frac{2}{h}f} d\mu_{\partial\Omega}} + o(1). \quad (4.1.5)$$

The formal asymptotic estimate (4.1.5) implies that the law of  $X_{\tau_\Omega}$  concentrates on points where  $f$  attains its minimum on  $\partial\Omega$ . These results are obtained in [MS77] injecting formal asymptotic expansions in powers of  $h$  in the partial differential equations satisfied by  $x \in \Omega \mapsto \mathbb{E}_x[F(X_{\tau_\Omega})]$  (see (1.3.32) in Section 1.3.3). We also refer to [SM79], where using formal computations, asymptotic formulas are obtained concerning the concentration of the law of  $X_{\tau_\Omega}$  on  $\text{argmin}_{\partial\Omega} f$  when  $\Omega$  is the union of basins of attraction of the dynamics  $\dot{x} = -\nabla f(x)$ .

Moreover, when (4.1.3) and (4.1.4) hold, the formula (4.1.5) was proved rigorously by Kamin in [Kam79], and extended to a non reversible diffusion process  $(Y_t)_{t \geq 0}$  solution to  $dY_t = b(Y_t) dt + \sqrt{h} dB_t$  in [Kam78, Per90, Day84, Day87] when  $\Omega$  contains precisely one attractor of the dynamics  $\dot{x} = b(x)$  and  $b \cdot \vec{n} < 0$  on  $\partial\Omega$ . However,

the results of [Kam79, Kam78, Per90, Day84, Day87] do not provide any information on the probability to leave  $\Omega$  through a point which is not a global minimum of  $f$  on  $\partial\Omega$  and we refer to the next chapter for results in this connection. We also refer to [Day99] for a comprehensive review of the above literature and to [IS15, IS17] for more recent results using similar techniques as those used in [Kam79, Kam78, Per90].

In the work [DLLN19a] presented in this chapter, we aim at analyzing the metastability of a domain  $\Omega$ , as defined in Definition 1.3.4 in Section 1.3.3, by studying on which points the law of  $X_{\tau_\Omega}$  does concentrate when  $h \rightarrow 0^+$  and the relative probabilities to leave through each of them. Since for physically reasonable domains this concentration is expected to occur on points belonging to  $\arg \min_{\partial\Omega} f$  (see the above results), we are more precisely interested in exhibiting explicit assumptions on the domain  $\Omega$  and on the smooth Morse function  $f$  ensuring the two following properties:

**[P1]** When  $X_0$  is initially distributed according to the quasi-stationary distribution  $\nu_h$  of the process (4.1.1) in  $\Omega$  (see Section 1.3.3 and in particular Definition 1.3.1 there), the law of  $X_{\tau_\Omega}$  concentrates in the limit  $h \rightarrow 0^+$  on some global minima of  $f$  on  $\partial\Omega$ .

**[P2]** There exist an open set  $\mathcal{V} \subset \Omega$  such that, when  $X_0 = x \in \mathcal{V}$ , the law of  $X_{\tau_\Omega}$  concentrates in the limit  $h \rightarrow 0^+$  on the same points of  $\partial\Omega$  as it does when  $X_0 \sim \nu_h$ , with the same relative probabilities to leave  $\Omega$  through each of them.

As it will be clear from our assumptions **(A0)** to **(A4)** below, we exhibit in [DLLN19a] very general couples  $(\Omega, f)$  satisfying **[P1]** and **[P2]** for which the Morse potential  $f$  can in particular have several critical points in  $\Omega$ , possibly larger in energy than  $\min_{\partial\Omega} f$ , and  $\partial_n f$  is not assumed to be positive on  $\partial\Omega$ . Under our assumptions, the asymptotic concentration of the law of  $X_{\tau_\Omega}$  can moreover occur on a strict subset of  $\arg \min_{\partial\Omega} f$ . However, we do not consider in [DLLN19a] the case where  $f$  has critical points on  $\partial\Omega$ .

An easy consequence of our results (see Theorem 4.2.3) is for instance the following generalization of [Kam79, Kam78, Per90, Day84, Day87] and [FW12, Theorem 2.1 in Chapter 4]: when<sup>2</sup>

$$\partial_n f > 0 \text{ on } \partial\Omega \quad \text{and} \quad (\nabla f)^{-1}(\{0\}) \subset \{f < \min_{\partial\Omega} f\}$$

(without restriction on the (finite) number of critical points of  $f$ ), and if  $X_0$  is distributed according to the quasi-stationary distribution  $\nu_h$  of the process (4.1.1) in  $\Omega$  or  $X_0 = x \in \Omega$ , then the exit point distribution concentrates on  $\arg \min_{\partial\Omega} f$ .

---

2. Actually, the following conclusions also hold assuming more generally that  $\partial_n f > 0$  on  $\partial\Omega$  and that  $\{f < \min_{\partial\Omega} f\}$  contains all the local minima of  $f$  and all its separating saddle points as defined in Section 3.1.3 in the case of Neumann type boundary conditions. This follows from the fact that in this case, the set  $\{f < \min_{\partial\Omega} f\}$  is connected.

## 4.2 The case of more general wells

### 4.2.1 Geometric hypotheses

Let  $\bar{\Omega}$  be a  $\mathcal{C}^\infty$  oriented compact and connected Riemannian manifold of dimension  $d$  with interior  $\Omega$  and boundary  $\partial\Omega$ <sup>3</sup>. We recall the definition of the domain of attraction of a subset  $D$  of  $\Omega$  for the  $-\nabla f$  dynamics of a  $\mathcal{C}^\infty$  function  $f : \bar{\Omega} \rightarrow \mathbb{R}$ . Let  $x \in \Omega$  and denote by  $\varphi_t(x)$  the solution to the ordinary differential equation

$$\frac{d}{dt}\varphi_t(x) = -\nabla f(\varphi_t(x)), \quad \varphi_0(x) = x, \quad (4.2.1)$$

on the interval  $t \in [0, t_x]$ , where

$$t_x = \inf\{t \geq 0, \varphi_t(x) \notin \Omega\} > 0.$$

Let  $x \in \Omega$  be such that  $t_x = +\infty$ . The  $\omega$ -limit set of  $x$ , denoted by  $\omega(x)$ , is defined by

$$\omega(x) = \{y \in \bar{\Omega}, \exists (s_n)_{n \in \mathbb{N}} \in (\mathbb{R}_+)^{\mathbb{N}}, \lim_{n \rightarrow +\infty} s_n = +\infty, \lim_{n \rightarrow +\infty} \varphi_{s_n}(x) = y\}.$$

Let us recall that the  $\omega$ -limit set  $\omega(x)$  is included in the set of the critical points of  $f$  in  $\bar{\Omega}$ . Moreover, when  $f$  has a finite number of critical points in  $\bar{\Omega}$ ,

$$\exists y \in \bar{\Omega}, \omega(x) = \{y\}.$$

Let  $D$  be a subset of  $\Omega$ . The domain of attraction of  $D$  is then defined by

$$\mathcal{A}(D) = \{x \in \Omega, t_x = +\infty \text{ and } \omega(x) \subset D\}. \quad (4.2.2)$$

Let us now introduce the basic Morse type assumption of [DLLN19a]<sup>4</sup>:

$$\left. \begin{array}{l} \text{The function } f : \bar{\Omega} \rightarrow \mathbb{R} \text{ is a } \mathcal{C}^\infty \text{ Morse function and } \nabla f \neq 0 \text{ on } \partial\Omega. \\ \text{The function } f|_{\partial\Omega} : \partial\Omega \rightarrow \mathbb{R} \text{ is a Morse function.} \\ \text{Moreover, } f \text{ has at least one local minimum in } \Omega. \end{array} \right\} \quad (\mathbf{M})$$

For any local minimum  $x$  of  $f$  in  $\Omega$ , one then defines

$$\mathbf{H}_f(x) := \inf_{\substack{\gamma \in \mathcal{C}^0([0,1], \bar{\Omega}) \\ \gamma(0)=x \\ \gamma(1) \in \partial\Omega}} \max_{t \in [0,1]} f(\gamma(t)), \quad (4.2.3)$$

where  $\mathcal{C}^0([0,1], \bar{\Omega})$  is the set of continuous paths from  $[0,1]$  to  $\bar{\Omega}$ . An equivalent definition of  $\mathbf{H}_f(x)$  in terms of the connected components of the sublevel sets of  $f$  is the following (see [DLLN19a] for more details):

$$\mathbf{H}_f(x) = \sup\{\lambda > f(x), \mathbf{C}(x, \lambda) \cap \partial\Omega = \emptyset\}, \quad (4.2.4)$$

3. Note that the convention adopted here is not the convention adopted in the preceding chapters where  $\Omega$  was always assumed to be closed. It is nevertheless more convenient to assume  $\Omega$  to be open here, for instance to be consistent with the usual convention in the Euclidean setting adopted in Section 4.1.

4. The assumption that  $f|_{\partial\Omega}$  is a Morse function can actually be replaced by the assumption that  $f|_{\{\sigma \in \partial\Omega, \partial_n f(\sigma) > 0\}}$  is a Morse function, see [DLLN19a] for more details.

where, for the local minimum  $x$  of  $f$  in  $\Omega$  and  $\lambda > f(x)$ ,

$$\mathbf{C}(x, \lambda) \text{ is the connected component of } \{f < \lambda\} \text{ in } \overline{\Omega} \text{ containing } x. \quad (4.2.5)$$

Moreover, the supremum in (4.2.4) is actually a maximum, i.e. the connected component of  $\mathbf{C}(x, \mathbf{H}_f(x))$  containing  $x$  is included in  $\Omega$ . Note also that,  $\overline{\Omega}$  being locally connected,  $\mathbf{C}(x, \mathbf{H}_f(x))$  is an open set of  $\overline{\Omega}$ , and then of  $\Omega$ , for every local minimum  $x$  of  $f$  in  $\Omega$ , and that  $\partial\mathbf{C}(x, \mathbf{H}_f(x)) \subset \{f = \mathbf{H}_f(x)\}$ . It follows in particular that for every  $y \in \mathbf{C}(x)$ , it holds  $t_y = +\infty$  and then,  $\mathbf{C}(x) \subset \mathcal{A}(\mathbf{C}(x))$ .

Let us now define a set of assumptions which will ensure that **[P1]** and **[P2]** are satisfied (see indeed Theorem 4.2.3 and Section 4.2.4 for a discussion on these assumptions):

— **(M)** holds and

$$\exists! \mathbf{C}_{\max} \in \mathcal{C} \text{ such that } \max_{\mathbf{C} \in \mathcal{C}} \left\{ \max_{\overline{\mathbf{C}}} f - \min_{\overline{\mathbf{C}}} f \right\} = \max_{\mathbf{C}_{\max}} f - \min_{\mathbf{C}_{\max}} f \quad (\mathbf{A1})$$

where

$$\mathcal{C} := \{ \mathbf{C}(x), x \text{ is a local minimum of } f \text{ in } \Omega \}, \quad (4.2.6)$$

with, for a local minimum  $x$  of  $f$  in  $\Omega$ ,

$$\mathbf{C}(x) := \mathbf{C}(x, \mathbf{H}_f(x)) \quad (\text{see (4.2.5)}). \quad (4.2.7)$$

— **(A1)** holds and

$$\partial\mathbf{C}_{\max} \cap \partial\Omega \neq \emptyset. \quad (\mathbf{A2})$$

— **(A1)** holds and

$$\partial\mathbf{C}_{\max} \cap \partial\Omega \subset \arg \min_{\partial\Omega} f. \quad (\mathbf{A3})$$

More precisely, the assumptions **(M)** and **(A1)** to **(A3)** ensure that when  $X_0 \sim \nu_h$  or  $X_0 = x \in \mathcal{A}(\mathbf{C}_{\max})$ , the law of  $X_{\tau_\Omega}$  concentrates on the points of  $\partial\mathbf{C}_{\max} \cap \partial\Omega$ , with the same relative probabilities to leave  $\Omega$  through each of them, see items 1 and 2 in Theorem 4.2.3.

Finally, let us introduce the following assumption:

**(A1)** holds and for any  $\mathbf{C} \in \mathcal{C} \setminus \{\mathbf{C}_{\max}\}$  (see (4.2.6)) it holds

$$\partial\mathbf{C}_{\max} \cap \partial\mathbf{C} = \emptyset. \quad (\mathbf{A4})$$

The assumption **(A4)**, together with **(M)** and **(A1)** to **(A3)**, ensures that the probability that the process (4.1.1) (starting from the quasi-stationary distribution  $\nu_h$  or from  $x \in \mathcal{A}(\mathbf{C}_{\max})$ ) leaves  $\Omega$  through any sufficiently small neighborhood of  $z \in \partial\Omega \setminus \partial\mathbf{C}_{\max}$  in  $\partial\Omega$  is exponentially small when  $h \rightarrow 0^+$ , see indeed item 3 in Theorem 4.2.3<sup>5</sup>.

In Figure 4.1 is represented a one-dimensional potential satisfying the assumptions **(A1)** to **(A4)**. These assumptions will be discussed in Section 4.2.4 where we will in particular show there that if one assumption among **(A1)**, **(A2)**, or **(A3)** does not hold, then there exists a function  $f$  satisfying **(M)** such that either **[P1]** or **[P2]** is not satisfied.

---

5. To connect with the notions introduced in Chapter 3, when **(A1)** to **(A3)** hold, **(A4)** is satisfied if and only if  $\partial\mathbf{C}_{\max} \cap \Omega$  does not contain any separating saddle point as defined in Definition 3.1.2.

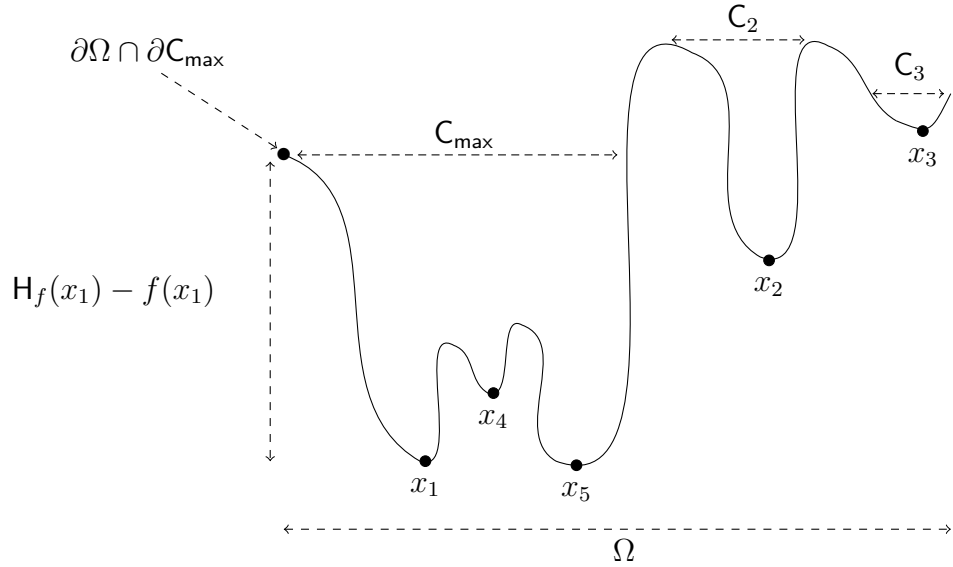


Figure 4.1 – A 1D example where **(A1)–(A4)** are satisfied. Here,  $f(x_1) = f(x_5)$ ,  $H_f(x_1) = H_f(x_4) = H_f(x_5)$ ,  $\mathcal{C} = \{C_{\max}, C_2, C_3\}$  (where  $\mathcal{C}$  is defined by (4.2.6)),  $\partial C_2 \cap \partial C_{\max} = \emptyset$  and  $\partial C_3 \cap \partial C_{\max} = \emptyset$ . Therefore, the assumption **(A4)** is indeed satisfied.

### 4.2.2 Local minima and saddle points of $f$

In this part, we label suitably the local minima and generalized saddle points of  $f$ , extensively used in [DLLN19a], in order to properly state the main results of this work. We refer to Section 3.1.3 in the case of Dirichlet type boundary conditions for more details about these generalized saddle points.

Let us assume that the function  $f$  satisfies the assumption **(M)**. We now specify the notation of Section 3.1.3 in this setting (see (3.1.4) and (3.1.5)). We denote by

$$\mathcal{U}_{\Omega}^{(0)} = \mathcal{U}_{\Omega}^{D,(0)} = \{x_1, \dots, x_{\mathbf{m}_0^D}\} \subset \Omega$$

the set of local minima of  $f$  in  $\Omega$ , that is, according to  $\nabla f \neq 0$  on  $\partial\Omega$ , the set of critical points of  $f$  with index 0 in  $\bar{\Omega}$ . Notice that since  $f$  satisfies **(M)**, it holds  $\mathbf{m}_0^D \geq 1$ .

We denote moreover the set of generalized saddle points of  $f$  by

$$\mathcal{U}_{\Omega}^{D,(1)} = \mathcal{U}_{\Omega}^{(1)} \cup \mathcal{U}_{\partial\Omega}^{D,(1)} = \{z_1, \dots, z_{\mathbf{m}_1^D}\},$$

where  $\mathcal{U}_{\Omega}^{(1)}$  denotes the set of critical points of  $f$  with index 1 in  $\Omega$ , assumed to have cardinality  $\mathbf{m}_1^{\Omega} \in \mathbb{N}$ , and

$$\mathcal{U}_{\partial\Omega}^{D,(1)} = \{\text{local minima } z \text{ of } f|_{\partial\Omega} \text{ s.t. } \partial_n f(z) > 0\} \subset \partial\Omega, \quad (4.2.8)$$

assumed to have cardinality

$$\mathbf{m}_1^{\partial\Omega} := \text{Card}(\mathcal{U}_{\partial\Omega}^{D,(1)}) \in \mathbb{N}. \quad (4.2.9)$$

When  $\mathbf{m}_1^{\partial\Omega} \geq 1$  and then  $\mathbf{m}_1^D \geq 1$ , the elements  $z_1, \dots, z_{\mathbf{m}_1^D}$  of  $\mathcal{U}_{\partial\Omega}^{D,(1)}$  are moreover labelled such that

$$\mathcal{U}_{\partial\Omega}^{D,(1)} = \{z_1, \dots, z_{\mathbf{m}_1^{\partial\Omega}}\}, \quad (4.2.10)$$

where, when in addition  $\mathcal{U}_{\partial\Omega}^{D,(1)} \cap \arg \min_{\partial\Omega} f \neq \emptyset$ , the elements  $z_1, \dots, z_{\mathbf{m}_1^{\partial\Omega}}$  of  $\mathcal{U}_{\partial\Omega}^{D,(1)}$  are ordered such that

$$\{z_1, \dots, z_{\mathbf{k}_1^{\partial\Omega}}\} = \mathcal{U}_{\partial\Omega}^{D,(1)} \cap \arg \min_{\partial\Omega} f, \quad (4.2.11)$$

where  $1 \leq \mathbf{k}_1^{\partial\Omega} \leq \mathbf{m}_1^{\partial\Omega}$ .

Let us now also assume that the assumptions **(A1)**, **(A2)**, and **(A3)** are satisfied. We recall that the set  $\mathbf{C}_{\max}$  is then defined by **(A1)**. It holds moreover in this case:

$$\mathbf{k}_1^{\partial\Omega} \geq 1 \quad \text{and} \quad \partial\mathbf{C}_{\max} \cap \partial\Omega \subset \mathcal{U}_{\partial\Omega}^{D,(1)} \cap \arg \min_{\partial\Omega} f = \{z_1, \dots, z_{\mathbf{k}_1^{\partial\Omega}}\}.$$

Indeed, **(A2)** and **(A3)** imply that  $\emptyset \neq \partial\mathbf{C}_{\max} \cap \partial\Omega \subset \arg \min_{\partial\Omega} f$  and then that  $\mathbf{C}_{\max}$  is a connected component of  $\{f < \min_{\partial\Omega} f\}$  and that  $\partial\mathbf{C}_{\max} \subset \{f = \min_{\partial\Omega} f\}$ . In particular, there is no local minimum of  $f$  in  $\bar{\Omega}$  on  $\partial\mathbf{C}_{\max}$ . Hence, every  $z \in \partial\mathbf{C}_{\max} \cap \partial\Omega$  being a local minimum of  $f|_{\partial\Omega}$ , the relation  $\nabla f(z) \neq 0$  implies  $\partial_n f(z) > 0$  and thus  $z \in \mathcal{U}_{\partial\Omega}^{D,(1)}$ .

We assume lastly that the elements  $z_1, \dots, z_{\mathbf{k}_1^{\partial\Omega}}$  of  $\mathcal{U}_{\partial\Omega}^{D,(1)} \cap \arg \min_{\partial\Omega} f$  are ordered such that

$$\{z_1, \dots, z_{\mathbf{k}_1^{\partial\mathbf{C}_{\max}}}\} = \partial\mathbf{C}_{\max} \cap \partial\Omega = \{z_1, \dots, z_{\mathbf{k}_1^{\partial\Omega}}\} \cap \partial\mathbf{C}_{\max}. \quad (4.2.12)$$

Notice that  $\mathbf{k}_1^{\partial\mathbf{C}_{\max}} \geq 1$  and that  $\mathbf{k}_1^{\partial\mathbf{C}_{\max}} \leq \mathbf{k}_1^{\partial\Omega}$ . See in Figure 4.2 an example illustrating the notation introduced in this section.

### 4.2.3 Main results on the exit point distribution

Let us begin this section by recalling some notions introduced in Section 1.3.3 of the introductory part.

Let  $L_{f, \frac{h}{2}}^{D,(0)}$  be the unbounded differential operator

$$L_{f, \frac{h}{2}}^{(0)} := \frac{h}{2} \Delta_{\mathbb{H}}^{(0)} + \nabla f \cdot \nabla$$

with domain

$$D(L_{f, \frac{h}{2}}^{D,(0)}) := \left\{ u \in H^1(\Omega, e^{-\frac{2}{h}f} d\mu), u = 0 \text{ on } \partial\Omega \right\} \cap H^2(\Omega, e^{-\frac{2}{h}f} d\mu).$$

This operator is self-adjoint, positive and has a compact resolvent in  $L^2(\Omega, e^{-\frac{2}{h}f} d\mu)$ . We denote by

$$\lambda_h = \lambda_{1,h} := \min\{\text{Sp}(L_{f, \frac{h}{2}}^{D,(0)})\} > 0 \quad (4.2.13)$$

its principal eigenvalue (which is simple) and by  $u_h$  some associated eigenfunction (which then has a sign on  $\Omega$ ), chosen to be positive on  $\Omega$  and unitary in  $L^2(\Omega, e^{-\frac{2}{h}f} d\mu)$ :

$$L_{f, \frac{h}{2}}^{D,(0)} u_h = \lambda_h u_h, \quad u_h > 0 \text{ on } \Omega, \quad \text{and} \quad \int_{\Omega} u_h^2 e^{-\frac{2}{h}f} d\mu = 1. \quad (4.2.14)$$

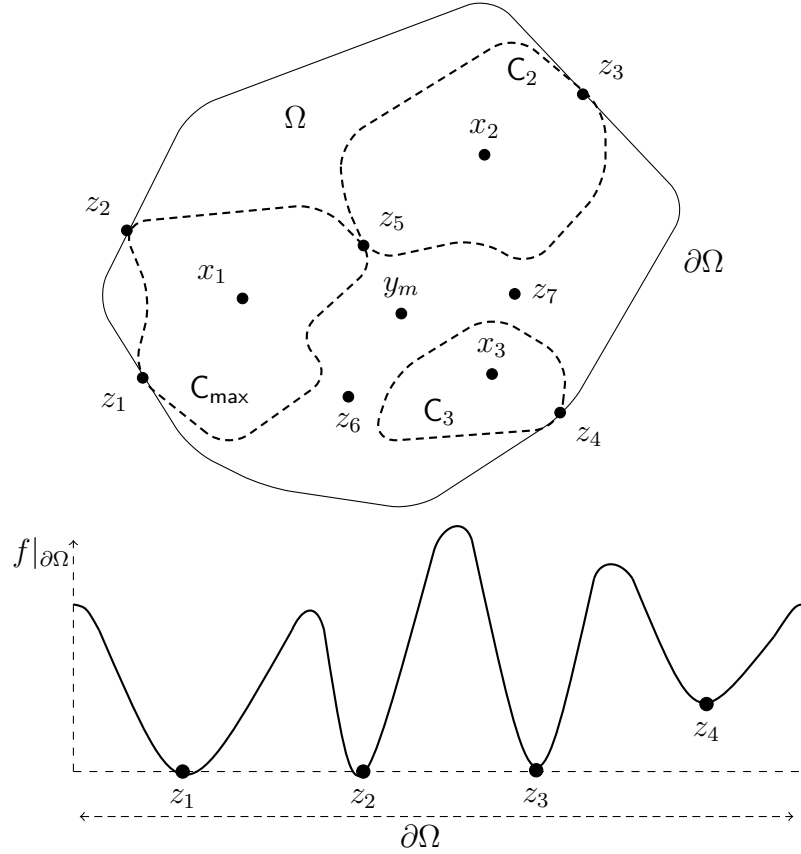


Figure 4.2 – Schematic representation of  $\mathcal{C}$  (see (4.2.6)) and  $f|_{\partial\Omega}$  under the assumptions **(M)** and **(A1)**–**(A3)**. Here,  $x_1 \in \Omega$  is the global minimum of  $f$  in  $\bar{\Omega}$  and the other local minima of  $f$  in  $\Omega$  are  $x_2$  and  $x_3$  (thus  $\mathcal{U}_\Omega^{(0)} = \{x_1, x_2, x_3\}$  and  $\mathbf{m}_0^D = 3$ ). Moreover,  $\min_{\partial\Omega} f = f(z_1) = f(z_2) = f(z_3) = \mathbf{H}_f(x_1) = \mathbf{H}_f(x_2) < \mathbf{H}_f(x_3) = f(z_4)$ ,  $\{f < \mathbf{H}_f(x_1)\}$  has two connected components:  $\mathcal{C}_{\max}$  (see **(A1)**) which contains  $x_1$  and  $\mathcal{C}_2$  which contains  $x_2$ . Thus, one has  $\mathcal{C} = \{\mathcal{C}_{\max}, \mathcal{C}_2, \mathcal{C}_3\}$ . In addition,  $\mathcal{U}_{\partial\Omega}^{(1)} = \{z_1, z_2, z_3, z_4\}$  ( $\mathbf{m}_1^{\partial\Omega} = 4$ ),  $\{z_1, z_2, z_3\} = \arg \min_{\partial\Omega} f$  ( $\mathbf{k}_1^{\partial\Omega} = 3$ ),  $\mathcal{U}_\Omega^{(1)} = \{z_5, z_6, z_7\}$  where  $\{z_5\} = \overline{\mathcal{C}_{\max}} \cap \overline{\mathcal{C}_2}$  ( $\mathbf{m}_1^\Omega = 3$  and **(A4)** is not satisfied) and  $\min(f(z_6), f(z_7)) > f(z_4)$ ,  $\partial\mathcal{C}_{\max} \cap \partial\Omega = \{z_1, z_2\}$  ( $\mathbf{k}_1^{\partial\mathcal{C}_{\max}} = 2$ ). Finally, one has  $\mathbf{m}_1^D = 7$ . The point  $y_m \in \Omega$  is a local maximum of  $f$  with  $f(y_m) > f(z_i)$  for all  $i \in \{1, \dots, 7\}$ .

The quasi-stationary distribution  $\nu_h$  associated with the overdamped Langevin dynamics (4.1.1) and  $\Omega$  is then the probability measure on  $\Omega$  defined by

$$\nu_h(d\mu) = \frac{u_h e^{-\frac{2}{h}f}}{\int_{\Omega} u_h e^{-\frac{2}{h}f} d\mu} d\mu.$$

Moreover, according to (1.3.29), it holds for any  $F \in L^\infty(\partial\Omega, \mathbb{R})$ ,

$$\mathbb{E}_{\nu_h}[F(X_{\tau_\Omega})] = \frac{h \int_{\partial\Omega} F \partial_n u_h e^{-\frac{2}{h}f} d\mu_{\partial\Omega}}{2\lambda_h \int_{\Omega} u_h e^{-\frac{2}{h}f} d\mu}. \quad (4.2.15)$$

Before stating the main result of [DLLN19a], that is Theorem 4.2.3, we first state the following result which is crucial in the proof of this theorem and might be of independent interest. It states that, when the assumptions **(M)** and **(A1)** are satisfied and  $\min_{\mathbf{C}_{\max}} f = \min_{\bar{\Omega}} f$ <sup>6</sup>, the quasi-stationary distribution  $\nu_h$  concentrates in (arbitrary small) neighborhoods of the global minima of  $f$  in  $\mathbf{C}_{\max}$ .

**Proposition 4.2.1.** *Assume that the assumptions **(M)** and **(A1)** are satisfied, and that*

$$\min_{\mathbf{C}_{\max}} f = \min_{\bar{\Omega}} f,$$

where we recall that  $\mathbf{C}_{\max}$  has been introduced in **(A1)**. Let  $\mathbf{O}$  be an open subset of  $\Omega$ . Then, if  $\mathbf{O} \cap \arg \min_{\mathbf{C}_{\max}} f \neq \emptyset$ , one has in the limit  $h \rightarrow 0^+$ :

$$\int_{\mathbf{O}} u_h e^{-\frac{2}{h}f} d\mu = h^{\frac{d}{4}} \pi^{\frac{d}{4}} \frac{\sum_{x \in \mathbf{O} \cap \arg \min_{\mathbf{C}_{\max}} f} (\det \text{Hess } f(x))^{-\frac{1}{2}}}{\left( \sum_{x \in \arg \min_{\mathbf{C}_{\max}} f} (\det \text{Hess } f(x))^{-\frac{1}{2}} \right)^{\frac{1}{2}}} e^{-\frac{1}{h} \min_{\bar{\Omega}} f} (1 + \mathcal{O}(h))$$

and

$$\nu_h(\mathbf{O}) = \frac{\sum_{x \in \mathbf{O} \cap \arg \min_{\mathbf{C}_{\max}} f} (\det \text{Hess } f(x))^{-\frac{1}{2}}}{\sum_{x \in \arg \min_{\mathbf{C}_{\max}} f} (\det \text{Hess } f(x))^{-\frac{1}{2}}} (1 + \mathcal{O}(h)),$$

where the terms  $\mathcal{O}(h)$  admit a full asymptotic expansion in  $h$ .

Moreover, when  $\bar{\mathbf{O}} \cap \arg \min_{\mathbf{C}_1} f = \emptyset$ , there exists  $c > 0$  such that when  $h \rightarrow 0^+$ :

$$\int_{\mathbf{O}} u_h e^{-\frac{2}{h}f} d\mu = \mathcal{O}(e^{-\frac{1}{h}(\min_{\bar{\Omega}} f + c)}) \quad \text{and} \quad \nu_h(\mathbf{O}) = \mathcal{O}(e^{-\frac{c}{h}}).$$

**Remark 4.2.2.** *In the work [LN19a], we study the repartition of  $\nu_h$  when  $h \rightarrow 0^+$  in the case of a double-well when **(A1)** does not hold. We show there that, generically,  $\nu_h$  concentrates in only one of the two wells in the limit  $h \rightarrow 0^+$ , and **[P1]** and **[P2]** hold (see Section 4.1). Nevertheless, under sufficient symmetries of  $f$ , the semiclassical tunneling effect between the wells is so strong that  $\nu_h$  concentrates in both wells in the limit  $h \rightarrow 0^+$ . This is reminiscent of previous results dealing with Schrödinger operators of the form  $-h^2\Delta + V$  and we refer in particular to [Hel88, Section 4.3] for more details and references.*

The main result of [DLLN19a] is the following.

**Theorem 4.2.3.** *Let us assume that the assumptions **(M)** and **(A1)**–**(A3)** are satisfied. Let  $F \in L^\infty(\partial\Omega, \mathbb{R})$  and  $(\Sigma_i)_{i \in \{1, \dots, \mathbf{k}_1^{\partial\Omega}\}}$  be a family of disjoint open subsets of  $\partial\Omega$  such that*

$$\text{for all } i \in \{1, \dots, \mathbf{k}_1^{\partial\Omega}\}, z_i \in \Sigma_i,$$

where we recall that  $\{z_1, \dots, z_{\mathbf{k}_1^{\partial\Omega}}\} = \mathcal{U}_{\partial\Omega}^{D, (1)} \cap \arg \min_{\partial\Omega} f$  (see (4.2.11)). Let  $K$  be a compact subset of  $\Omega$  such that  $K \subset \mathcal{A}(\mathbf{C}_{\max})$  (see **(A1)** and (4.2.2)). Let  $\mu_0$  be a probability distribution which is either supported in  $K$  or equals to the quasi-stationary distribution  $\nu_h$  of the process (4.1.1) in  $\Omega$ . Then:

---

6. Note that this is automatically satisfied under **(A1)**–**(A3)**.



1. There exists  $c > 0$  such that in the limit  $h \rightarrow 0^+$ :

$$\mathbb{E}_{\mu_0} [F(X_{\tau_\Omega})] = \sum_{i=1}^{\mathbf{k}_1^{\partial\Omega}} \mathbb{E}_{\mu_0} [\mathbf{1}_{\Sigma_i} F(X_{\tau_\Omega})] + \mathcal{O}(e^{-\frac{c}{h}}) \quad (4.2.16)$$

and

$$\sum_{i=\mathbf{k}_1^{\partial\mathbf{C}_{\max}+1}}^{\mathbf{k}_1^{\partial\Omega}} \mathbb{E}_{\mu_0} [\mathbf{1}_{\Sigma_i} F(X_{\tau_\Omega})] = \mathcal{O}(h^{\frac{1}{4}}), \quad (4.2.17)$$

where we recall that  $\{z_1, \dots, z_{\mathbf{k}_1^{\partial\mathbf{C}_{\max}}}\} = \partial\mathbf{C}_{\max} \cap \partial\Omega$  (see (4.2.12)).

2. When, for some  $i \in \{1, \dots, \mathbf{k}_1^{\partial\mathbf{C}_{\max}}\}$ , the function  $F$  is  $\mathcal{C}^\infty$  in a neighborhood of  $z_i$ , one has when  $h \rightarrow 0^+$ :

$$\mathbb{E}_{\mu_0} [\mathbf{1}_{\Sigma_i} F(X_{\tau_\Omega})] = F(z_i) a_i + \mathcal{O}(h^{\frac{1}{4}}), \quad (4.2.18)$$

where

$$a_i = \frac{\partial_n f(z_i)}{\sqrt{\det \text{Hess } f|_{\partial\Omega}(z_i)}} \left( \sum_{j=1}^{\mathbf{k}_1^{\partial\mathbf{C}_{\max}}} \frac{\partial_n f(z_j)}{\sqrt{\det \text{Hess } f|_{\partial\Omega}(z_j)}} \right)^{-1}. \quad (4.2.19)$$

3. When **(A4)** is satisfied, the remainder term  $\mathcal{O}(h^{\frac{1}{4}})$  in (4.2.17) is of the order  $\mathcal{O}(e^{-\frac{c}{h}})$  for some  $c > 0$  and the remainder term  $\mathcal{O}(h^{\frac{1}{4}})$  in (4.2.18) is of the order  $\mathcal{O}(h)$  and admits a full asymptotic expansion in  $h$ .

Finally, the constants involved in the remainder terms in (4.2.16), (4.2.17), and in (4.2.18) are uniform with respect to the probability distribution  $\mu_0$  supported in  $K$ .

According to (4.2.18) and (4.2.19), when the function  $F$  belongs to  $\mathcal{C}^\infty(\partial\Omega, \mathbb{R})$  and  $x \in \mathcal{A}(\mathbf{C}_{\max})$ , one then has in the limit  $h \rightarrow 0^+$ :

$$\mathbb{E}_x [F(X_{\tau_\Omega})] = \sum_{i=1}^{\mathbf{k}_1^{\partial\mathbf{C}_{\max}}} a_i F(z_i) + \mathcal{O}(h^{\frac{1}{4}}) = \frac{\int_{\partial\Omega \cap \mathcal{V}(\overline{\mathbf{C}_{\max}})} F \partial_n f e^{-\frac{2}{h}f} d\mu_{\partial\Omega}}{\int_{\partial\Omega \cap \mathcal{V}(\overline{\mathbf{C}_{\max}})} \partial_n f e^{-\frac{2}{h}f} d\mu_{\partial\Omega}} + o_h(1), \quad (4.2.20)$$

where  $\mathcal{V}(\overline{\mathbf{C}_{\max}})$  is a sufficiently small neighborhood of  $\overline{\mathbf{C}_{\max}}$  in  $\overline{\Omega}$  and the order in  $h$  of the remainder term  $o_h(1)$  depends on the support of  $F$  and on whether or not the assumption **(A4)** is satisfied (compare with (4.1.5)).

Theorem 4.2.3 implies that in the limit  $h \rightarrow 0^+$ , when  $X_0 \sim \nu_h$  or  $X_0 = x \in \mathcal{A}(\mathbf{C}_{\max})$ , the law of  $X_{\tau_\Omega}$  concentrates on the set  $\{z_1, \dots, z_{\mathbf{k}_1^{\partial\mathbf{C}_{\max}}}\} = \partial\Omega \cap \partial\mathbf{C}_{\max}$  with explicit formulas for the probabilities to exit through each of the  $z_i$ 's. Therefore, **[P1]** and **[P2]** (see Section 4.1) are satisfied when the assumptions **(A1)**–**(A3)** hold.

Another consequence of Theorem 4.2.3 is the following. 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  $h \rightarrow 0^+$  (see (4.2.16)) and the probability to exit through  $z_{\mathbf{k}_1^{\mathbf{C}_{\max}+1}}, \dots, z_{\mathbf{k}_1^{\partial\Omega}}$  tends to 0 (and is even exponentially small when **(A4)** holds) even though all these points belong to  $\arg \min_{\partial\Omega} f$ .

Let us conclude this section by stressing that Theorem 4.2.3 can also be applied to a well chosen subdomain of  $\Omega$  in order to deal with the concentration of the law of  $X_{\tau_\Omega}$  in the limit  $h \rightarrow 0^+$  when  $X_0 = x \in \mathcal{A}(\mathbf{C})$  and  $\mathbf{C} \in \mathcal{C}$  (see (4.2.6)) is not necessarily  $\mathbf{C}_{\max}$ .

This permits for example to prove the following result:

**Theorem 4.2.4.** *Let us assume that  $(\mathbf{M})$  holds and let  $\mathbf{C} \in \mathcal{C}$  (see (4.2.6)) be such that*

$$\partial\mathbf{C} \cap \partial\Omega \neq \emptyset \quad \text{and} \quad |\nabla f| \neq 0 \quad \text{on} \quad \partial\mathbf{C}. \quad (4.2.21)$$

We recall that  $\partial\mathbf{C} \cap \partial\Omega \subset \mathcal{U}_{\partial\Omega}^{D,(1)}$  (see (4.2.8) and (4.2.10)).

Let  $K$  be a compact subset of  $\Omega$  such that  $K \subset \mathcal{A}(\mathbf{C})$  and, for all  $z \in \partial\mathbf{C} \cap \partial\Omega$ , let  $\Sigma_z$  be an open subset of  $\partial\Omega$  such that  $z \in \Sigma_z$ . Then, there exists  $c > 0$  such that in the limit  $h \rightarrow 0^+$ ,

$$\sup_{x \in K} \mathbb{P}_x \left[ X_{\tau_\Omega} \in \partial\Omega \setminus \bigcup_{z \in \partial\mathbf{C} \cap \partial\Omega} \Sigma_z \right] \leq e^{-\frac{c}{h}}.$$

Assume moreover that the sets  $(\Sigma_z)_{z \in \partial\mathbf{C} \cap \partial\Omega}$  are two by two disjoint and take  $z \in \partial\mathbf{C} \cap \partial\Omega$ . It then holds

$$\mathbb{P}_x[X_{\tau_\Omega} \in \Sigma_z] = \frac{\partial_n f(z)}{\sqrt{\det \text{Hess } f|_{\partial\Omega}(z)}} \left( \sum_{y \in \partial\mathbf{C} \cap \partial\Omega} \frac{\partial_n f(y)}{\sqrt{\det \text{Hess } f|_{\partial\Omega}(y)}} \right)^{-1} (1 + \mathcal{O}(h))$$

for all  $x \in K$  in the limit  $h \rightarrow 0^+$  and uniformly in  $x \in K$ .

Theorem 4.2.4 implies that when  $\mathbf{C} \in \mathcal{C}$  satisfies (4.2.21) (this is for instance the case for  $\mathbf{C}_3$  on Figures 4.1 and 4.2), the law of  $X_{\tau_\Omega}$  when  $X_0 = x \in \mathcal{A}(\mathbf{C})$  concentrates on  $\partial\mathbf{C} \cap \partial\Omega$  when  $h \rightarrow 0^+$ .

#### 4.2.4 About the hypotheses

In this section, we discuss, assuming  $(\mathbf{M})$ , the necessity of the assumptions  $(\mathbf{A1})$ – $(\mathbf{A3})$  to obtain  $[\mathbf{P1}]$  and  $[\mathbf{P2}]$  (see Section 4.1). We also discuss the necessity of the assumption  $(\mathbf{A4})$  to get the item 3 in Theorem 4.2.3.

##### On the assumption $(\mathbf{A1})$

###### a) Spectral meaning of the assumption $(\mathbf{A1})$

Before going through different examples, let us first specify the meaning of  $(\mathbf{A1})$  – which formally means that the potential function  $f$  admits precisely one deepest characteristic well – in terms of the spectrum of  $L_{f, \frac{h}{2}}^{D,(0)}$  made of the eigenvalues  $0 < \lambda_h = \lambda_{1,h} < \lambda_{2,h} \leq \dots$  counted with multiplicity.

According to Theorem 3.2.2 in Chapter 3 or to [DLLN19b, Theorem 4], it holds, under the basic assumption  $(\mathbf{M})$ ,

$$\forall k \in \mathbb{N}^*, \quad \lim_{h \rightarrow 0^+} h \ln \lambda_{k,h} \quad \text{exists in } \mathbb{R}^- \quad \text{and} \quad \lim_{h \rightarrow 0^+} h \ln \lambda_{k,h} < 0 \quad \text{iff} \quad 1 \leq k \leq \mathbf{m}_0^D,$$

where we recall that  $\mathbf{m}_0^D$  denotes the number of local minima of  $f$  in  $\Omega$ , and

$$(\mathbf{A1}) \quad \text{is satisfied} \quad \text{iff} \quad \lim_{h \rightarrow 0^+} h \ln \lambda_h < \lim_{h \rightarrow 0^+} h \ln \lambda_{2,h}.$$

In other words, the assumption **(A1)** is satisfied if and only if there is an exponentially big gap in the limit  $h \rightarrow 0^+$  between  $\lambda_h$  and  $\lambda_{2,h}$ .

**b) An example where **(A1)** and **[P2]** are not satisfied**

Let us consider  $z_1 < 0$ ,  $z_2 := -z_1$ ,  $z = 0$  and  $f \in \mathcal{C}^\infty([z_1, z_2], \mathbb{R})$  a Morse function such that

$$f \text{ is an even function} \quad \text{and} \quad \{x \in [z_1, z_2], f'(x) = 0\} = \{x_1, z, x_2\},$$

where

$$z_1 < x_1 < z < x_2 < z_2, \quad f(z_1) = f(z_2), \quad \text{and} \quad f(x_1) = f(x_2) < f(z_1) < f(z).$$

Notice that in this case  $x_1 = -x_2$ ,  $x_1$  and  $x_2$  are the two global minima of  $f$  on  $[z_1, z_2]$ ,  $z$  is the global maximum of  $f$  on  $[z_1, z_2]$  and  $\mathbf{H}_f(x_1) = \mathbf{H}_f(x_2) = f(z_1)$ , see Figure 4.3. For such a function, the assumption **(A1)** is not satisfied since  $\arg \max \{ \mathbf{H}_f(x) - f(x), x \text{ is local minimum of } f \text{ in } \Omega \} = \{x_1, x_2\}$  and  $x_1$  belongs to a connected component of  $\{f < \mathbf{H}_f(x_1)\}$  which differs from the connected component of  $\{f < \mathbf{H}_f(x_1)\}$  which contains  $x_2$ .

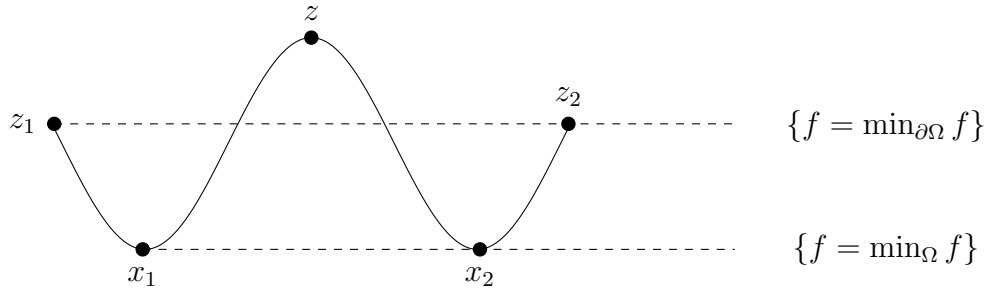


Figure 4.3 – A 1D example where **(A1)** and **[P2]** are not satisfied.

Since for  $x \in (z_1, z_2)$  and  $h > 0$ ,  $\nu_h(x) = \nu_h(-x)$  and  $\mathbb{P}_x[X_{\tau_{(z_1, z_2)}} = z_1] = \mathbb{P}_{-x}[X_{\tau_{(z_1, z_2)}} = z_2]$ , one has for all  $h > 0$ :

$$\mathbb{P}_{\nu_h}[X_{\tau_{(z_1, z_2)}} = z_1] = \frac{1}{2} \quad \text{and} \quad \mathbb{P}_{\nu_h}[X_{\tau_{(z_1, z_2)}} = z_2] = \frac{1}{2}.$$

However, it follows for example from computations done in the appendix of [DLLN19a] and relying on explicit formulas for  $\mathbb{P}_x[X_{\tau_{(z_1, z_2)}} = z_1]$  and  $\mathbb{P}_x[X_{\tau_{(z_1, z_2)}} = z_2]$  together with Laplace's method, that for  $x \in (z_1, z)$ , there exists  $c > 0$  such that in the limit  $h \rightarrow 0^+$ ,

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

and that for  $x \in (z, z_2)$ , there exists  $c > 0$  such that in the limit  $h \rightarrow 0^+$ ,

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

Therefore, in this example, the assumption **[P2]** is not satisfied and the domain  $\Omega$  is not metastable for deterministic initial conditions  $X_0 = x \in (z_1, z_2) \setminus \{z\}$  – and thus not metastable! – in the sense of Definition 1.3.4<sup>7</sup>.

7. Note however that when the process starts from  $z$ , it has a probability one half to fall in the well associated with  $x_1$  and a probability one half to fall in the other well. Using the symmetry, one could then show that the process is metastable for the deterministic initial conditions  $X_0 = z$ .

**c) There are cases where [P1] and [P2] are satisfied but not (A1)**

In the symmetric case depicted in Figure 4.3, the quasi-stationary distribution  $\nu_h$  concentrates in the two wells  $(z_1, z)$  and  $(z, z_2)$  (see [LN19a]): for any  $a_1 < b_1$  such that  $x_1 \in (a_1, b_1) \subset (z_1, z)$  and  $a_2 < b_2$  such that  $x_2 \in (a_2, b_2) \subset (z, z_2)$ , it holds

$$\lim_{h \rightarrow 0^+} \nu_h((a_1, b_1)) = \frac{1}{2} \quad \text{and} \quad \lim_{h \rightarrow 0^+} \nu_h((a_2, b_2)) = \frac{1}{2}.$$

However, it is proved in [LN19a] (see Remark 4.2.2 in this connection) that this equal repartition of  $\nu_h$  when  $h \rightarrow 0^+$  is very unstable with respect to perturbations: changing a little bit the value of the determinant of the Hessian matrix of  $f$  at  $x_1$  or  $x_2$ , or the normal derivative of  $f$  at  $z_1$  or  $z_2$  (while keeping the fact that (A1) is not satisfied) makes  $\nu_h$  concentrates in the limit  $h \rightarrow 0^+$  in only one of the two wells  $(z_1, z)$  or  $(z, z_2)$ , and [P1] and [P2] then also hold.

**d) On the analysis of [P1] and [P2] when (A1) does not hold**

To analyse in general whether [P1] or [P2] is satisfied, one needs in particular to study the asymptotic repartition of  $\nu_h$  in neighborhoods of the local minima of  $f$  in  $\Omega$  when  $h \rightarrow 0^+$ . To do this, we look for an accurate approximation of the principal eigenfunction  $u_h$  of  $L_{f, \frac{h}{2}}^{D, (0)}$  (chosen unitary in  $L^2(\Omega, e^{-\frac{2}{h}f} d\mu)$ ). When (A1) is not satisfied, this is delicate since exponentially small eigenvalues of the same order are into play:  $\lambda_h$  and  $\lambda_{2,h}$  are exponentially small when  $h \rightarrow 0^+$  and

$$\lim_{h \rightarrow 0^+} h \ln \lambda_h = \lim_{h \rightarrow 0^+} h \ln \lambda_{2,h}.$$

This makes in particular difficult to properly estimate  $u_h$  by simply projecting a well chosen quasimode on  $\text{Span}\{u_h\}$  since the quality of such an approximation is typically bounded from above by the quotient  $\frac{\lambda_h}{\lambda_{2,h}}$  which in general does not tend to 0 when  $h \rightarrow 0^+$ <sup>8</sup> (whereas this quotient is exponentially small when (A1) is satisfied).

Moreover, when (A1) is not satisfied, it is difficult to predict in which well  $\nu_h$  concentrates when it does, as explained in [LN19a]. This is again due to the fact that this prediction relies on a very accurate comparison between  $\lambda_h$  and  $\lambda_{2,h}$ . To overcome this difficulty in our work [LN19a], which precisely focuses on this situation in the double-well case, the key point relies on the fact that we are able to precisely analyse the restriction of  $L_{f, \frac{h}{2}}^{D, (0)}$  to the eigenspace associated with  $\lambda_h$  and  $\lambda_{2,h}$ .

**On the assumption (A2)**

Let us consider here  $z_1 < z_2$  and  $f: [z_1, z_2] \rightarrow \mathbb{R}$  a  $\mathcal{C}^\infty$  Morse function such that  $\{x \in [z_1, z_2], f'(x) = 0\} = \{x_1, x_2, c, d\}$  with  $z_1 < x_1 < c < x_2 < d < z_2$  and  $f(x_2) < f(x_1) < f(z_1) < f(z_2) < f(d) < f(c)$  (see Figure 4.4). This implies that  $f'(z_2) < 0$  and  $f(d) - f(x_2) > f(z_1) - f(x_1)$ . Moreover, it holds

$$\mathbf{H}_f(x_1) = f(z_1), \mathbf{H}_f(x_2) = f(d), f(z_1) = \min_{\partial\Omega} f, \mathbf{C}_{\max} \subset (c, d) \quad \text{and} \quad \partial\mathbf{C}_{\max} \cap \partial\Omega = \emptyset.$$

8. More precisely, it follows from [DLLN19a, Theorem 5] that this quotient is either of constant order or of order  $\sqrt{h}$ , according to the geometry of the level sets of the function  $f$ .

The assumption **(A1)** is satisfied but not **(A2)** (since the boundary of  $\mathbf{C}_{\max}$  does not meet  $\partial\Omega$ ). From [DLLN19a, Appendix B], there exists  $c > 0$  such that in the limit  $h \rightarrow 0^+$ :

$$\mathbb{P}_{\nu_h}[X_{\tau_{(z_1, z_2)}} = z_2] = 1 + O(e^{-\frac{c}{h}}). \quad (4.2.22)$$

Therefore, in the small temperature regime and starting from the quasi-stationary distribution, the process (4.1.1) leaves  $\Omega = (z_1, z_2)$  through  $z_2$  when  $h \rightarrow 0^+$ . Notice that  $z_2$  is not the global minimum of  $f|_{\partial\Omega}$  and is even not a generalized critical point with index 1. Consequently, the condition **[P1]** is not satisfied.

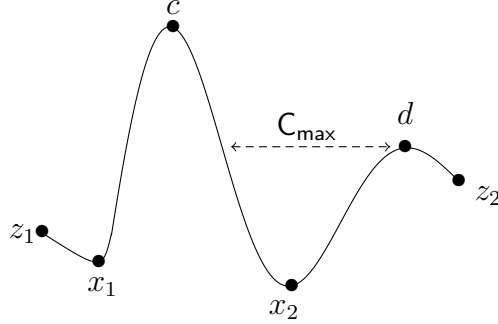


Figure 4.4 – A 1D example where **(A1)** is satisfied but not **(A2)**. In this example, **[P1]** is not satisfied.

### On the assumption **(A3)**

Let us now consider  $z_1 < z_2$  and  $f: [z_1, z_2] \rightarrow \mathbb{R}$  be a  $\mathcal{C}^\infty$  Morse function such that  $\{x \in [z_1, z_2], f'(x) = 0\} = \{x_1, z, x_2\}$ , where  $z_1 < x_1 < z < x_2 < z_2$  and  $f(x_2) < f(x_1) < f(z_1) < f(z_2) < f(z)$  (see Figure 4.5). This implies that  $f(z_1) - f(x_1) < f(z_2) - f(x_2)$ ,  $f'(z_1) < 0$ ,  $f'(z_2) > 0$ , that  $x_2$  is the global minimum of  $f$  in  $[z_1, z_2]$  and  $x_1$  is a local minimum of  $f$ , and that  $z$  is the global maximum of  $f$  in  $[z_1, z_2]$ . It then holds

$$\mathbf{H}_f(x_1) = f(z_1), \quad \mathbf{H}_f(x_2) = f(z_2), \quad f(z_1) = \min_{\partial\Omega} f, \quad \partial\mathbf{C}_{\max} \cap \partial\Omega = \{z_2\},$$

and  $\mathbf{C}_{\max} \subset (z, z_2)$ . The assumptions **(A1)** and **(A2)** are then satisfied but not **(A3)**.

Moreover, from [DLLN19a, Appendix B], there exists  $c > 0$  such that in the limit  $h \rightarrow 0^+$ :

$$\mathbb{P}_{\nu_h}[X_{\tau_{(z_1, z_2)}} = z_2] = 1 + O(e^{-\frac{c}{h}}). \quad (4.2.23)$$

Therefore, when  $X_0 \sim \nu_h$ , the law of  $X_{\tau_\Omega}$  concentrates on  $z_2$  in the limit  $h \rightarrow 0^+$ . Since  $f(z_2) > \min_{\partial\Omega} f$ , the property **[P1]** is thus not satisfied.

### On the assumption **(A4)**

We conclude this section by giving an example such that **(A4)** is not satisfied and the remainder term  $\mathcal{O}(h^{\frac{1}{4}})$  in (4.2.17) is not of the order  $\mathcal{O}(e^{-\frac{c}{h}})$  for some  $c > 0$ . To this end, let us consider  $z_1 < z_2$  and a  $\mathcal{C}^\infty$  Morse function  $f: [z_1, z_2] \rightarrow \mathbb{R}$  such that  $\{x \in [z_1, z_2], f'(x) = 0\} = \{x_1, z, x_2\}$  with  $z_1 < x_1 < z < x_2 < z_2$  and  $f(x_1) < f(x_2) < f(z) = f(z_1) = f(z_2)$  (see Figure 4.6). This implies that  $f'(z_1) < 0$

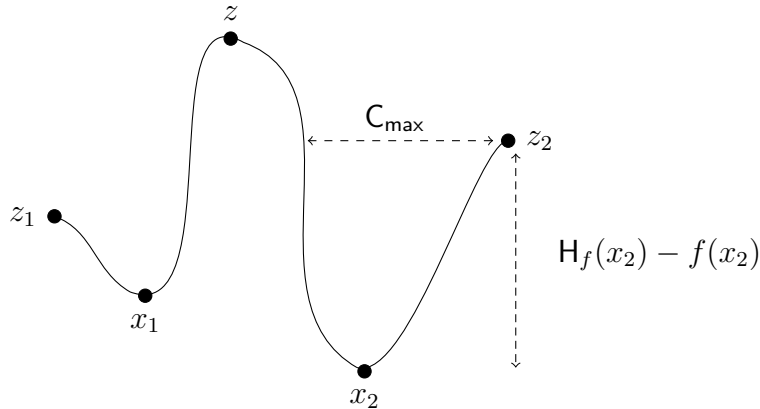


Figure 4.5 – A 1D example where **(A1)**–**(A2)** are satisfied but not **(A3)**. In this example, **[P1]** is not satisfied.

and  $f'(z_2) > 0$ , that  $x_1$  is the global minimum of  $f$  in  $[z_1, z_2]$  and  $x_2$  is a local minimum of  $f$ , and that  $z$  is a local maximum of  $f$ . In this example, it holds:

$$\mathbf{H}_f(x_1) = f(z_1) = \min_{\partial\Omega} f, \quad \mathbf{C}_{\max} = (z_1, z), \quad \partial\mathbf{C}_{\max} \cap \partial\Omega = \{z_1\},$$

and

$$\mathbf{C} = (z, z_2),$$

where  $\mathbf{C} \neq \mathbf{C}_{\max}$  is the other connected component of  $\{f < \mathbf{H}_f(x_1)\}$ . The assumptions **(A1)**, **(A2)**, and **(A3)** are then satisfied whereas, since  $\partial\mathbf{C}_{\max} \cap \partial\mathbf{C} = \{z\}$ , **(A4)** is not satisfied.

From [DLLN19a, Appendix B] together with Laplace's method, one has for  $x \in \mathbf{C}_{\max}$  in the limit  $h \rightarrow 0^+$ :

$$\mathbb{P}_x[X_{\tau(z_1, z_2)} = z_2] = \frac{\sqrt{|f''(z)|}}{2|f'(z_1)|\sqrt{\pi}}\sqrt{h} + \mathcal{O}(h).$$

Moreover, the result holds starting from  $\nu_h$  using for example Proposition 4.2.6 below): in the limit  $h \rightarrow 0^+$ ,

$$\mathbb{P}_{\nu_h}[X_{\tau(z_1, z_2)} = z_2] = \frac{\sqrt{|f''(z)|}}{2|f'(z_1)|\sqrt{\pi}}\sqrt{h} + \mathcal{O}(h).$$

In this case, the exit through  $z_2$  when  $h \rightarrow 0^+$  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.  $f(z_2) \in \mathcal{U}_{\partial\Omega}^{D,(1)}$ , see (4.2.8)) and  $f(z_2) = \min_{\partial\Omega} f$ . The remainder term  $\mathcal{O}(h^{\frac{1}{4}})$  in (4.2.17) is then not exponentially small and is actually exactly of the order  $\mathcal{O}(\sqrt{h})$  in this example.

**Remark 4.2.5.** *This can be generalized to higher-dimensional settings. In [Nec17, Proposition C.40, item 3], it is shown on some higher-dimensional cases for which the assumption **(A4)** does not hold, that the remainder terms  $\mathcal{O}(h^{\frac{1}{4}})$  in (4.2.17) and (4.2.18) are of the order  $\mathcal{O}(\sqrt{h})$ . We moreover expect that the remainder terms  $\mathcal{O}(h^{\frac{1}{4}})$  in (4.2.17) and (4.2.18) are of the order  $\mathcal{O}(\sqrt{h})$  in the setting considered in Theorem 4.2.3. Proving this fact would require some substantially finer analysis.*

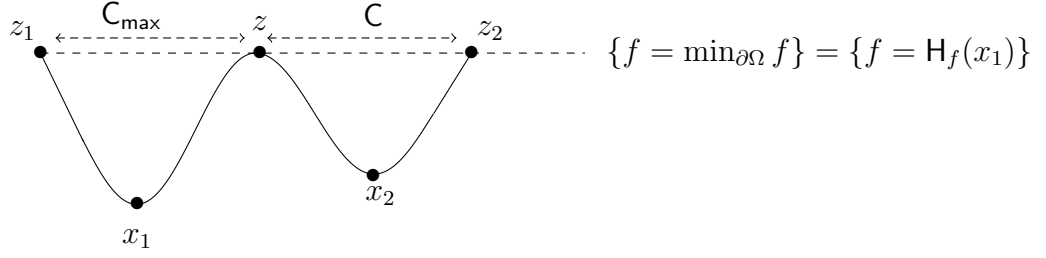


Figure 4.6 – A 1D example where **(A1)**–**(A3)** hold but not **(A4)**.

### 4.2.5 About the proofs

Let us now give a brief idea on how Theorem 4.2.3 is proven in [DLLN19a].

The main part of the proof of Theorem 4.2.3 consists in proving the asymptotic estimates on  $\mathbb{E}_{\nu_h} [F(X_{\tau_\Omega})]$ . In view of (4.2.15), in order to obtain these estimates, we study the precise asymptotic behaviour when  $h \rightarrow 0^+$  of the quantities

$$\lambda_h, \quad \int_{\Omega} u_h e^{-\frac{2}{h}f} d\mu, \quad \text{and} \quad \partial_n u_h,$$

where  $\lambda_h$  is defined by (4.2.13) and  $u_h$  by (4.2.14).

The study of the precise asymptotic behaviour of  $\lambda_h$  and of the low spectrum of  $L_{f, \frac{h}{2}}^{D, (0)}$ , which amounts, according to (see (1.3.18))

$$\Delta_{f, h}^{(0)} = 2h e^{-\frac{f}{h}} L_{f, \frac{h}{2}}^{(0)} e^{\frac{f}{h}} = 2h e^{-\frac{f}{h}} \left( \frac{h}{2} \Delta_{\mathbb{H}}^{(0)} + \nabla f \cdot \nabla \right) e^{\frac{f}{h}},$$

to study the low spectrum of the Witten Laplacian  $\Delta_{f, h}^{D, (0)}$  with Dirichlet type boundary conditions (see Section 1.2.3), has already been explained in Chapter 3 (see Theorem 3.2.2 there). We recall that this study relies on the supersymmetric structure of the Witten Laplacian which leads in this setting to the following. Let  $c > 0$  be small enough such that, for  $i \in \{0, 1\}$ , it holds, in the limit  $h \rightarrow 0^+$ ,

$$\dim \text{Ran} (\pi_h^{(i)}) = \mathbf{m}_i^D, \quad (4.2.24)$$

where  $\pi_h^{(i)} := \pi_{[0, c)}(L_{f, \frac{h}{2}}^{D, (i)})$  is the spectral projector of the self-adjoint operator  $L_{f, \frac{h}{2}}^{D, (i)} = \frac{1}{2h} e^{\frac{f}{h}} \Delta_{f, h}^{D, (i)} e^{-\frac{f}{h}}$  in  $\Lambda L^2(\Omega, e^{-\frac{2}{h}f} d\mu)$  associated with the interval  $[0, c)$  (see Theorem 1.2.5 and (1.3.18)). It then holds (see Section 1.2.3 and (1.3.18))

$$D(L_{f, \frac{h}{2}}^{D, (1)}) = \left\{ \omega \in \Lambda^1 H^2(\Omega, e^{-\frac{2}{h}f} d\mu), \mathbf{t}\omega = 0 \text{ and } \mathbf{t}d_{2f, h}^* \omega = 0 \right\}$$

and<sup>9</sup>

$$\nabla : \text{Ran} (\pi_h^{(0)}) \rightarrow \text{Ran} (\pi_h^{(1)}) \quad \text{and} \quad L_{f, \frac{h}{2}}^{D, (1)} \nabla = \nabla L_{f, \frac{h}{2}}^{D, (0)} \quad \text{on} \quad \text{Ran} (\pi_h^{(0)}). \quad (4.2.25)$$

9. Here, we a slight abuse of notation, we identify the differential  $du$  of the function  $u$  with its gradient  $\nabla u$ .

Note also the relation  $L_{f, \frac{h}{2}}^{D, (0)} = \frac{h}{2} \nabla^* \nabla$  on  $\text{Ran}(\pi_h^{(0)})$ , where  $\nabla^*$  is the adjoint of  $\nabla : \text{Ran}(\pi_h^{(0)}) \rightarrow \text{Ran}(\pi_h^{(1)})$  with respect to the scalar product on  $\Lambda L^2(\Omega, e^{-\frac{2}{h}f} d\mu)$ .

Once the asymptotic behaviour of  $\lambda_h$  and of the low spectrum of  $L_{f, \frac{h}{2}}^{D, (0)}$  has been understood by carefully analyzing the matrix of  $\nabla : \text{Ran}(\pi_h^{(0)}) \rightarrow \text{Ran}(\pi_h^{(1)})$  in bases constructed using suitable quasimodes as in Chapter 3 (see Section 3.3 and in particular Section 3.3.3 there), it is quite easy to prove Proposition 4.2.1 concerning the concentration of  $u_h e^{-\frac{2}{h}f}$  in  $\mathbf{C}_{\max}$ , which gives in particular a precise estimate on  $\int_{\Omega} u_h e^{-\frac{2}{h}f} d\mu$ . For this, we simply use the fact that  $\frac{\lambda_h}{\lambda_{2,h}}$  is exponentially small when  $h \rightarrow 0^+$  and an accurate approximation  $\tilde{u}_h$  of  $u_h$  in  $L^2(\Omega, e^{-\frac{2}{h}f} d\mu)$  given by the construction made in Section 3.3 in Chapter 3 (see Section 3.3.1, (3.3.6) and (3.3.7) there, and also (5.2.4) and the lines below in the next chapter in the simplest possible situation).

Lastly, to obtain the precise asymptotic behaviour of  $\partial_n u_h = \vec{n} \cdot \nabla u_h$ , the idea is to decompose  $\nabla u_h$ , which belongs to  $\text{Ran} \pi_h^{(1)}$  by supersymmetry (see (4.2.25)), along a natural orthonormal basis of  $\text{Ran} \pi_h^{(1)}$ . This requires in particular to show that the above accurate approximation  $\tilde{u}_h$  of  $u_h$  in  $L^2(\Omega, e^{-\frac{2}{h}f} d\mu)$  is actually an accurate approximation of  $u_h$  in  $H^1(\Omega, e^{-\frac{2}{h}f} d\mu)$ , which relies on the specific form of  $\lambda_h$  and of the above matrix of  $\nabla : \text{Ran}(\pi_h^{(0)}) \rightarrow \text{Ran}(\pi_h^{(1)})$  in suitable bases (whose study already led to the precise computation of  $\lambda_h$ !).

Then, in order to finish the proof of Theorem 4.2.3, it remains to prove asymptotic estimates on  $\mathbb{E}_x [F(X_{\tau_{\Omega}})]$  when  $x \in \mathcal{A}(\mathbf{C}_{\max})$ . To do this, we first use classical techniques for elliptic PDEs when  $x \in \mathbf{C}_{\max}$  (see in particular [DF78] in this connection). These results are then extended to arbitrary  $x \in \mathcal{A}(\mathbf{C}_{\max})$  using basic results of large deviation theory (see [FW12]).

This leads in particular to the following proposition, which connects the law of  $X_{\tau_{\Omega}}$  when  $X_0 \sim \nu_h$  and  $X_0 = x \in \mathcal{A}(\mathbf{C}_{\max})$  in the limit  $h \rightarrow 0^+$  and implies that [P2] (see Section 4.1) is satisfied for every  $x \in \mathcal{A}(\mathbf{C}_{\max})$ .

**Proposition 4.2.6.** *Assume that the assumptions (M) and (A1) are satisfied. Let us moreover assume that*

$$\min_{\mathbf{C}_{\max}} f = \min_{\Omega} f,$$

where we recall that  $\mathbf{C}_{\max}$  is introduced in (A1). Let  $K$  be a compact subset of  $\Omega$  such that  $K \subset \mathcal{A}(\mathbf{C}_{\max})$  and let  $F \in \mathcal{C}^{\infty}(\partial\Omega, \mathbb{R})$ . Then, there exists  $c > 0$  such that for all  $x \in K$ :

$$\mathbb{E}_{\nu_h} [F(X_{\tau_{\Omega}})] = \mathbb{E}_x [F(X_{\tau_{\Omega}})] + O(e^{-\frac{c}{h}})$$

in the limit  $h \rightarrow 0^+$  and uniformly in  $x \in K$ .

## 4.3 Some perspectives

### 4.3.1 Potentials with critical points on the boundary

As in Chapter 3, all the results mentioned and presented in this chapter do not consider the case of critical points on the boundary. We recall moreover that, even though the latter case is generic, it is relevant to consider the case where the potential



$f$  admits critical points on the boundary since it is the case in most applications, see indeed (1.3.38) and the discussion around in Section 1.3.3.

In order to obtain generalizations of the results presented in Section 4.2.3 in this case, we first need to obtain precise asymptotics on the low spectrum of  $L_{f, \frac{h}{2}}^{D, (0)}$ , or equivalently of  $\Delta_{f, h}^{D, (0)}$ , and we refer to Section 3.5.1 in this connection. Moreover, even though such asymptotics can be obtained without explicitly considering the Witten Laplacian acting on 1-forms  $\Delta_{f, h}^{D, (1)}$ , generalizing the results of Section 4.2.3 when  $f$  admits critical points on the boundary also relies on a good understanding of the low spectrum of  $\Delta_{f, h}^{D, (1)}$  (see for instance (4.2.24) in Section 4.2.5). In particular, the counterpart of Theorem 1.2.5 in the case of critical points on the boundary is a prerequisite for a generalization of the results stated in Section 4.2.3. This will require a careful analysis near the critical points of  $f$  in  $\partial\Omega$ . Moreover, we expect to need stronger compatibility conditions on the shape of  $\partial\Omega$  near the critical point of  $f$  than for the sole precise computation of the low spectrum of  $\Delta_{f, h}^{D, (0)}$  (see Section 3.5.1). Then, and only then, we should be able to suitably generalize Theorem 4.2.3 when  $f$  admits critical points on the boundary.

### 4.3.2 Non reversible overdamped Langevin dynamics

In Section 3.5.2 of the preceding chapter, we mentioned our recent work [LM19], in collaboration with Laurent Michel, where we prove sharp asymptotic estimates on the low spectrum of the counterpart of  $L_{f, \frac{h}{2}}^{(0)}$  for the dynamics

$$dX_t = b(X_t) + \sqrt{h} dB_t = -(1 + J)\nabla f(X_t)dt + \sqrt{h} dB_t, \quad (4.3.1)$$

that is  $L_{b, \frac{h}{2}}^{(0)} := -\frac{h}{2}\Delta + \nabla f \cdot \nabla + (J\nabla f) \cdot \nabla$ , where  $J$  is a constant skew-symmetric matrix of size  $d$ . We recall that in this case,

$$m_{f, \frac{h}{2}}(d\mu) = \left( \int_{\mathbb{R}^d} e^{-2\frac{f}{h}} d\mu \right)^{-1} e^{-2\frac{f}{h}} d\mu$$

is still an invariant measure since  $L_{b, \frac{h}{2}}^{\dagger, (0)} e^{-2\frac{f}{h}} = 0$ . Moreover, since  $J$  is constant, it holds

$$L_{b, \frac{h}{2}}^{(0)} = -\frac{h}{2} e^{2\frac{f}{h}} \operatorname{div} \left( e^{-2\frac{f}{h}} (I - J) \nabla \right) = -d_{f, \frac{h}{2}}^* (I - J) d.$$

It follows that  $L_{b, \frac{h}{2}}^{(0)}$  has in this case a natural supersymmetric extension  $L_{b, \frac{h}{2}}^{(1)}$  (but for a non symmetric ‘‘scalar product’’).

Furthermore, looking at the corresponding exit problem of some bounded domain  $\Omega$ , the process (4.3.1) still admits a unique quasi-stationary distribution on  $\Omega$  (see for example [CV17]), given by the (suitably normalized) positive principal eigenfunction of the (non self-adjoint) Dirichlet realization of  $L_{b, \frac{h}{2}}^{\dagger, (0)}$  on  $\Omega$  (whose existence follows from the Krein-Rutman theorem). Denoting by  $u_h$  some principal eigenfunction of  $L_{b, \frac{h}{2}}^{D, (0)}$ , the quasi-stationary distribution is then still given by (see (1.3.27) in the reversible case)

$$\nu_h(d\mu) := \nu_h(x) d\mu := \frac{u_h(x) e^{-2\frac{f(x)}{h}}}{\int_{\Omega} u_h e^{-2\frac{f}{h}} d\mu} d\mu.$$

In future works, we would like to adapt the quasi-stationary distribution approach in this setting in order to generalize the results stated in Section 4.2.3, when  $\partial\Omega$  admits critical points of  $f$  or not. To do this, even once the low spectrum of  $L_{b, \frac{\hbar}{2}}^{D, (0)}$  will have been precisely computed, some important analysis will still be required, in particular to properly understand the behaviour of  $L_{b, \frac{\hbar}{2}}^{D, (1)}$  near the (generalized) critical points of  $f$  in  $\Omega$  and in  $\partial\Omega$  (see the previous Section 4.3.1 in this connection). Again, the most delicate part of this analysis should concern the critical points of  $f$  in  $\partial\Omega$ , since for its critical points in  $\Omega$ , it should be possible to adapt the analysis done in [HHS11] for the Kramers-Fokker-Planck operator.



# Chapter 5

## Exit from a metastable state: sharp asymptotics of the first exit point distribution

We present in this chapter the main results of [DLLN17b]. They are also summarized in the the proceedings type works [DLLN17a, LLN18].

### 5.1 Markov jump process and Eyring-Kramers law

#### 5.1.1 Kinetic Monte Carlo methods

Let  $f : \mathbb{R}^d \rightarrow \mathbb{R}$  be a Morse function,  $\Omega \subset \mathbb{R}^d$  be a (smooth open connected) domain of the configuration space, and let us assume that the overdamped Langevin process<sup>1</sup>

$$dX_t = -\nabla f(X_t)dt + \sqrt{h} dB_t \quad (5.1.1)$$

is initially distributed according to a probability measure  $\mu$  (i.e.  $X_0 \sim \mu$ ) which is supported in  $\Omega$  and for which the exit event from  $\Omega$  is metastable (see Definition 1.3.4 in Section 1.3.3). Let us denote by  $(\Omega_i)_{i=1, \dots, n}$  the surrounding domains of  $\Omega$  (see Figure 5.1), each of them corresponding to a macroscopic state of the system. Many reduced models and algorithms rely on the fact that the exit event from  $\Omega$ , i.e. the next visited state by the process (5.1.1) among the  $\Omega_i$ 's as well as the time spent by the process (5.1.1) in  $\Omega$ , is efficiently approximated by a Markov jump process using kinetic Monte Carlo methods [Sch98, SS13, Vot05, Wal03, Cam14, FYY14].

Kinetic Monte Carlo methods simulate a Markov jump process in a discrete state space. To use a kinetic Monte Carlo algorithm in order to sample the exit event from  $\Omega$ , one needs, for  $i \in \{1, \dots, n\}$ , the transition rate  $k_{0i}$  to go from the state  $\Omega$  to the state  $\Omega_i$ . A kinetic Monte Carlo algorithm generates the next visited state  $Y$  among the  $\Omega_i$ 's and the time  $T$  spent in  $\Omega$  for the process (5.1.1) as follows:

1. First sample  $T$  as an exponential random variable with parameter  $\sum_{i=1}^n k_{0i}$ , i.e.:

$$T \sim \mathcal{E}\left(\sum_{i=1}^n k_{0i}\right). \quad (5.1.2)$$

---

1. As in Chapter 4, the scaling in  $h$  considered here is different from the one adopted in (1.3.1) in Section 1.3.

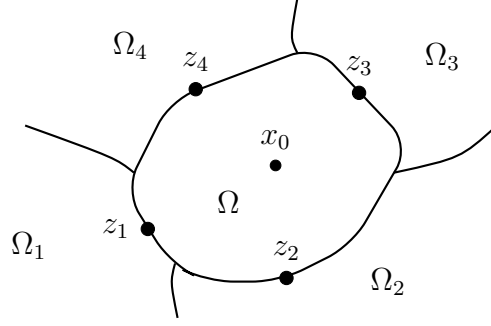


Figure 5.1 – A domain  $\Omega$  and its the surrounding domains  $(\Omega_i)_{i=1,\dots,4}$ , where  $x_0$  is the global minimum of  $f$  in  $\Omega$  and  $\{z_i\} = \operatorname{argmin}_{\partial\Omega\cap\Omega_i} f$  ( $i \in \{1, 2, 3, 4\}$ ).

2. Then, sample the next visited state  $Y$  independently from  $T$ , i.e

$$Y \perp\!\!\!\perp T \quad (5.1.3)$$

using the following law : for all  $i \in \{1, \dots, n\}$ ,

$$\mathbb{P}[Y = i] = \frac{k_{0i}}{\sum_{\ell=1}^n k_{0\ell}}. \quad (5.1.4)$$

**Remark 5.1.1.** *Let us give an equivalent way to sample  $T$  and  $Y$  in a Monte Carlo method. Let  $(\tau_i)_{i \in \{1, \dots, n\}}$  be  $n$  independent random variables such that for all  $i \in \{1, \dots, n\}$ ,  $\tau_i$  is exponentially distributed with parameter  $k_{0i}$ . Then, the couple  $(T, Y)$  has the same law as  $(\min_{j \in \{1, \dots, n\}} \tau_j, \operatorname{argmin}_{j \in \{1, \dots, n\}} \tau_j)$ .*

## 5.1.2 Eyring-Kramers law

In practice, the transition rates  $(k_{0i})_{i \in \{1, \dots, n\}}$  are computed using the Eyring-Kramers formula [HTB90, Vot05]:

$$k_{0i} = A_i e^{-\frac{2}{\hbar}(f(z_i) - f(x_0))}, \quad (5.1.5)$$

where  $A_i > 0$  is a prefactor,  $x_0$  is the global minimum of  $f$  on  $\Omega$  (assumed to be unique), and  $\{z_i\} = \operatorname{argmin}_{z \in \partial\Omega_i} f(z)$ , where  $\partial\Omega_i$  denotes the part of the boundary  $\partial\Omega$  which connects the region  $\Omega$  (numbered 0) with the neighboring region numbered  $i$ , see Figure 5.1. The prefactor  $A_i$  depends on the dynamics under consideration and on the potential function  $f$  around  $x_0$  and  $z_i$ .

Moreover, the domain  $\Omega$  is in practice the basin of attraction of  $x_0$  for the dynamics  $\dot{x} = -\nabla f(x)$ . For  $i \in \{1, \dots, n\}$ , the point  $z_i$  is then a saddle point (i.e. a critical point with index 1) of  $f$ , and the prefactor  $A_i$  writes

$$A_i = \frac{|\lambda(z_i)|}{2\pi} \frac{\sqrt{|\det \operatorname{Hess} f(x_0)|}}{\sqrt{|\det \operatorname{Hess} f(z_i)|}}, \quad (5.1.6)$$

where  $\lambda(z_i)$  is the negative eigenvalue of  $\operatorname{Hess} f(z_i)$ . This formula has been obtained in the small temperature regime by Kramers in [Kra40] but also by many authors previously (see Sections 1.3.2 and 1.3.3, and the exhaustive review of the literature

reported in [HTB90]). We also refer to [HTB90] for generalizations to the Langevin dynamics (see also Section 5.3.2).

In the work [DLLN17b], we consider a slightly different situation where the domain  $\Omega$  is a confining well (containing  $x_0$ ) inside the basin of attraction of  $x_0$  for the dynamics  $\dot{x} = -\nabla f(x)$ , i.e. satisfies  $\partial_n f > 0$  on  $\partial\Omega$ . Then, for  $i \in \{1, \dots, n\}$ , the point  $z_i$  is not a saddle point of  $f$  in the usual sense (since  $\nabla f(z_i) \neq 0$ ) but a generalized saddle point in the sense of Section 3.1.3 in the case of Dirichlet type boundary conditions (see (3.1.5) there and the discussion below). This leads in particular to the following formula instead of (5.1.6) (see (1.3.33), where  $2h$  has to be replaced by  $h$  according to the different scaling in  $h$  there, and the discussion around in Section 1.3.3):

$$A_i = \frac{\partial_n f(z_i)}{\sqrt{\pi h}} \frac{\sqrt{\det \text{Hess } f(x_0)}}{\sqrt{\det \text{Hess } f|_{\partial\Omega}(z_i)}}. \quad (5.1.7)$$

**Remark 5.1.2.** *In the Physics literature, the approximation of the macroscopic evolution of the system with a Markov jump process with transition rates computed with the Eyring-Kramers formula (5.1.5)–(5.1.6) is sometimes called the Harmonic Transition State Theory, see [Mar15, Vin57].*

### 5.1.3 Markov jump process and quasi-stationary distribution

We assume more generally from now on that  $\bar{\Omega}$  is a  $C^\infty$  oriented compact and connected Riemannian manifold of dimension  $d$  with interior  $\Omega$  and boundary  $\partial\Omega$ . As explained in Section 1.3.3, if the process solution to (5.1.1) remains for a sufficiently long time in the domain  $\Omega$ , it is natural to consider the exit event starting from the quasi-stationary distribution attached to  $\Omega$  (see Definition 1.3.1 and Proposition 1.3.3 in Section 1.3.3).

We recall here from Sections 1.3.3 and 4.2.3 that the unbounded operator

$$L_{f, \frac{h}{2}}^{D, (0)} := \frac{h}{2} \Delta_{\text{H}}^{(0)} + \nabla f \cdot \nabla \quad \text{with domain} \quad D(L_{f, \frac{h}{2}}^{D, (0)}) := (H_0^1 \cap H^2)(\Omega, e^{-\frac{2}{h}f} d\mu)$$

is self-adjoint positive with a compact resolvent in  $L^2(\Omega, e^{-\frac{2}{h}f} d\mu)$ , that its principal eigenvalue

$$\lambda_h = \lambda_{1,h} := \min\{\text{Sp}(L_{f, \frac{h}{2}}^{D, (0)})\} > 0 \quad (5.1.8)$$

is simple and that if  $u_h$  denotes some associated eigenfunction (which then has a sign on  $\Omega$ ), the quasi-stationary distribution  $\nu_h$  associated with  $\Omega$  and (5.1.1) is the probability measure on  $\Omega$  defined by

$$\nu_h(d\mu) = \frac{u_h e^{-\frac{2}{h}f}}{\int_{\Omega} u_h e^{-\frac{2}{h}f} d\mu} d\mu. \quad (5.1.9)$$

In the sequel, we assume moreover without loss of generality that

$$L_{f, \frac{h}{2}}^{D, (0)} u_h = \lambda_h u_h, \quad u_h > 0 \text{ on } \Omega, \quad \text{and} \quad \int_{\Omega} u_h^2 e^{-\frac{2}{h}f} d\mu = 1. \quad (5.1.10)$$

---

2. We adopt here the same convention as in Chapter 4, differing from the one adopted in the other chapters where  $\Omega$  was assumed to be closed.

We also recall from Proposition 1.3.5 that when the dynamics  $(X_t)_{t \geq 0}$  solution to (5.1.1) is initially distributed according to  $\nu_h$ :

- the first exit time from  $\Omega$ ,  $\tau_\Omega$ , and the first exit point  $X_{\tau_\Omega}$  are independant,
- $\tau_\Omega$  is exponentially distributed with parameter  $\lambda_h$  (and then  $\mathbb{E}_{\nu_h}(\tau_\Omega) = \frac{1}{\lambda_h}$ ),
- and the law of  $X_{\tau_\Omega}$  has a density with respect to the Lebesgue measure on  $\partial\Omega$  given by

$$z \in \partial\Omega \mapsto -\frac{h}{2\lambda_h} \frac{\partial_n u_h(z) e^{-\frac{2}{h}f(z)}}{\int_\Omega u_h e^{-\frac{2}{h}f} d\mu}. \quad (5.1.11)$$

This shows that, starting from the quasi-stationary distribution in the domain  $\Omega$ , the exit event  $(\tau_\Omega, X_{\tau_\Omega})$  can be modeled by a Markov jump process *without any approximation*. Indeed, using the notation of Section 5.1.1, let us consider that  $\Omega \subset \mathbb{R}^d$  is associated with the state 0 and surrounded by  $n$  neighbouring states associated with domains  $(\Omega_i)_{i=1, \dots, n}$  (see Figure 5.1 for a schematic representation when  $n = 4$ ), and let us define the following transition rates:

$$\forall i \in \{1, \dots, n\}, k_{0i} := \frac{\mathbb{P}_{\nu_h}(X_{\tau_\Omega} \in \partial\Omega \cap \partial\Omega_i)}{\mathbb{E}_{\nu_h}(\tau_\Omega)}. \quad (5.1.12)$$

Then the exit event  $(\tau_\Omega, X_{\tau_\Omega})$  is such that:

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

These are exactly the properties (5.1.2)–(5.1.4) which are required to define a transition using a Markov jump process. The quasi-stationary distribution can thus be used to parameterize the underlying jump Markov process when the domains are metastable (see Definition 1.3.4).

The question we try to answer in our work [DLLN17b] is then the following: when  $\Omega$  is a confining well and  $X_0 \sim \nu_h$ , what is the error introduced when one approximates the exact rates (5.1.12) using the Eyring-Kramers formula given by (5.1.5) and (5.1.7). Since in this case  $\mathbb{E}_{\nu_h}(\tau_\Omega) = \frac{1}{\lambda_h}$ , note that one has from (5.1.11) the following formula for the exact rates:

$$k_{0i} = -\frac{h}{2} \frac{\int_{\partial\Omega \cap \partial\Omega_i} \partial_n u_h e^{-\frac{2}{h}f} d\mu_{\partial\Omega}}{\int_\Omega u_h e^{-\frac{2}{h}f} d\mu}. \quad (5.1.13)$$

In [DLLN17b], we prove that in the small temperature regime  $h \rightarrow 0^+$ , the exact rates (5.1.13) can indeed be accurately approximated by the Eyring-Kramers formula given by (5.1.5) and (5.1.7) with explicit error bounds (see Corollary 5.2.8 below). 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 1.3.3 and in particular (1.3.30) there.

## 5.2 Results for a confining well

### 5.2.1 An adapted Agmon distance

Our results hold under some geometric assumptions which require to introduce some natural Agmon distance quantifying the decay of the eigenfunctions of  $L_{f, \frac{h}{2}}^{D, (1)}$  (or equivalently of the Witten Laplacian  $\Delta_{f, h}^{D, (1)}$  with Dirichlet type boundary conditions, see Section 1.2.3) away from the (generalized) critical points of  $f$  (see for example [Sim84, HS84, DS99] for more material about the Agmon distance on manifolds without boundary).

**Definition 5.2.1.** *Let  $\bar{\Omega}$  be a  $C^\infty$  oriented connected compact Riemannian manifold of dimension  $d$  with boundary  $\partial\Omega$  and  $f : \bar{\Omega} \rightarrow \mathbb{R}$  be a  $C^\infty$  function. Define  $g : \bar{\Omega} \rightarrow \mathbb{R}$  by:*

$$\text{for all } x \in \Omega, g(x) = |\nabla f(x)| \quad \text{and} \quad \text{for all } x \in \partial\Omega, g(x) = |\nabla_T f(x)|, \quad (5.2.1)$$

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  $\gamma : I \rightarrow \bar{\Omega}$ , where  $I \subset \mathbb{R}$  is an interval, by

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

Let us recall that the Rademacher's theorem (see for example [EG15]) 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 adapted to our problem.

**Definition 5.2.2.** *Let  $g$  be the function introduced in Definition 5.2.1. The Agmon distance between  $x \in \bar{\Omega}$  and  $y \in \bar{\Omega}$  is defined by*

$$d_a(x, y) := \inf_{\gamma \in \text{Lip}(x, y)} L(\gamma, (0, 1)), \quad (5.2.2)$$

where  $\text{Lip}(x, y)$  is the set of curve  $\gamma : [0, 1] \rightarrow \bar{\Omega}$  which are Lipschitz with  $\gamma(0) = x$  and  $\gamma(1) = y$ .

The Agmon distance  $d_a$  is obviously symmetric, nonnegative, and satisfies the triangular inequality. It is moreover a distance when the critical points of  $f$  and of  $f|_{\partial\Omega}$  are isolated.

When  $\bar{\Omega}$  is a manifold without boundary, the Agmon distance  $d_a$  introduced in Definition 5.2.2 coincides with the Agmon distance defined in [HS85c, Appendix 2]. It satisfies in particular  $|\nabla d_a| = |\nabla f|$  near the (non degenerate) critical points of  $f$  in  $\Omega$ . When  $\partial\Omega \neq \emptyset$ , it moreover also satisfies  $|\nabla d_a| = |\nabla f|$  near the (non degenerate) critical points of  $f|_{\partial\Omega}$ . This property, crucial in the analysis led in [DLLN17b], requires to use the tangential gradient of  $f$  on  $\partial\Omega$  in the definition of  $d_a$  (see (5.2.1)). We refer to [DLLN17b, Section 3] for more details about  $d_a$ .

### 5.2.2 Main results

Before stating the main results of [DLLN17b], we first introduce some notation and some preliminary results.



The following hypotheses specify in particular what we mean by a confining well for the potential  $f$  (see also Section 1.3.3).

**[H1]** The function  $f : \bar{\Omega} \rightarrow \mathbb{R}$  is a Morse function without any critical on  $\partial\Omega$  and  $f|_{\partial\Omega}$  is a Morse function.

**[H2]** The function  $f$  has a unique global minimum  $x_0 \in \Omega$  in  $\bar{\Omega}$ , i.e.

$$\min_{\partial\Omega} f > \min_{\bar{\Omega}} f = \min_{\Omega} f = f(x_0),$$

and  $x_0$  is the unique critical point of  $f$  in  $\bar{\Omega}$ . We assume moreover that  $f|_{\partial\Omega}$  has precisely  $n \geq 1$  local minima  $z_1, \dots, z_n$ , ordered such that

$$f(z_1) \leq f(z_2) \leq \dots \leq f(z_n).$$

**[H3]** It holds  $\partial_n f > 0$  on  $\partial\Omega$ .

When these assumptions are satisfied, note that according to the notation of Section 3.1.3 in the Dirichlet setting (see (3.1.4) and (3.1.5)), it holds  $\mathbf{m}_0^D = 1$  and  $\{x_0\} = \mathcal{U}_{\bar{\Omega}}^{D,(0)}$ , and

$$\mathbf{m}_1^D = n \quad \text{and} \quad \mathcal{U}_{\bar{\Omega}}^{D,(1)} = \mathcal{U}_{\partial\Omega}^{D,(1)} = \{z_1, \dots, z_n\}.$$

In the sequel, we denote moreover by  $n_0 \in \{1, \dots, n\}$  the number of points in  $\arg \min f|_{\partial\Omega}$ :

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

Note that Theorem 3.2.2 and (3.2.1) in Chapter 3 (see also [HN06, DLLN19b]) then immediately lead to the following proposition:

**Proposition 5.2.3.** *Assume that [H1], [H2], and [H3] hold. Then, the principal eigenvalue  $\lambda_h$  of  $L_{f, \frac{h}{2}}^{D,(0)}(\Omega)$  satisfies in the limit  $h \rightarrow 0^+$ :*

$$\lambda_h = \frac{\sqrt{\det \text{Hess } f(x_0)}}{\sqrt{\pi h}} \sum_{i=1}^{n_0} \frac{\partial_n f(z_i)}{\sqrt{\det \text{Hess } f|_{\partial\Omega}(z_i)}} e^{-\frac{2}{h}(f(z_1)-f(x_0))} (1 + \mathcal{O}(h)), \quad (5.2.3)$$

where the term  $\mathcal{O}(h)$  admits a full asymptotic expansion in  $h$ .

Moreover, Proposition 4.2.1 in Chapter 4 immediately implies the following result:

**Proposition 5.2.4.** *Assume that [H1], [H2], and [H3] hold. Then, when  $h \rightarrow 0^+$ , it holds*

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

where  $u_h$  is defined by (5.1.10) and the term  $\mathcal{O}(h)$  admits a full asymptotic expansion in  $h$ .

We now 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 that for any  $x \in \partial\Omega$ ,  $\nabla_T f(x)$  denotes the tangential gradient of  $f$  on  $\partial\Omega$ .

**Definition 5.2.5.** *Assume that [H1] holds. For each local minimum  $z \in \partial\Omega$ , one denotes by  $B_z \subset \partial\Omega$  the basin of attraction in  $\partial\Omega$  of  $z$  for the dynamics  $\dot{x} = -\nabla_T f(x)$  in  $\partial\Omega$ . We recall that  $B_z$  is an open subset of  $\partial\Omega$  and we additionally define  $B_z^c := \partial\Omega \setminus B_z$ .*

Note in particular that one obviously has  $f(x) \geq f(z)$  for each local minimum  $z \in \partial\Omega$  and  $x \in B_z$ .

In view of (5.1.11) and (5.1.13), we need to estimate three quantities in order to analyze the exit point density and the asymptotic of the transition rates in the regime  $h \rightarrow 0^+$ :  $\lambda_h$  and  $\int_{\Omega} u_h e^{-\frac{2}{h}f}$ , where  $(\lambda_h, u_h)$  is defined by (5.1.8) and (5.1.10), and  $\int_{\Sigma} (\partial_n u_h) e^{-\frac{2}{h}f}$  for a subset  $\Sigma$  of  $\partial\Omega$ . The two first quantities are already estimated thanks to Propositions 5.2.3 and 5.2.4, and the following result gives an estimate on  $\int_{\Sigma} (\partial_n u_h) e^{-\frac{2}{h}f}$  when  $\Sigma \subset B_{z_i}$  for some local minimum  $z_i$  of  $f|_{\partial\Omega}$ .

**Theorem 5.2.6.** *Assume that [H1], [H2], and [H3] hold, and that*

—  $\forall i \in \{1, \dots, n\}$ ,

$$\inf_{z \in B_{z_i}^c} d_a(z, z_i) > \max[f(z_n) - f(z_i), f(z_i) - f(z_1)], \quad (5.2.4)$$

— and

$$f(z_1) - f(x_0) > f(z_n) - f(z_1). \quad (5.2.5)$$

*Then, for all  $i \in \{1, \dots, n\}$  and all open set  $\Sigma_i \subset \partial\Omega$  containing  $z_i$  and such that  $\bar{\Sigma}_i \subset B_{z_i}$ , it holds in the limit  $h \rightarrow 0^+$ ,*

$$\int_{\Sigma_i} \partial_n u_h e^{-\frac{2}{h}f} d\mu_{\partial\Omega} = A_i(h) e^{-\frac{2f(z_i) - f(x_0)}{h}} (1 + \mathcal{O}(h)), \quad (5.2.6)$$

*where  $u_h$  is defined by (5.1.10), the term  $\mathcal{O}(h)$  admits a full asymptotic expansion in  $h$ , and*

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

Theorem 5.2.6 is the main contribution of our work [DLLN19a]. Together with Propositions 5.2.3 and 5.2.4, it has the consequences stated below on the first exit point distribution and on the estimate of the exact rates  $(k_{0i})_{i \in \{1, \dots, n\}}$  using the Eyring-Kramers formula (see Section 5.1.3). We recall that  $(X_t)_{t \geq 0}$  denotes the solution to (5.1.1), that  $\tau_{\Omega}$  is the first exit time from the domain  $\Omega$ , and that  $\nu_h$  is the quasi-stationary distribution associated with  $(X_t)_{t \geq 0}$  and  $\Omega$  (see (5.1.9)).

**Corollary 5.2.7.** *Under the hypotheses of Theorem 5.2.6, for every  $i \in \{1, \dots, n\}$  and every open set  $\Sigma_i \subset \partial\Omega$  containing  $z_i$  such that  $\bar{\Sigma}_i \subset B_{z_i}$ , it holds in the limit  $h \rightarrow 0^+$ :*

$$\mathbb{P}_{\nu_h} [X_{\tau_{\Omega}} \in \Sigma_i] = \frac{\frac{\partial_n f(z_i)}{\sqrt{\det \text{Hess } f|_{\partial\Omega}(z_i)}}}{\sum_{k=1}^{n_0} \frac{\partial_n f(z_k)}{\sqrt{\det \text{Hess } f|_{\partial\Omega}(z_k)}}} e^{-\frac{2}{h}(f(z_i) - f(z_1))} (1 + \mathcal{O}(h)), \quad (5.2.7)$$

*where the term  $\mathcal{O}(h)$  admits a full asymptotic expansion in  $h$ .*

Note in passing that as a simple consequence of Corollary 5.2.7, we recover the fact that  $(X_t)_{t \geq 0}$  leaves  $\Omega$  around the global minima  $z_1, \dots, z_{n_0}$  of  $f$  on  $\partial\Omega$  (see Section 1.3.3 and Chapter 4, and [DLLN19b]).

**Corollary 5.2.8.** *Let  $i \in \{1, \dots, n\}$  and  $\Sigma_i \subset \partial\Omega$  be an open set containing  $z_i$  such that  $\bar{\Sigma}_i \subset B_{z_i}$ . Using the notation of Section 5.1.3, assume that  $\Sigma_i$  is the common boundary between  $\Omega$  and another domain  $\Omega_i \subset \mathbb{R}^d$ . Under the hypotheses of Theorem 5.2.6, the transition rate to go from  $\Omega$  to  $\Omega_i$  given by (5.1.12) satisfies, in the limit  $h \rightarrow 0^+$ ,*

$$k_{0i} = \frac{1}{\sqrt{\pi h}} \partial_n f(z_i) \frac{\sqrt{\det \text{Hess } f(x_0)}}{\sqrt{\det \text{Hess } f|_{\partial\Omega}(z_i)}} e^{-\frac{2}{h}(f(z_i) - f(x_0))} (1 + \mathcal{O}(h)), \quad (5.2.8)$$

where the term  $\mathcal{O}(h)$  admits a full asymptotic expansion in  $h$ .

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  $z_1, \dots, z_n$  of  $f$  on  $\partial\Omega$  are therefore not saddle points of  $f$  but generalized saddle points (see (3.1.5) and the discussion below in Section 3.1.3). We refer to (5.3.1) in Section 5.3.1 for the expected formula when  $z_1, \dots, z_n$  are usual saddle points of  $f$ .

Let us conclude this section with the following result which generalizes Corollary 5.2.7 to sufficiently low in energy deterministic initial conditions. We refer to [DLLN17b, Section 1.6.6] for other generalisations of Theorem 5.2.6 and Corollary 5.2.7.

**Corollary 5.2.9.** *Let us assume that all the hypotheses of Corollary 5.2.7 are satisfied, and that in addition there exists  $i_0 \in \{2, \dots, n\}$  such that*

$$2(f(z_{i_0}) - f(z_1)) < f(z_1) - f(x_0). \quad (5.2.9)$$

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

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

Then, for  $i \in \{1, \dots, j\}$  and for every open set  $\Sigma_i \subset \partial\Omega$  containing  $z_i$  and such that  $\bar{\Sigma}_i \subset B_{z_i}$ , we have uniformly in  $x \in \{f \leq \alpha\} \cap \Omega$  in the limit  $h \rightarrow 0^+$ :

$$\mathbb{P}_x[X_{\tau_\Omega} \in \Sigma_i] = \frac{\frac{\partial_n f(z_i)}{\sqrt{\det \text{Hess } f|_{\partial\Omega}(z_i)}}}{\sum_{k=1}^{n_0} \frac{\partial_n f(z_k)}{\sqrt{\det \text{Hess } f|_{\partial\Omega}(z_k)}}} e^{-\frac{2}{h}(f(z_i) - f(z_1))} (1 + \mathcal{O}(h)). \quad (5.2.10)$$

Let us give a simple example to illustrate this result. In a situation where  $n = 2$  and  $f(z_2) > f(z_1)$ , 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 when  $X_0 = x$  for  $x \in \{f < 2f(z_1) - f(z_2)\} \cap \Omega$  under the assumption  $f(z_1) - f(x_0) > 2(f(z_2) - f(z_1))$ , which is a stronger assumption than (5.2.5).

### 5.2.3 About the hypotheses

#### On the geometric assumption (5.2.4)

The question we would like to address here is the following: is the assumption (5.2.4) necessary for the result on the exit point density (5.2.7) 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  $\Omega$  is defined by (see Figure 5.2):

$$\Omega = (-1, 1)^2 \cup \{(x, y) \mid x^2 + (y - 1)^2 < 1\} \cup \{(x, y) \mid x^2 + (y + 1)^2 < 1\}.$$

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  $\Omega$ , namely the global minimum  $x_0 = (a/2, 0)$ . Let us check that the assumptions of Theorem 5.2.6 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, from the analysis on the Agmon distance  $d_a$  led in [DLLN17b, Section 3], the inequalities

$$d_a(z_1, B_{z_1}^c) > f(z_2) - f(z_1) \quad \text{and} \quad d_a(z_2, B_{z_2}^c) > f(z_2) - f(z_1)$$

are satisfied (see [DLLN17b, Section 1.6.2] for details).

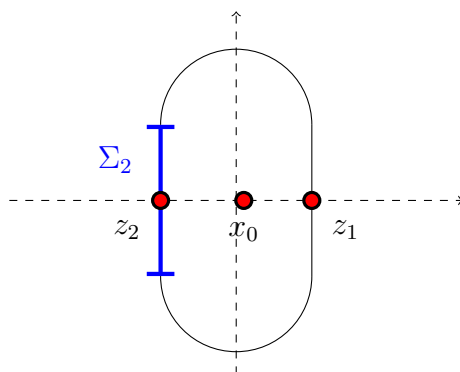


Figure 5.2 – The domain  $\Omega$ .

Let us now consider the segment  $\Sigma_2$  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 Corollary 5.2.7, we expect that, in the limit  $h \rightarrow 0^+$ ,

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

where

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

The function  $G$  is compared for various values of  $h$  to the numerically estimated function  $F$  defined by  $F\left(\frac{2}{h}\right) = \ln(\mathbb{P}_{\nu_h}[X_{\tau_\Omega} \in \Sigma_2])$ . In practice, the quasi-stationary distribution  $\nu_h$  is sampled using a Fleming-Viot particle system (the convergence diagnostics is based on a Gelman-Rubin statistics, see [BLS15]) 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  $6 \times 10^5$  particles distributed according to the quasi-stationary distribution  $\nu_h$ . The dynamics (5.1.1) is discretized in time using an Euler-Maruyama scheme with a timestep  $\Delta t = 2.10^{-3}$  on Figure 5.3. We observe on the latter figure an excellent agreement between the theory and the numerical results.

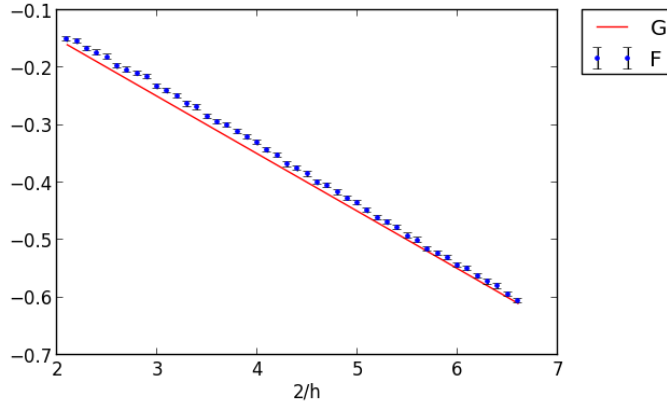


Figure 5.3 – Logarithm of the probability  $\mathbb{P}_{\nu_h}(X_{\tau_\Omega} \in \Sigma_2)$  as a function of  $\frac{2}{h}$ : comparison of the theoretical result function ( $G$ ) with the numerical result (function  $F$ ,  $\Delta t = 2.10^{-3}$ );  $a = 1/20$ .

Now, the potential function  $f$  is modified such that the assumption (5.2.4) is not satisfied anymore. More precisely, the potential function is

$$f(x, y) = (y^2 - 2a(x))^3 \quad \text{with} \quad a(x) = a_1x^2 + b_1x + 0.5,$$

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  $f(z_2) = -8(a(-1))^3 > 0 > f(z_1)$ . 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  $B_{z_2}^c$  (at the points  $(1, -1/\sqrt{2}) \in B_{z_2}^c$  and  $(1, 1/\sqrt{2}) \in B_{z_2}^c$ ) so that  $\inf_{z \in B_{z_2}^c} d_a(z, z_2) < f(z_2) - f(z_1)$ . Indeed, in that case assumption (5.2.4) is not satisfied since

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

Notice that  $\text{Hess } f|_{\partial\Omega}(z_1)$  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  $h \rightarrow 0^+$ , we observe a discrepancy on the prefactors, see Figure 5.4.

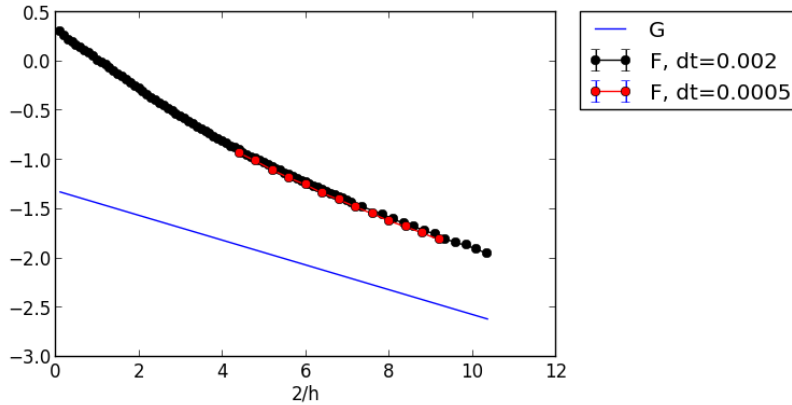


Figure 5.4 – Logarithm of the probability  $\mathbb{P}_{\nu_h}(X_{\tau_\Omega} \in \Sigma_2)$  as a function of  $\frac{2}{h}$ : comparison of the theoretical result function ( $G$ ) with the numerical result (function  $F$ ,  $\Delta t = 2.10^{-3}$  and  $\Delta t = 5.10^{-4}$ ).

Therefore, it seems that assumption (5.2.4) 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 (5.2.5) and (5.2.9)

To discuss the necessity of the assumptions (5.2.9) in Corollary 5.2.9 and (5.2.5) in Corollary 5.2.7, we consider a one-dimensional case, where the law of  $X_{\tau_\Omega}$  when  $X_0 = x$  has an explicit expression. Let  $f : \mathbb{R} \rightarrow \mathbb{R}$  be  $\mathcal{C}^\infty$  and let  $z_1, z_2 \in \mathbb{R}$  be 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 that  $f$  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]** to **[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 problem

$$L_{f, \frac{h}{2}}^{(0)} w_h = -\frac{h}{2} w_h'' + w_h' f' = 0, \quad w_h(z_1) = 0, \quad w_h(z_2) = 1.$$

Therefore, one has for  $x \in [z_1, z_2]$ :

$$w_h(x) = \int_{z_1}^x e^{\frac{2}{h} f} d\mu \left( \int_{z_1}^{z_2} e^{\frac{2}{h} f} d\mu \right)^{-1}.$$

Let  $x \in [z_1, z_2]$ . Using Laplace's method, it holds in the limit  $h \rightarrow 0^+$ :

- if  $f(x) < f(z_1)$ ,

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

- if  $f(x) = f(z_1)$  and  $x \neq z_1$ ,

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

– and if  $f(x) > f(z_1)$ ,

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

Therefore, in dimension one, the estimate (5.2.10) holds if and only if  $x \in \{f < f(z_1)\}$ . In accordance with Corollary 5.2.9, the asymptotic (5.2.10) only holds for initial conditions which are sufficiently low in energy. However, we observe that in this simple one-dimensional setting, the assumption (5.2.9) is not needed, but we do not know if the results of Corollary 5.2.9 hold in general without this assumption.

Let us now discuss the assumption (5.2.5) in the framework of Theorem 5.2.6 and Corollary 5.2.7. From (5.1.9), one has:

$$\mathbb{P}_{\nu_h}[X_{\tau_{(z_1, z_2)}} = z_2] = \int_{z_1}^{z_2} \mathbb{P}_x[X_{\tau_{(z_1, z_2)}} = z_2] d\nu_h = \frac{\int_{z_1}^{z_2} u_h w_h e^{-\frac{2}{\hbar}f} d\mu}{\int_{z_1}^{z_2} u_h e^{-\frac{2}{\hbar}f} d\mu}.$$

From basic estimates proven in [DLLN17b], one has for any  $\delta > 0$ , in the limit  $h \rightarrow 0^+$  (see Section 1.6.2 there for details):

$$\mathbb{P}_{\nu_h}[X_{\tau_{(z_1, z_2)}} = z_2] = -\frac{f'(z_2)}{f'(z_1)} e^{-\frac{2}{\hbar}(f(z_2)-f(z_1))} (1 + \mathcal{O}(h) + \mathcal{O}(e^{-\frac{1}{\hbar}(3f(z_1)-f(z_2)-2f(x_0)-\delta)})).$$

Therefore, the result of Corollary 5.2.7 holds if

$$2(f(z_1) - f(x_0)) > f(z_2) - f(z_1). \quad (5.2.11)$$

This explicit computation in dimension one then shows that the result of Corollary 1 indeed requires an assumption of the type: the height  $f(z_1) - f(x_0)$  of the energy barrier to leave the well is sufficiently large compared to the largest difference in energy of the saddle points  $f(z_2) - f(z_1)$ . Notice that (5.2.11) differs from (5.2.5) by a multiplicative factor  $\frac{1}{2}$ . We do not know if the results of Corollary 5.2.7 hold in general under the weaker assumption (5.2.11). Finally, let us mention that when  $d = 1$ , (5.2.4) is always satisfied.

## 5.2.4 About the proofs

Let us now give a brief idea on how Theorem 5.2.6 is proven in [DLLN17b].

As in Section 4.2.5 in Chapter 4, we have, under [H1]–[H3] and with the notation of Section 5.2.2:

— the existence of  $c > 0$  such that

$$\dim \text{Ran}(\pi_h^{(0)}) = 1 \quad \text{and} \quad \dim \text{Ran}(\pi_h^{(1)}) = n,$$

where, for  $i \in \{0, 1\}$ ,  $\pi_h^{(i)} := \pi_{[0, c)}(L_{f, \frac{h}{2}}^{D, (i)})$  is the spectral projector of the self-adjoint operator  $L_{f, \frac{h}{2}}^{D, (i)} = \frac{1}{2h} e^{\frac{f}{h}} \Delta_{f, h}^{D, (i)} e^{-\frac{f}{h}}$  in  $\Lambda L^2(\Omega, e^{-\frac{2}{h}f} d\mu)$  associated with the interval  $[0, c)$ ,

— the supersymmetric relations<sup>3</sup>

$$L_{f, \frac{h}{2}}^{D,(1)} \nabla = \nabla L_{f, \frac{h}{2}}^{D,(0)} \quad \text{and} \quad L_{f, \frac{h}{2}}^{D,(0)} = \frac{h}{2} \nabla^* \nabla \quad \text{on} \quad \text{Ran}(\pi_h^{(0)}), \quad (5.2.12)$$

where  $\nabla^*$  is the adjoint of  $\nabla : \text{Ran}(\pi_h^{(0)}) \rightarrow \text{Ran}(\pi_h^{(1)})$  with respect to the scalar product on  $\Lambda L^2(\Omega, e^{-\frac{2}{h}f} d\mu)$ .

Since  $\text{Ran}(\pi_h^{(0)}) = \text{Span}\{u_h\}$ , where we recall that  $u_h$  is the principal eigenfunction of  $L_{f, \frac{h}{2}}^{D,(0)}$  defined by (5.1.10), we deduce in particular from (5.2.12) that for any orthonormal basis  $(\psi_j)_{j \in \{1, \dots, n\}}$  of  $\text{Ran} \pi_h^{(1)}$  in the weighted Hilbert space  $\Lambda L_w^2(\Omega) := \Lambda L^2(\Omega, e^{-\frac{2}{h}f} d\mu)$ , it holds, for every  $k \in \{1, \dots, n\}$ ,

$$\int_{\Sigma_k} \partial_n u_h e^{-\frac{2}{h}f} d\mu_{\partial\Omega} = \sum_{j=1}^n \langle \nabla u_h, \psi_j \rangle_{L_w^2} \int_{\Sigma_k} \psi_j \cdot \vec{n} e^{-\frac{2}{h}f} d\mu_{\partial\Omega}, \quad (5.2.13)$$

where we recall that  $\Sigma_k$  is an open set of  $\partial\Omega$  such that  $z_k \in \Sigma_k$  and  $\overline{\Sigma_k} \subset B_{z_k}$ . We hence look for an accurate enough approximation of  $u_h$  and a suitable basis  $(\psi_j)_{j \in \{1, \dots, n\}}$  of  $\text{Ran} \pi_h^{(1)}$ .

### Step 1: approximation of $u_h$

Under [H1], [H2], and [H3], it is not difficult to find a good enough approximation of  $u_h$ . Indeed, it suffices to consider the normalized cut-off function

$$\tilde{u}_h = \tilde{u}_{h,\varepsilon} := \frac{\chi}{\|\chi\|_{L_w^2}},$$

where  $\chi \in C_c^\infty(\Omega, \mathbb{R}^+)$  and  $\chi = 1$  on  $\{x \in \Omega, d(x, \partial\Omega) \geq \varepsilon\}$  where  $\varepsilon > 0$  is arbitrary small. This leads, by the same analysis as in Section 3.3 in Chapter 3 (see Section 3.3.1, (3.3.6), and (3.3.7)), to the following estimate in the limit  $h \rightarrow 0^+$ :

$$\pi_h^{(0)} \tilde{u}_h = \tilde{u}_h + \mathcal{O}(e^{-\frac{1}{h}(f(z_1) - f(x_0) - \delta_\varepsilon)}) \text{ in } L_w^2(\Omega), \quad \text{where } 0 < \delta_\varepsilon \xrightarrow{\varepsilon \rightarrow 0^+} 0^+.$$

Since  $\text{Ran}(\pi_h^{(0)}) = \text{Span}\{u_h\}$  and  $\chi \geq 0$ , it then holds in  $L_w^2(\Omega)$  in the limit  $h \rightarrow 0^+$ :

$$u_h = \frac{\pi_h^{(0)} \tilde{u}_h}{\|\pi_h^{(0)} \tilde{u}_h\|_{L_w^2}} = \tilde{u}_h + \mathcal{O}(e^{-\frac{1}{h}(f(z_1) - f(x_0) - \delta)}), \quad \text{where } 0 < \delta_\varepsilon \xrightarrow{\varepsilon \rightarrow 0^+} 0^+. \quad (5.2.14)$$

### Step 2: construction of a suitable basis of $\text{Ran} \pi_h^{(1)}$

In view of (5.2.13), we are looking for an almost orthonormal family of 1-forms  $(\tilde{\psi}_j)_{j \in \{1, \dots, n\}}$  which forms, when projected on  $\text{Ran} \pi_h^{(1)}$ , a basis of  $\text{Ran} \pi_h^{(1)}$  which allows to obtain, when  $h \rightarrow 0^+$ , sharp enough asymptotic estimates on  $\partial_n u_h$  on all the  $\Sigma_k$ 's to prove Theorem 5.2.6.

More precisely, the analysis of the properties needed to prove Theorem 5.2.6 from (5.2.13) made in [DLLN17b, Section 2] (see Proposition 25 there) leads us to look

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3. As in Section 4.2.5, we identify the differential  $du$  of the function  $u$  with its gradient  $\nabla u$ .



for an almost orthonormal family  $(\tilde{\psi}_j)_{j \in \{1, \dots, n\}}$  satisfying in particular for some  $c > 0$  in the limit  $h \rightarrow 0^+$  (see (5.2.4)),

$$\forall j \in \{1, \dots, n\}, \quad \|(1 - \pi_h^{(1)})\tilde{\psi}_j\|_{H_w^1} = \mathcal{O}(e^{-\frac{1}{h}(\max\{f(z_n) - f(z_j), f(z_j) - f(z_1)\} + c)}), \quad (5.2.15)$$

where  $\Lambda H_w^1(\Omega) := \Lambda H^1(\Omega, e^{-\frac{2}{h}f} d\mu)$ . The relation (5.2.15) obviously implies that in the limit  $h \rightarrow 0^+$ ,  $(\pi_h^{(1)}\tilde{\psi}_j)_{j \in \{1, \dots, n\}}$  is an almost orthonormal basis of  $\text{Ran } \pi_h^{(1)}$ , but permits also to show that for some  $c > 0$  independent of  $h$  and for every  $k \in \{1, \dots, n\}$ , it holds (compare with (5.2.6) in Theorem 5.2.6 and with (5.2.13))

$$\int_{\Sigma_k} \partial_n u_h e^{-\frac{2}{h}f} d\mu_{\partial\Omega} = \sum_{j=1}^n \langle \nabla \tilde{u}_h, \tilde{\psi}_j \rangle_{L_w^2} \int_{\Sigma_k} \tilde{\psi}_j \cdot \vec{n} e^{-\frac{2}{h}f} d\mu_{\partial\Omega} + \mathcal{O}(e^{-\frac{2f(z_k) - f(x_0) + c}{h}}), \quad (5.2.16)$$

where  $\tilde{u}_h$  is the approximation of  $u_h$  defined below and satisfying (5.2.14).

The construction of such a family  $(\tilde{\psi}_j)_{j \in \{1, \dots, n\}}$  satisfying (5.2.15) is one of the major issues of [DLLN17b] (see below for more explanations). Once this is done, in order to prove Theorem 5.2.6, it remains to precisely estimate the terms  $\int_{\Sigma_k} \tilde{\psi}_j \cdot \vec{n} e^{-\frac{2}{h}f} d\mu_{\partial\Omega}$  and  $\langle \nabla \tilde{u}_h, \tilde{\psi}_j \rangle_{L_w^2}$  for  $j, k \in \{1, \dots, n\}$ . Such estimates follow from the construction of an accurate WKB approximation of each  $\tilde{\psi}_j$  in a neighborhood in  $\bar{\Omega}$  of an arbitrarily large closed neighborhood of  $z_j$  in  $B_{z_j}$ .

We conclude this section by explaining the construction a family  $(\tilde{\psi}_j)_{j \in \{1, \dots, n\}}$  as above made in [DLLN17b].

### Step 2.a): Construction of the family $(\tilde{\psi}_j)_{j \in \{1, \dots, n\}}$

Inspired by the construction made in Section 3.3.2, we want to define, for every  $j \in \{1, \dots, n\}$ , a quasimode  $\tilde{\psi}_j$  satisfying  $z_k \in \text{supp } \tilde{\psi}_j$  if and only if  $k = j$  (and  $x_0 \notin \text{supp } \tilde{\psi}_j$ ). But contrary to the construction of Section 3.3.2, we want  $\text{supp } \tilde{\psi}_j$  to be arbitrary large in  $B_{z_j} \cup \Omega$  (see why next step).

More precisely, the basic idea of [DLLN17b] is to construct  $\tilde{\psi}_j$  by exploiting the supersymmetric structure of the weighted Laplacian (or equivalently of the Witten Laplacian) in the following way. Let  $\Omega_0$  be a small smooth open neighborhood of  $x_0$  such that  $\partial_n f < 0$  on  $\Gamma_0 = \partial\Omega_0$ ,  $\vec{n}$  being the outward normal to  $\Omega \setminus \Omega_0$ . Let moreover  $\Gamma_j$  denote a closed subset of  $B_{z_j}$  containing  $z_j$ , arbitrary large in  $B_{z_j}$ . Let us then define  $\dot{\Omega} := \Omega \setminus \bar{\Omega}_0$  and let us consider the weighted Laplacian  $L_{f, \frac{h}{2}}^{DN} = \frac{1}{2h} e^{\frac{f}{h}} \Delta_{f, h}^{DN} e^{-\frac{f}{h}}$  on  $\dot{\Omega}$  (see (1.3.18)) with Dirichlet type boundary conditions on  $\Gamma_j \cup \partial\Omega_0$  and with Neumann type boundary conditions on  $\Gamma'_j := \partial\dot{\Omega} \setminus \Gamma_j$  (see Section 1.2.3). Then, according to [H1], [H2], and [H3]:

- it holds  $\nabla f \neq 0$  in  $\dot{\Omega}$ ,
- since  $\partial_n f > 0$  on  $\Gamma'_j$ , the function  $f$  has no generalized critical point in the Neumann setting on this part of the boundary of  $\dot{\Omega}$  (see Section 1.2.3 and (3.1.3) in Section 3.1.3),
- since  $\partial_n f < 0$  on  $\partial\Omega_0$  and  $\partial_n f > 0$  on  $\Gamma_j$ , the function  $f$  has precisely one generalized critical point in the Dirichlet setting on  $\partial\dot{\Omega} \setminus \Gamma'_j$  (see Section 1.2.3 and (3.1.5) in Section 3.1.3), namely  $z_j$ , which is a generalized saddle point.

Combining the results of Theorem 1.2.5 in the Dirichlet and in the Neumann setting then formally implies that  $L_{f, \frac{h}{2}}^{DN, (p)}$  admits some exponentially small eigenvalue if and only if  $p = 1$ , in which case it admits precisely one exponentially small eigenvalue (counted with multiplicity). The supersymmetry then implies that this eigenvalue is necessarily 0.

Actually, the above reasoning is only formal since the proof of Theorem 1.2.5 makes for instance use of Green type formulas, which rely in particular on the fact that the elements in the form domain of the Witten Laplacian considered are in  $\Lambda H^1(\Omega)$  and then admit a well-defined boundary trace. We recall moreover that the inclusion of the form domains in  $\Lambda H^1$  follows from the Gaffney inequalities (1.2.15) and (1.2.17). But when for example  $u$  belongs to the form domain of the operator  $L_{f, \frac{h}{2}}^{DN, (1)}$  on  $\dot{\Omega}$ , i.e. when  $u$  is a 1-form such that (see Section 1.2.3)

$$u, du, d^*u \in \Lambda L^2(\dot{\Omega}) \quad \text{and} \quad \mathbf{t}u = 0 \quad \text{on} \quad \Gamma_j \cup \partial\Omega_0, \quad \mathbf{n}u = 0 \quad \text{on} \quad \Gamma'_j, \quad (5.2.17)$$

it is in general even no more true that  $u \in \Lambda^1 H^{\frac{1}{2}}(\dot{\Omega})$  (see for example [JMM09]). This singular behaviour arises from the fact that  $\Gamma_j$  and  $\overline{\Gamma'_j}$ , where Dirichlet and Neumann type boundary conditions are respectively considered, meet at an angle (greater than or equal to)  $\pi$ .

However, the analysis led in the articles [JMM09, GMM11], dealing in particular with Hodge Laplacians on domains with Lipschitz boundaries, implies that when  $\Gamma_j$  and  $\overline{\Gamma'_j}$  meet at an angle strictly less than  $\pi$ , any 1-form  $u$  satisfying (5.2.17) then belong to  $\Lambda^1 H^{\frac{1}{2}}(\dot{\Omega})$ , admits in some sense a boundary trace  $u|_{\partial\dot{\Omega}} \in \Lambda^1 L^2(\partial\dot{\Omega})$ , and satisfies the following Gaffney type subelliptic estimate (where  $C > 0$  is independent of  $u$ ):

$$\|u\|_{H^{\frac{1}{2}}(\dot{\Omega})} + \|u|_{\partial\dot{\Omega}}\|_{L^2(\partial\dot{\Omega})} \leq C \left( \|u\|_{L^2(\dot{\Omega})} + \|du\|_{L^2(\dot{\Omega})} + \|d^*u\|_{L^2(\dot{\Omega})} \right). \quad (5.2.18)$$

Thus, in order to be able to apply properly the above reasoning exploiting the supersymmetry, we slightly modify  $\dot{\Omega}$  and  $\Gamma'_j$  in such a way that  $\Gamma_j$  and the new  $\Gamma'_j$  meet at an angle strictly less than  $\pi$ .

The 1-form  $\tilde{\psi}_j$  associated with  $z_j$  is then defined from an eigen-1-form  $v_j = v_{j, h}$  associated with the eigenvalue 0 of the operator  $L_{f, \frac{h}{2}}^{DN, (1)}$  on the above modification  $\dot{\Omega}_j$  of  $\dot{\Omega}$ :

$$\tilde{\psi}_j := \frac{\chi_j v_j}{\|\chi_j v_j\|_{L^2_w}},$$

where  $\chi_j$  is a cut-off function with an arbitrary large support in  $\overline{\dot{\Omega}_j} \setminus \overline{\Gamma'_j}$ , and then in  $B_{z_j} \cup \Omega \setminus \{x_0\}$ . This is a major difference with previous constructions in the literature, such as in [HN06].

### Step 2.b): Accuracy of the quasimodes $\tilde{\psi}_j$ for $j \in \{1, \dots, n\}$

To obtain the estimate (5.2.15) (and then (5.2.16)), one needs to quantify the decrease of the quasimode  $\tilde{\psi}_j$  outside a neighborhood of  $z_j$ . This is done in [DLLN17b] using Agmon estimates which allow to localize  $\tilde{\psi}_j$  in a neighborhood of  $z_j$ . More precisely, we prove in [DLLN17b, Section 4] that for some  $N \in \mathbb{N}$  and every  $j \in \{1, \dots, n\}$ , it holds

$$\|\tilde{\psi}_j e^{\frac{1}{h} d_a(\cdot, z_j)}\|_{H^1_w} = O(h^{-N}), \quad (5.2.19)$$

where  $d_a$  is the Agmon distance defined in (5.2.2). Proving the relation (5.2.19) requires in particular a nice understanding of this Agmon distance, which is the object of [DLLN17b, Section 3], and dealing with the boundary of  $\Omega$  introduces technical difficulties. This relation is then obtained by adapting to our case techniques developed in [HN06, Lep10].

Note now that (5.2.19) leads, using for instance (3.3.7), to the following estimate:

$$\begin{aligned} \exists C > 0, \forall j \in \{1, \dots, n\}, \quad \|(1 - \pi_h^{(1)})\tilde{\psi}_j\|_{L_w^2}^2 &\leq C \langle L_{f,h}^{D,(1)}\tilde{\psi}_j, \tilde{\psi}_j \rangle_{L_w^2} \\ &\leq C h^{-2N-1} e^{-\frac{2}{h} \inf_{\text{supp} \nabla \chi_j} d_a(\cdot, z_j)}. \end{aligned}$$

Since by construction  $\text{supp} \tilde{\psi}_j$  is arbitrary large in  $B_{z_j} \cup \Omega \setminus \{x_0\}$ , the latter inequality permits to obtain the relation (5.2.15) when for every  $j \in \{1, \dots, n\}$ ,

$$f(z_j) - f(x_0) = d_a(x_0, z_j) > \max[f(z_n) - f(z_j), f(z_j) - f(z_1)]$$

and

$$d_a(B_{z_j}^c, z_j) > \max[f(z_n) - f(z_j), f(z_j) - f(z_1)],$$

that is precisely when the assumptions (5.2.4) and (5.2.5) hold. This explains in particular why the quasimode  $\tilde{\psi}_j$  must have its support arbitrary large in  $B_{z_j} \cup \Omega$ .

## 5.3 Some perspectives

### 5.3.1 The standard Eyring-Kramers law

We have already stressed several times in this work that the algorithms aiming at approximating the exit event from a metastable state  $\Omega$  for the overdamped Langevin dynamics by a Markov jump process following the Eyring-Kramers law (see Definition 1.3.6 in Section 1.3.3 and Section 5.1.2) assume in practice that  $\Omega$  is the basin of attraction of some local minimum of the potential function  $f$  for the dynamics  $\dot{x} = -\nabla f(x)$  (see (1.3.38) and the discussion around in Section 1.3.3, and Section 5.1).

Motivated by this setting, non generic but natural with respect to applications, we intend, in a future work in collaboration with Boris Nectoux and Tony Lelièvre, to extend the results of this chapter when  $\Omega$  is, say, a smooth basin of attraction of some local minimum of the potential  $f$ , or, since a basin of attraction is not smooth in general, a suitable smooth approximation of this basin of attraction.

In this case, denoting by  $(z_i)_{1 \leq i \leq n}$  the saddle points of  $f$  on  $\partial\Omega$ , we expect to prove for the exit rates  $(k_{0i})_{i \in \{1, \dots, n\}}$ , instead of (5.2.8) in Corollary 5.2.8, the following result:

$$k_{0i} = \frac{|\lambda(z_i)|}{\pi} \frac{\sqrt{\det \text{Hess } f(x_0)}}{\sqrt{|\det \text{Hess } f(z_i)|}} e^{-\frac{2}{h}(f(z_i) - f(x_0))} (1 + \mathcal{O}(\sqrt{h})), \quad (5.3.1)$$

where  $\lambda(z_i)$  is the negative eigenvalue of  $\text{Hess } f(z_i)$ . Notice that the latter formula differs asymptotically from (5.1.5)–(5.1.6) and (1.3.38) in Section 1.3.3 by a multiplicative factor  $\frac{1}{2}$  since we actually compute the exit rates from  $\Omega$  and not the

transition rates to the neighboring states. Concerning this multiplicative factor  $\frac{1}{2}$ , we refer for example to the remark on page 408 in [BEGK04], [LLN18, Remark 10], and the results on asymptotic exit times in [MS93]. This factor is due to the fact that, once at the saddle point, the process has, in the limit  $h \rightarrow 0^+$ , a probability one half to go back to  $\Omega$ , and a probability one half to effectively leave  $\Omega$ . Note in passing that this multiplicative factor does not have any influence on the law of the next visited state which only involves ratio of the rates  $k_{0i}$ , see Section 5.1.3 and (5.2.7). Concerning lastly the error term  $\mathcal{O}(\sqrt{h})$  involved in (5.3.1), one can not hope better in general, as it can for example be seen from 1D computations (this follows from the fact that the Laplace method on a half-space produces in general a term of this order).

Then, we plan to look at the corresponding problem for the related non reversible overdamped Langevin equation,

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

where  $J$  is a constant skew-symmetric matrix of size  $d$  and whose infinitesimal generator is given by

$$L_{b, \frac{h}{2}}^{(0)} := -\frac{h}{2}\Delta + \nabla f \cdot \nabla + (J\nabla f) \cdot \nabla = L_{f, \frac{h}{2}}^{(0)} + (J\nabla f) \cdot \nabla.$$

We refer to Sections 3.5.2 and 4.3.2 for more details on this operator.

To conclude this part, let us also recall that, whether we want to prove (5.3.1) or its counterpart in the non-reversible case, we first need to obtain an Eyring-Kramers type formula for the principal eigenvalue of  $L_{V, \frac{h}{2}}^{D, (0)}$ <sup>4</sup> (or for its counterpart  $L_{b, \frac{h}{2}}^{D, (0)}$ ) as well as an accurate knowledge of  $L_{V, \frac{h}{2}}^{D, (1)}$  (or of  $L_{b, \frac{h}{2}}^{D, (1)}$ ) near the critical points of  $f$ , which all belong to  $\partial\Omega$  except one when  $\Omega$  behaves as a basin of attraction of some local minimum of  $f$ . This knowledge is crucial to be able to adapt the analysis of [DLLN17b] (see indeed Section 5.2.4).

### 5.3.2 Case of the general Langevin dynamics

In this last part, we are interested in the general Langevin process

$$\begin{cases} dq_t = p_t dt \\ dp_t = -\nabla f(q_t) dt - \gamma p_t dt + \sqrt{h\gamma} dB_t, \end{cases} \quad (5.3.2)$$

where  $(q_t, p_t) \in \Omega \times \mathbb{R}^d$ ,  $\Omega$  being an open subset of  $\mathbb{R}^d$ ,  $f : \mathbb{R}^d \rightarrow \mathbb{R}$  is the potential energy function,  $\gamma > 0$  is the friction parameter,  $h = k_B T > 0$  is proportional to the temperature, and  $B_t \in \mathbb{R}^d$  is a  $d$ -dimensional Brownian motion. The Langevin dynamics gives the evolution of the positions  $q_t \in \mathbb{R}^d$  and of the momenta  $p_t \in \mathbb{R}^d$ , contrary to the overdamped Langevin dynamics

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

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4. This formula has been recently obtained in our work [LN19b] in collaboration with Boris Nectoux.

which is only in position space:  $X_t \in \mathbb{R}^d$ . The Langevin dynamics, which is thus more general than the overdamped Langevin dynamics, is also the dynamics the most used in practice to simulate the microscopic evolution of a molecular system. Moreover, using a rescaling in time, the overdamped Langevin dynamics is derived from the Langevin dynamics in the large friction limit: when  $\gamma \rightarrow +\infty$ ,  $(q_{\gamma t})_{t \geq 0}$  converges to  $(X_t)_{t \geq 0}$  (see for example [LRS10, Section 2.2.4]). The infinitesimal generator of the Langevin dynamics (5.3.2) is given by the Kramers-Fokker-Planck type operator

$$P_{f, \frac{\hbar}{2}} := -\gamma \frac{\hbar}{2} \Delta_p + \gamma p \cdot \nabla_p - p \cdot \nabla_q + \nabla f \cdot \nabla_p.$$

This operator is neither (formally) self-adjoint nor elliptic, but only hypoelliptic, which makes its study delicate.

In the case where  $\Omega = \mathbb{R}^d$ , an important step in the study of kinetic equations by semiclassical methods was obtained by Hérau-Nier in [HN04]. In this work, the authors proved hypoelliptic estimates for the operator  $\partial_t - P_{f, \frac{\hbar}{2}}^\dagger$ , where  $P_{f, \frac{\hbar}{2}}^\dagger$  denotes the formal adjoint of  $P_{f, \frac{\hbar}{2}}$ , and brought to light the link between the exponential rate of return to equilibrium for the Langevin dynamics (5.3.2) and the spectral properties of the Witten Laplacian associated with  $f$ . Their study was continued by Hérau-Hitrik-Sjöstrand in a series of works ending with [HHS11], where, taking advantage of the specific supersymmetric and PT-symmetric structures of  $P_{f, \frac{\hbar}{2}}$ , the authors obtained Eyring-Kramers type formulas for the smallest eigenvalues of  $P_{f, \frac{\hbar}{2}}$  in the limit  $\hbar \rightarrow 0^+$ .

A challenging perspective would be to prove that the exit event from a bounded metastable domain  $\Omega \subset \mathbb{R}^d$  for the Langevin dynamics (5.3.2) satisfies asymptotically the corresponding Eyring-Kramers law. The general strategy to tackle this problem is the following.

- First, proving the existence (and the unicity) of the quasi-stationary distribution associated with the Langevin dynamics and  $\Omega$ . The recent important work [Nie18], where the operator  $P_{f, \frac{\hbar}{2}}$  acting on  $\Omega$  with absorbing boundary conditions is in particular shown to be maximal accretive and to satisfy subelliptic estimates, already gives a part of the answer. However, a Krein-Rutman type argument is still missing to prove that  $P_{f, \frac{\hbar}{2}}$  admits a unique eigenvalue with minimal real part (which is hence real) and whose associated eigenvectors have a sign.
- Second, proving Eyring-Kramers type formulas for the small eigenvalues of  $P_{f, \frac{\hbar}{2}}$  with absorbing boundary conditions on  $\Omega$ , which means performing an analysis in the spirit of [HHS11] in the case with boundary. This should be a long work, also relying on [Nie18]. We recall that even in the self-adjoint elliptic setting, the presence of a boundary leads to substantial difficulties (see in this connection Sections 3.5.1 and 4.3.1 when the boundary admits critical points of  $f$ ). In this context, it would be interesting to both look at the cases where  $\partial\Omega$  admits critical points of  $f$  or not.
- Lastly, generalizing the results presented in this chapter in this non-elliptic setting. Again, this should be a long work.

Generalizing the results presented in Chapter 4 on the concentration of the exit distribution, in the cases where  $\partial\Omega$  admits critical points of  $f$  or not, is another related interesting perspective.



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