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QUANTITATIVE ANALYSIS OF METASTABILITY IN REVERSIBLE DIFFUSION PROCESSES VIA A WITTEN COMPLEX APPROACH: THE CASE WITH BOUNDARY

Bernard Helffer
Francis Nier

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Bernard Helffer
Laboratoire de Mathématiques, UMR CNRS 8628, Université Paris-Sud,
Bâtiment 425, F-91405 Orsay, France.
E-mail : Bernard.Helffer@math.u-psud.fr

Francis Nier
IRMAR, UMR CNRS 6625, Université de Rennes 1, Campus de Beaulieu,
F-35042 Rennes Cedex, France.
E-mail : francis.nier@univ-rennes1.fr

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QUANTITATIVE ANALYSIS OF METASTABILITY IN REVERSIBLE DIFFUSION PROCESSES VIA A WITTEN COMPLEX APPROACH: THE CASE WITH BOUNDARY

Bernard Helffer, Francis Nier

Abstract. — This article is a continuation of previous works by Bovier-Eckhoff-Gayrard-Klein, Bovier-Gayrard-Klein and Helffer-Klein-Nier. The main object is the analysis of the small eigenvalues (as $h \to 0$) of the Laplacian attached to the quadratic form

$$C_0^\infty(\Omega) \ni v \mapsto h^2 \int_\Omega |\nabla v(x)|^2 \; e^{-2f(x)/h} \; dx \; ,$$

where Ω is a bounded connected open set with C^∞-boundary and f is a Morse function on $M = \overline{\Omega}$. The previous works were devoted to the case of a manifold M which is compact but without boundary or $\mathbb{R}^n$. Our aim is here to analyze the case with boundary. After the introduction of a Witten cohomology complex adapted to the case with boundary, we give a very accurate asymptotics for the exponentially small eigenvalues. In particular, we analyze the effect of the boundary in the asymptotics.

Résumé **(Étude quantitative de la métastabilité des processus réversibles au moyen du complexe de Witten : le cas à bord.)**

Cet article prolonge des travaux antérieurs de Bovier-Eckhoff-Gayrard-Klein, Bovier-Gayrard-Klein et Helffer-Klein-Nier. L'objet principal en est l'analyse des petites valeurs propres du Laplacien associé à la forme quadratique

$$C_0^\infty(\Omega) \ni v \mapsto h^2 \int_\Omega |\nabla v(x)|^2 \; e^{-2f(x)/h} \; dx \; ,$$

où Ω est un domaine borné régulier et f est une fonction de Morse sur $M = \overline{\Omega}$. Les travaux précédents traitaient le cas d'une variété compacte M sans bord ou le cas $M = \mathbb{R}^n$. Ici nous analysons le cas d'une variété compacte à bord. Après l'introduction d'un complexe de cohomologie de Witten adapté au cas à bord, nous donnons une description très précise des valeurs propres exponentiellement petites. En particulier, nous traitons l'effet du bord sur les développements asymptotiques.

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CHAPTER 1

INTRODUCTION

We are interested in the exponentially small eigenvalues of the Dirichlet realization of the semiclassical Witten Laplacian on 0-forms

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

Our aim is to extend to the case of a regular bounded open set $\Omega \subset \mathbb{R}^n$, or more generally a compact Riemannian manifold with boundary, results which were previously obtained in the case when Ω is a compact Riemannian manifold or in the case of $\mathbb{R}^n$. We shall analyze the Dirichlet realization of this operator.
The function f is assumed to be a Morse function on $\overline{\Omega}$ (with no critical points at the boundary). It is known (see [**32**], [**33**], [**7**], [**21**] and more recently [**6**]) that, like in the case without boundary, there are exactly m_0 eigenvalues in some interval $[0, Ch^{\frac{6}{5}}]$ for $h > 0$ small enough, where m_0 is the number of local minima in Ω. This is strongly due to the fact that the Dirichlet case is concerned. These eigenvalues are actually exponentially small as $h \to 0$.
Moreover this can be extended (see [**6**]) to Laplacians on p-forms, $p \geq 1$. But this time in addition to the interior critical points with index p, some critical points of the restriction of the Morse function to the boundary (which will be assumed to be a Morse function) will play a role.

Our purpose is to derive with the same accuracy as in [**18**] asymptotic formulas for the m_0 first eigenvalues of the Dirichlet realization of $\Delta^{(0)}_{f,h}$. A similar problem was considered by many authors via a probabilistic approach in [**10**], [**23**], [**28**], [**25**]. More recently, in the case of $\mathbb{R}^n$, A. Bovier, M. Eckhoff, V. Gayrard and M. Klein obtained in [**3**] and [**4**], accurate asymptotic forms of the exponentially small eigenvalues. These results were improved and extended to the case of a compact manifold in [**18**].
The Witten Laplacian is associated to the Dirichlet form

$$C_0^\infty(\Omega) \ni u \mapsto \int_\Omega |(h\nabla + \nabla f)u(x)|^2\ dx\ .$$

Note that the probabilists look equivalently at:

$$C_0^\infty(\Omega) \ni v \mapsto h^2 \int_\Omega |\nabla v(x)|^2 \; e^{-2f(x)/h} \; dx \; .$$

Bovier, Eckhoff, Gayrard and Klein considered this problem via a probabilistic approach. They obtained, in the case of $\mathbb{R}^n$ and under additional conditions on f and ∇f at ∞, the following asymptotic behavior for the first eigenvalues $\lambda_k(h)$, $k \in \{2, \ldots, m_0\}$, with $\lambda_1(h) = 0$, of $\Delta_{f,h}^{(0)}$:

$$(1.1) \quad \lambda_k(h) = \frac{h}{\pi} |\widehat{\lambda}_1(U_{j(k)}^{(1)})| \sqrt{\frac{\left|\det(\mathrm{Hess}\, f(U_k^{(0)}))\right|}{\left|\det(\mathrm{Hess}\, f(U_{j(k)}^{(1)}))\right|}} \times \exp - \frac{2}{h} \left(f(U_{j(k)}^{(1)}) - f(U_k^{(0)}) \right) \times (1 + \mathcal{O}(h^{\frac{1}{2}} |\log h|)) \; ,$$

where the $U_k^{(0)}$ denote the local minima of f ordered in some specific way, the $U_{j(k)}^{(1)}$ are "saddle points" attached in a specific way to the $U_k^{(0)}$ (which appear to be critical points of index 1) and $\widehat{\lambda}_1(U_{j(k)}^{(1)})$ is the negative eigenvalue of Hess $f(U_{j(k)}^{(1)})$.

Their article belongs to a family of works done by probabilists starting at least from Freidlin and Wentzel (See [**10**] for a presentation and additional references). The first articles were only giving the asymptotic behavior of the logarithm of the eigenvalues. The main contribution of [**4**] and [**3**] was to determine the main term in the prefactor. The later [**18**] gave a complete asymptotics in (1.1) and extended the results to more general geometries, including cases when $\lambda_1(h) \neq 0$.

In the case with boundary, we observe that the function $\exp - \frac{f}{h}$ does not satisfy the Dirichlet condition, so the smallest eigenvalue can not be 0. For this case, we can mention as starting reference Theorem 7.4 in [**10**], which says (in particular) that, if f has no critical points except a non-degenerate local minimum x_{min}, then the lowest eigenvalue $\lambda_1(h)$ of the Dirichlet realization $\Delta_{f,h}^{(0)}$ in Ω satisfies:

$$(1.2) \qquad \lim_{h \to 0} -h \, \log \lambda_1(h) = 2 \inf_{x \in \partial\Omega} (f(x) - f(x_{min})) \; .$$

Other results are given in the case of many local minima but they are limited to the determination of logarithmic equivalents (see Theorems 7.3 and 7.4 in [**10**]).

The approach given in [**18**] intensively uses, together with the techniques of [**21**], the two facts that the Witten Laplacian is associated to a cohomology complex and that the function $x \mapsto \exp - \frac{f(x)}{h}$ is a distributional solution in the kernel of the Witten Laplacian on $0-$forms permitting to construct very efficiently quasimodes. We recall that the Witten Laplacian is defined as

$$(1.3) \qquad \Delta_{f,h} = d_{f,h} d_{f,h}^* + d_{f,h}^* d_{f,h} \; ,$$

where $d_{f,h}$ is the distorted exterior differential

$$d_{f,h} := e^{-f(x)/h}\,(hd_x)\,e^{f(x)/h}\ , \tag{1.4}$$

and where $d_{f,h}^{*}$ is its adjoint for the L^2-scalar product canonically associated to the Riemannian structure. The restriction of $d_{f,h}$ to p-forms is denoted by $d_{f,h}^{(p)}$. With these notations, the Witten Laplacian on functions is

$$\Delta_{f,h}^{(0)} = d_{f,h}^{(0)*}d_{f,h}^{(0)}\ . \tag{1.5}$$

In the Witten-complex spirit and due to the relation

$$d_{f,h}^{(0)}\Delta_{f,h}^{(0)} = \Delta_{f,h}^{(1)}d_{f,h}^{(0)}\ , \tag{1.6}$$

it is more convenient to consider the singular values of the restricted differential $d_{f,h}^{(0)} : F^{(0)} \to F^{(1)}$. The space $F^{(\ell)}$ is the m_ℓ-dimensional spectral subspace of $\Delta_{f,h}^{(\ell)}$, $\ell \in \{0,1\}$,

$$F^{(\ell)} = \text{Ran } 1_{I(h)}(\Delta_{f,h}^{(\ell)})\ , \tag{1.7}$$

with $I(h) = [0, Ch^{\frac{6}{5}}]$ and the property[(1)]

$$1_{I(h)}(\Delta_{f,h}^{(1)})d_{f,h}^{(0)} = d_{f,h}^{(0)}1_{I(h)}(\Delta_{f,h}^{(0)})\ . \tag{1.8}$$

The restriction $d_{f,h}\big|_{F^{(\ell)}}$ will be more shortly denoted by $\beta_{f,h}^{(\ell)}$

$$\beta_{f,h}^{(\ell)} := (d_{f,h}^{(\ell)})_{/F^{(\ell)}}\ . \tag{1.9}$$

We will mainly concentrate on the case $\ell = 0$.
In order to exploit all the information which can be extracted from well chosen quasimodes, working with singular values of $\beta_{f,h}^{(0)}$ happens to be more efficient than considering their squares, the eigenvalues of $\Delta_{f,h}^{(0)}$. Those quantities agree better with the underlying Witten complex structure.

The main result. — Let us describe the result. We shall show that under a suitable generic assumption (see Assumption 5.3.1), one can label the m_0 local minima and introduce an injective map j from the set of the local minima into the set of the m_1 generalized critical points with index 1 of the Morse function on $\overline{\Omega}$. At a generalized critical point U with index 1, we can introduce the Hessians $\text{Hess}\,f(U)$, if $U \in \Omega$, or $(\text{Hess}\,f\big|_{\partial\Omega})(U)$, if $U \in \partial\Omega$. When $U \in \Omega$, $\widehat{\lambda}_1(U)$ denotes the negative eigenvalue of $\text{Hess}\,f(U)$.

THEOREM 1. — *Under Assumption* (5.3.1)*, there exists h_0 such that, for $h \in (0, h_0]$, the spectrum in $[0, h^{\frac{3}{2}})$ of the Dirichlet realization of $\Delta_{f,h}^{(0)}$ in Ω, consists of m_0 eigenvalues $\lambda_1(h) < \cdots < \lambda_{m_0}(h)$ of multiplicity 1, which are exponentially small and*

(1) The right end $a(h) = Ch^{\frac{6}{5}}$ of the interval $I(h) = [0, a(h)]$ is suitable for technical reasons. What is important is that $a(h) = o(h)$. The value of $C > 0$ does not play any role.

admit the following asymptotic expansions:

$$\lambda_k(h) = \frac{h}{\pi}|\widehat{\lambda}_1(U_{j(k)}^{(1)})| \sqrt{\frac{\left|\det(\operatorname{Hess} f(U_k^{(0)}))\right|}{\left|\det(\operatorname{Hess} f(U_{j(k)}^{(1)}))\right|}} \left(1 + hc_k^1(h)\right) \times$$

$$\times \exp -\frac{2}{h}\left(f(U_{j(k)}^{(1)}) - f(U_k^{(0)})\right) , \quad \text{if } U_{j(k)}^{(1)} \in \Omega ,$$

and

$$\lambda_k(h) = \frac{2h^{1/2}|\nabla f(U_{j(k)}^{(1)})|}{\pi^{1/2}} \sqrt{\frac{\left|\det(\operatorname{Hess} f(U_k^{(0)}))\right|}{\left|\det(\operatorname{Hess} f\big|_{\partial\Omega}(U_{j(k)}^{(1)}))\right|}} \left(1 + hc_k^1(h)\right) \times$$

$$\times \exp -\frac{2}{h}\left(f(U_{j(k)}^{(1)}) - f(U_k^{(0)})\right) , \quad \text{if } U_{j(k)}^{(1)} \in \partial\Omega ,$$

where $c_k^1(h)$ *admits a complete expansion:* $c_k^1(h) \sim \sum_{m=0}^{\infty} h^m c_{k,m}$.

This theorem extends to the case with boundary the previous result of [**4**] and its improvement in [**18**] (see also non-rigorous formal computations of [**26**], who look also at cases with symmetry and the books [**10**] and [**25**] and references therein).

About the proof. — As in [**21**] and [**18**], the proof will be deeply connected with the analysis of the small eigenvalues of a suitable realization (which is **not** the Dirichlet realization) of the Witten Laplacian on the 1-forms. In order to follow the same strategy as in the boundaryless case, three main points have to be explained.
The first point was to find the right substitute for the Witten complex. Our starting problem being the analysis of the Dirichlet realization of the Witten Laplacian, we were led to find the right realization of the Witten Laplacian on 1-forms in the case with boundary in order to keep the commutation relation (1.6). A part of the answer already existed in the literature ([**29**], [**14**] and [**6**]) in connection with the analysis of the relative cohomology.
The second point was to get the "rough" localization of the spectrum of this Laplacian on 1-forms. The analysis was performed in [**6**], in the spirit of Witten's idea, extending the so called harmonic approximation. But these authors, interested in the Morse theory, simplified the problem in the sense that they use the possibility (inherent to Morse theory) to choose a well-chosen metric and a right Morse function in order to simplify the analysis at the boundary. We emphasize that we treat the general case here.
The third point is the construction of WKB solutions for the critical points of the restriction of the Morse function to the boundary. For simplicity, we restrict our attention to the case of 1-forms which is the only one needed for our problem.