Low lying eigenvalues of Witten Laplacians and metastability (After Helffer-Klein-Nier and Helffer-Nier)

Bernard Helffer
Mathématiques -
Université Paris Sud- UMR CNRS 8628
Partially supported by the programme SPECT (ESF)
and by the PROGRAMME HPRN-CT-2002-00277

Giens 2004

Main goals

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

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

Our aim is to describe the recent results which have been recently obtained in three cases :

- The case of $\mathbb{R}^n$ (Bovier-Gayrard-Klein,Helffer-Klein-Nier),
- The case of a compact riemannian manifold (HKN),
- The case of a bounded set Ω with regular boundary (HelfferNier) (in this case, we consider the Dirichlet realization of this operator).

Main assumptions

Assumption 1
The function f is assumed to be a C^∞- function on $\overline{\Omega}$ and a Morse function on Ω.

In the case when $\Omega = \mathbb{R}^n$,
Assumption 2

$$\liminf_{|x|\to+\infty} |\nabla f(x)|^2 > 0 \ ,$$

and

$$|D_x^\alpha f| \leq C_\alpha(|\nabla f|^2 + 1) \ ,$$

for $|\alpha| = 2$.

In the case with boundary,
Assumption 3
The function f has no critical points at the boundary and the function $f_{/\partial\Omega}$ is a Morse function on $\partial\Omega$.

Initiated by E. Witten

It is known (see Simon, Witten, Helffer-Sjostrand and more recently Chang-Liu, Helffer-Nier2) that the Witten Laplacians on functions $\Delta^{(0)}_{f,h}$ admits 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 easy to guess by considering, near each of the local minima $U^{(0)}_j$, the function $\chi_j(x)\exp -\frac{f}{h}$, where χ_j is a suitable cut-off function localizing near $U^{(0)}_j$ as suitable quasimode. This shows that these eigenvalues are actually exponentially small as $h \to 0$.

Note we consider the Dirichlet problem. So Assumption 3 implies that the eigenfunctions corresponding to low lying eigenvalues are localized far from the boundary.

Witten Laplacians on p-forms

Moreover this can be extended (see Simon, Witten, Helffer-Sjostrand, Chang-Liu) to Laplacians on p-forms, $p > 1$.
These Laplacians are obtained by deforming the De Rham complex d :

$$d_{f,h} = \exp -\frac{f}{h}(hd) \exp \frac{f}{h} = hd + df\wedge \ ,$$

and by associating the Laplacian :

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

where $d^*_{f,h}$ is its L^2-adjoint. By restriction to the p-forms we get $\Delta^{(p)}_{f,h}$.

Morse Inequalities

In the compact case, this was the main point of the semi-classical proof suggested by Witten of the Morse inequalities.

Each of the W-Laplacians is essentially selfadjoint and an analysis based on the harmonic approximation shows that the dimension of the eigenspace corresponding to $]0, h^{\frac{6}{5}}]$ is, for h small enough, equal to m_p the number of critical points of index p (the index at a critical point U being defined as the number of negative eigenvalues of the Hessian of f at U.

Note that the dimension of the kernel of $\Delta_{h,f}^{(p)}$ being equal to the Betti number b_p, this gives immediately the so called "weak Morse Inequalities" :

$$b_p \leq m_p \;, \quad \text{for all } p \in \{0, \ldots, n\} \;.$$

Questions in the case with boundary

In the case with boundary, two natural questions appear :

What is the interesting selfadjoint realization to consider (in order for example to show a Morse inequality) ?

How do we define the notion of critical point and of index for a point at the boundary?

We mainly concentrate here on the analysis of the Witten Laplacians on 0-forms and 1-forms.

Our aim is to get the optimal accuracy asymptotic formulas for the m_0 first eigenvalues of the Dirichlet realization of $\Delta^{(0)}_{f,h}$.

Previously via a probabilistic approach : Freidlin-Wentcel, Holley-Kusuoka-Strook, Miclo, Kolokoltsov, Bovier-Eckhoff-Gayrard-Klein and Bovier-Gayrard-Klein, but the proof of optimal accuracy (except may be for the case of dimension 1) was open.

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 :

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

The case of $\mathbb{R}^n$

In the case of $\mathbb{R}^n$ and under assumptions 1 and 2 (together with a generic assumption), one gets :

Theorem

The first eigenvalues $\lambda_k(h)$, $k \in \{2, \ldots, m_0\}$, of $\Delta^{(0)}_{f,h}$ have the following expansions :

$$\lambda_k(h) = \frac{h}{\pi} |\widehat{\lambda}_1(U^{(1)}_{j(k)})| \sqrt{\frac{\left|\det(\mathrm{Hess} f(U^{(0)}_k))\right|}{\left|\det(\mathrm{Hess} f(U^{(1)}_{j(k)}))\right|}} \times \exp -\frac{2}{h}\left(f(U^{(1)}_{j(k)}) - f(U^{(0)}_k)\right) \times (1 + r_1(h)) \,,$$

with $r_1(h) = o(1)$.

Here the $U^{(0)}_k$ denote the local minima of f ordered in some specific way, the $U^{(1)}_{j(k)}$ are "saddle points" (critical points of index 1) attached in a specific way to the $U^{(0)}_k$ and $\widehat{\lambda}_1(U^{(1)}_{j(k)})$ is the negative eigenvalue of $\mathrm{Hess} f(U^{(1)}_{j(k)})$.

Actually, the estimate

$$r_1(h) = \mathcal{O}(h^{\frac{1}{2}}|\log h|) ,$$

is obtained in BovGayKl (under weaker assumptions on f) and a complete asymptotics

$$r_1(h) \sim \sum_{j \geq 1} r_{1j} h^j ,$$

is obtained in HKN.
Here we have left out the case $k = 1$, which leads to a specific assumption (see Assumption 2) in the case of $\mathbb{R}^n$ for f at ∞. This implies that $\Delta_{f,h}^{(0)}$ is essentially selfadjoint and that the bottom of the essential spectrum is bounded below by some $\epsilon_0 > 0$ (independently of $h \in]0, h_0]$, h_0 small enough). If the function $\exp -\frac{f}{h}$ is in L^2, then

$$\lambda_1(h) = 0 .$$

But other examples like $f(x) = -(x^2-1)^2$ (with $n=1$) are interesting and an asymptotic of $\lambda_1(h)$ can be given for this example.

The approach given in HKN intensively uses, together with the techniques of HelSj4,two facts that

- the Witten Laplacian is associated to a cohomology complex
- $\exp -\frac{f(x)}{h}$ is in the kernel of the Witten Laplacian on $0-$forms

This permits to construct – and this is specific of the case of $\Delta_{f,h}^{(0)}$– very efficiently quasimodes. The restriction of $d_{f,h}$ to p-forms is denoted by $d_{f,h}^{(p)}$.
We note that we have the relation

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

Witten complex, Reduced Witten complex

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

$$F^{(\ell)} = \operatorname{Ran} 1_{I(h)}(\Delta^{(\ell)}_{f,h}) \;,$$

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

$$1_{I(h)}(\Delta^{(1)}_{f,h}) d_{f,h} = d_{f,h} 1_{I(h)}(\Delta^{(0)}_{f,h}) \;.$$

We will analyze :

$$\beta^{(\ell)}_{f,h} := (d^{(\ell)}_{f,h})_{/F^{(\ell)}} \;.$$

We will mainly concentrate on the case $\ell = 0$.

Singular values

In order to exploit all the information which can be extracted from well chosen quasimodes, working with singular values of $\beta^{(0)}_{f,h}$ happens to be more efficient than considering their squares, the eigenvalues of $\Delta^{(0)}_{f,h}$. The main point is probably that the errors appear "multiplicatively" when computing the matrix of $\beta^{(0)}_{f,h}$ in approximate well localized "almost" orthogonal basis of $F^{(0)}$ and $F^{(1)}$.
By this we mean :

$$\lambda = \lambda^{app}(1 + error) ,$$

instead of additively

$$\lambda = \lambda^{app} + error ,$$

as for example in HeSj4. Here λ_{app} will be explicitly obtained from the WKB analysis.

The main result in the case with boundary

In the case with boundary, the function $\exp -\frac{f}{h}$ does not satisfy the Dirichlet condition, so the smallest eigenvalue can not be 0.

For this case, a starting reference Freidlin-Wentzel, which says (in particular) that, if f has a unique non degenerate local minimum x_{min}, then the lowest eigenvalue $\lambda_1(h)$ of the Dirichlet realization $\Delta^{(0)}_{f,h}$ in Ω satisfies :

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

Other results are given in the case of many local minima but they are again limited to the determination of logarithmic equivalents.

We can show (Helffer-Nier) that, under a suitable generic assumption "Assgeneric", one can

- label the m_0 local minima
- introduce an injective map j from the set of the local minima into the set of the m_1 (generalized) saddle points of the Morse functions in $\overline{\Omega}$ of index 1.

We recall that ∇f does not vanish at the boundary. Our problem leads us to define a point of index 1 at the boundary as a point U which is a local minimum of $f_{/\partial\Omega}$ and for which the external normal derivative of f is strictly positive.

At a generalized critical point U with index 1, we can associate the Hessians $\mathrm{Hess} f(U)$, if $U \in \Omega$, or $(\mathrm{Hess} f\big|_{\partial\Omega})(U)$, if $U \in \partial\Omega$. When $U \in \Omega$, $\widehat{\lambda}_1(U)$ denotes the negative eigenvalue of $\mathrm{Hess} f(U)$.

Theorem
Under Assumptions 1, 3 and "Assgeneric", 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 $\Delta^{(0)}_{f,h}$ in Ω, consists of m_0 eigenvalues $\lambda_1(h) < \ldots < \lambda_{m_0}(h)$ of multiplicity 1, which are exponentially small and admit the following asymptotic expansions :

$$\lambda_k(h) = \tfrac{h}{\pi}|\widehat{\lambda}_1(U^{(1)}_{j(k)})|\sqrt{\frac{\left|\det(\mathrm{Hess} f(U^{(0)}_k))\right|}{\left|\det(\mathrm{Hess} f(U^{(1)}_{j(k)}))\right|}}\left(1 + hc^1_k(h)\right) \times$$
$$\times \exp -\tfrac{2}{h}\left(f(U^{(1)}_{j(k)}) - f(U^{(0)}_k)\right)\ , \quad \text{if } U^{(1)}_{j(k)} \in \Omega\ ,$$

and

$$\lambda_k(h) = \frac{2h^{1/2}|\nabla f(U^{(1)}_{j(k)})|}{\pi^{1/2}}\sqrt{\frac{\left|\det(\mathrm{Hess} f(U^{(0)}_k))\right|}{\left|\det(\mathrm{Hess} f\big|_{\partial\Omega}(U^{(1)}_{j(k)}))\right|}}\left(1 + hc^1_k(h)\right) \times$$
$$\times \exp -\tfrac{2}{h}\left(f(U^{(1)}_{j(k)}) - f(U^{(0)}_k)\right)\ , \quad \text{if } U^{(1)}_{j(k)} \in \partial\Omega\ .$$

Here $c_k^1(h)$ 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 results of BovGayKl and HKN (see also the books FrWe and Ko and references therein).

About the proof in the case with boundary

As in HelSj4, the proof is deeply connected with the analysis of the small eigenvalues of a suitable realization (which is **not** the Dirichlet realization) of the Laplacian on the 1-forms. In order to understand the strategy, three main points have to be explained.

First point: define the Witten complex and the associate Laplacian.

The case of a compact manifold was treated in the foundational paper of Witten.
The case of $\mathbb{R}^n$ requires some care (See Johnsen, Helffer or Helffer-Nier1).

The case with boundary creates specific new problems.

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 extend the commutation relation

$$\Delta^{(1)}_{f,h} d^{(0)}_{f,h} = d^{(0)}_{f,h} \Delta^{(0)}_{f,h}.$$

in a suitable "strong" sense (at the level of the selfadjoint realizations).

Towards the boundary conditions

The answer was present in the literature Chang-Liu in connection with the analysis of the relative cohomology.
Let us explain how we can find the right condition by looking at the eigenvectors.

If u is eigenvector of the Dirichlet realization of $\Delta^{(0)}_{f,h}$, then by commutation relation, $d^{(0)}_{f,h}u$ (which can not vanish) should be an eigenvector in the domain of the realization of $\Delta^{(1)}_{f,h}$. But $d^{(0)}_{f,h}u$ does not satisfy the Dirichlet condition in all its components, but only in its tangential components.

This is the natural condition in the definition of the variational domain to take for the quadratic form $\omega \mapsto ||d^{(1)}_{f,h}\omega||^2 + ||d^{(0)}_{f,h}{}^{*}\omega||^2$.

The selfadjoint realization $\Delta_{f,h}^{(1)\,DT}$ obtained as the Friedrichs extension associated to the quadratic form gives the right answer.

Observing also that $d_{f,h}^{(0),*}(d_{f,h}^{(0)}u) = \lambda u$ (with $\lambda \neq 0$), we get the second natural (Neumann type)-boundary condition saying that a one form ω in the domain of the operator $\Delta_{f,h}^{(1)\,DT}$ should satisfy

$$d_{f,h}^{(0),*}\omega_{/\partial\Omega} = 0 \; .$$

Second point :“rough” localization of the spectrum of this Laplacian on 1-forms.

The analysis was performed in CL, in the spirit of Witten's idea, extending the so called Harmonic approximation. But these authors, because they were interested in the Morse theory, used the possibility to add symplifying assumptions on f and the metric near the boundary. We emphasize that HelNi2 treats the general case.

Third point : construction of WKB solutions for the critical points.

This was one in HelSj4 for the case without boundary, as an extension of previous constructions of HelSj1.

The new point is the construction of WKB near critical points of the restriction of the Morse function at the boundary is done in HelNi2 for 1-forms.

The analysis of a point of index 1 at the boundary of a WKB solution is done in [HelNi]. Let us explain the main lines of the construction.

The construction is done locally around a local minimum U_0 of $f\big|_{\partial\Omega}$ with $\partial_n f(U_0) > 0$. The function Φ is a local solution of the eikonal equation

$$|\nabla\Phi|^2 = |\nabla f|^2 \ ,$$

which also satisfies

$$\Phi = f \text{ on } \partial\Omega$$

and

$$\partial_n\Phi = -\partial_n f \text{ on } \partial\Omega$$

and we normalize f so that $f(U_0) = f(0) = 0$.
We first consider a local solution u_0^{wkb} near the point $x = 0$ of

$$e^{\frac{\Phi}{h}}\Delta^{(0)}_{f,h} u_0^{wkb} = \mathcal{O}(h^\infty) \ ,$$

with u_0^{wkb} in the form

$$u_0^{wkb} = a(x,h) e^{-\frac{\Phi}{h}} \ ,$$

$$a(x,h) \sim \sum_j a_j(x) h^j \ ,$$

and the condition at the boundary

$$a(x,h) e^{-\frac{\Phi}{h}} = e^{-\frac{f}{h}} \quad \text{on } \partial\Omega \ ,$$

which leads to the condition

$$a(x,h)\big|_{\partial\Omega} = 1 \ .$$

In order to verify locally the boundary condition for our future u_1^{wkb}, we substract $e^{-\frac{f}{h}}$ and still obtain

$$e^{\frac{\Phi}{h}} \Delta_f^{(0)} (u_0^{wkb} - e^{-\frac{f}{h}}) = \mathcal{O}(h^\infty) \ .$$

We now define the WKB solution u_1^{wkb} by considering :

$$u_1^{wkb} := d_{f,h} u_0^{wkb} = d_{f,h}(u_0^{wkb} - e^{-\frac{f}{h}}) \; .$$

The 1-form $u_1^{wkb} = d_{f,h} u_0^{wkb}$ satisfies locally the Dirichlet tangential condition on the boundary and u_1^{wkb} gives a good approximation for a ground state of a suitable realization of $\Delta_{f,h}^{(1)}$ in a neighborhood of this boundary critical point.

Bibliographie

References

[BEGK] A. Bovier, M. Eckhoff, V. Gayrard, and M. Klein : Metastability in reversible diffusion processes I. Sharp asymptotics for capacities and exit times. To appear in JEMS (2004).

[BoGayKl] A. Bovier, V. Gayrard, and M. Klein. Metastability in reversible diffusion processes II Precise asymptotics for small eigenvalues. Preprint 2002 (new version in 2004). To appear in JEMS (2004).

[CL] Kung Ching Chang and Jiaquan Liu. A cohomology complex for manifolds with boundary. Topological methods in non linear analysis. Volume 5, p. 325-340 (1995).

[CFKS] H.L Cycon, R.G Froese, W. Kirsch, and B. Simon. *Schrödinger operators with application to quantum mechanics and global geometry*. Text and Monographs in Physics. Springer-Verlag (1987).

[FrWe] M.I. Freidlin and A.D. Wentzell. *Random perturbations of dynamical systems. Transl. from the Russian by Joseph Szuecs. 2nd ed.* Grundlehren der Mathematischen Wissenschaften. 260. New York (1998).

[He3] B. Helffer. *Semi-classical analysis, Witten Laplacians and statistical mechanics*. World Scientific (2002).

[HKN] B. Helffer, M. Klein, and F. Nier. Quantitative analysis of metastability in reversible diffusion processes via a Witten complex approach. Preprint 2004.

[HelNi] B. Helffer and F. Nier. *Hypoellipticity and spectral theory for Fokker-Planck operators* *and Witten Laplacians*. Prépublication 03-25 de l'IRMAR, Univ. Rennes 1 (sept. 2003).

[HelSj1] B. Helffer and J. Sjöstrand. Multiple wells in the semi-classical limit I, Comm. Partial Differential Equations 9 (4), p. 337-408, (1984).

[HelSj2] B. Helffer and J. Sjöstrand. Puits multiples en limite semi-classique II -Interaction moléculaire-Symétries-Perturbations. Ann. Inst. H. Poincaré Phys. Théor. 42 (2), p. 127-212 (1985).

[HelSj4] B. Helffer and J. Sjöstrand. Puits multiples en limite semi-classique IV -Etude du complexe de Witten -. Comm. Partial Differential Equations 10 (3), p. 245-340 (1985).

[HolKusStr] R. Holley, S. Kusuoka, and D. Stroock. Asymptotics of the spectral gap with applications to the theory of simulated annealing. J. Funct. Anal. 83 (2), p. 333-347 (1989).

[Jo] J. Johnsen. On the spectral properties of Witten Laplacians, their range projections and Brascamp-Lieb's inequality. Integral Equations Operator Theory 36(3), p. 288-324 (2000).

[Kol] V.N. Kolokoltsov. Semi-classical analysis for diffusions and stochastic processes. Lecture Notes in Mathematics 1724. Springer Verlag, Berlin 2000.

[Mic] L. Miclo. Comportement de spectres d'opérateurs à basse température. Bull. Sci. Math. 119, p. 529-533 (1995).

[Schw] G. Schwarz. *Hodge decomposition. A method for Solving Boundary Value Problems.* Lect. Notes in Mathematics 1607, Springer (1995).

[Sim2] B. Simon. Semi-classical analysis of low lying eigenvalues, I.. Nondegenerate minima: Asymptotic expansions. Ann. Inst. H. Poincaré Phys. Théor. 38, p. 296-307 (1983).

[Wit] E. Witten. Supersymmetry and Morse inequalities. J. Diff. Geom. 17, p. 661-692 (1982).