

*Journées*

# **ÉQUATIONS AUX DÉRIVÉES PARTIELLES**

Forges-les-Eaux, 7 juin–11 juin 2004

Francis Nier

**Quantitative analysis of metastability in reversible diffusion processes  
via a Witten complex approach.**

*J. É. D. P.* (2004), Exposé n° VIII, 17 p.

<[http://jedp.cedram.org/item?id=JEDP\\_2004\\_\\_\\_\\_A8\\_0](http://jedp.cedram.org/item?id=JEDP_2004____A8_0)>

**cedram**

*Article mis en ligne dans le cadre du  
Centre de diffusion des revues académiques de mathématiques  
<http://www.cedram.org/>*

# Quantitative analysis of metastability in reversible diffusion processes via a Witten complex approach.

Francis Nier<sup>1</sup>

## Abstract

We present here a simplified version of recent results obtained with B. Helffer and M. Klein. They are concerned with the exponentially small eigenvalues of the Witten Laplacian on 0-forms. We show how the Witten complex structure is better taken into account by working with singular values. This provides a convenient framework to derive accurate approximations of the first eigenvalues of  $\Delta_{f,h}^{(0)}$  and solves efficiently the question of weakly resonant wells.

## 1. Motivations.

With the stochastic differential equation

$$dx = -2\nabla f(x) dt + dB_h(t),$$

is associated the drift diffusion operator

$$D_{f,h} = 2\nabla f(x) \cdot \nabla - h\Delta \quad \text{on} \quad L^2(M, e^{-\frac{2f(x)}{h}} dx).$$

The small parameter  $h > 0$  represents the temperature and is given by the covariance  $\langle B_h(t), B_h(t') \rangle = \frac{h}{2}\delta(t-t')$ . Under the suitable assumptions on  $f$ , this drift-diffusion operator generates a semigroup  $(e^{-tD_{f,h}})_{t \geq 0}$  with equilibrium 1.

After multiplication by  $h$  and conjugation with  $e^{\frac{f(x)}{h}}$ , this operator is transformed into the Witten Laplacian on 0-forms :

$$\Delta_{f,h}^{(0)} = -h^2\Delta + |\nabla f(x)|^2 - h\Delta f(x) \quad \text{on} \quad L^2(M, dx),$$

with equilibrium  $C_h e^{-\frac{f(x)}{h}}$  :

$$\Delta_{f,h}^{(0)} \left( e^{-\frac{f(x)}{h}} \right) = 0.$$

---

<sup>1</sup>IRMAR, Université de Rennes 1, Campus de Beaulieu, F-35042 Rennes Cedex, France.

The main purpose here is the estimate of the rate of return to the equilibrium, given by the first nonzero eigenvalue  $\lambda_2(h)$  of  $\Delta_{f,h}^{(0)}$ .

In the probabilistic approach, when  $\mu = C_h^2 e^{-2f(x)/h} dx$  is a probability measure, this  $\lambda_2(h)$  is also the best constant in the Poincaré inequality

$$\text{var}_\mu(u) = \int \left( u(x) - \int u d\mu \right)^2 d\mu(x) \leq \frac{1}{\lambda_2(h)} \int |h \nabla u(x)|^2 d\mu(x).$$

In the two approaches it is well known that  $\lambda_2(h) = O(e^{-C/h})$  when  $f$  admits more than one local minimum (see [HelSj4] or [FrWe] for example) and  $\lambda_2(h)^{-1}$  is interpreted as an exponentially large lifetime of metastable states.

Another motivation is related to previous works with F. Hérau [HerNi] and B. Helffer [HelNi] related to the kinetic Fokker-Planck equation (also called Kramers equation) :

$$\begin{cases} \partial_t U + v \cdot \partial_x U - \frac{1}{m} \partial_x f(x) \cdot \partial_v U - \frac{\gamma_0}{m\beta} \left( \partial_v - \frac{m\beta}{2} v \right) \cdot \left( \partial_v + \frac{m\beta}{2} v \right) U = 0 \\ U(x, v, t = 0) = U_0(x, v), \end{cases}$$

in  $L^2(\mathbb{R}^{2n})$  ( $M = \mathbb{R}^n$ ,  $\mathbb{R}^{2n} = T^*M$ ), where  $m$ ,  $\gamma_0$  and  $\beta$  respectively denote the particle mass, the friction coefficient and the inverse temperature. Up to some explicit polynomial factors in those parameters, it was shown that the rate of return to the equilibrium for this equation is bounded from below by  $\lambda_2(h)$  and  $\sqrt{\lambda_2(h)} \log(\lambda_2(h))$  as  $h = \beta^{-1} \rightarrow 0$ .

We conclude this presentation by mentioning that all our results can be applied even when  $C_h^2 e^{-\frac{2f(x)}{h}} dx$  is not a probability measure ( $e^{-\frac{f(x)}{h}} \notin L^2(\mathbb{R}^n, dx)$ ). This may happen when the global minimum of  $f(x)$  is at infinity. The equilibrium is then 0 and all initial states are metastable. In this case  $\lambda_2(h)$  is the first eigenvalue of  $\Delta_{f,h}^{(0)}$  and it cannot be related to any Poincaré inequality.

## 2. A linear algebra problem.

The core of the analysis relies on the question of determining the eigenvalues of some square non-negative matrix in finite dimension. If  $A_0(h) \in \mathcal{M}_{m_0}(\mathbb{C})$  is an  $h$ -dependent  $m_0 \times m_0$  non-negative matrix :

$$\begin{aligned} 0 \leq A_0(h)^* = A_0(h) &= (a_{i,j}(h))_{1 \leq i,j \leq m_0}, \\ \text{with } \forall \varepsilon > 0, \exists C_\varepsilon > 1, \quad C_\varepsilon e^{-\frac{\alpha_{ij}-\varepsilon}{h}} &\geq |a_{ij}(h)| \geq C_\varepsilon^{-1} e^{-\frac{\alpha_{ij}+\varepsilon}{h}}. \end{aligned}$$

If  $\alpha_{i_0 j_0} < \alpha_{ij}$  for  $(i, j) \neq (i_0, j_0)$ , then

- $j_0 = i_0$ .
- $\lambda_{m_0}(h) \simeq e^{-\frac{\alpha_{i_0 i_0}}{h}}$ .
- The basis vector  $e_{i_0}$  is exponentially close to the corresponding eigenvector.

But one cannot get further information on the smaller eigenvalues  $\lambda_k(h)$ ,  $1 \leq k \leq m_0 - 1$ , because the orthonormalization process brings error terms which can be much bigger.

We next show that an accurate determination of all the eigenvalues  $\lambda_k$ ,  $1 \leq k \leq m_0$ , is possible with an additional structure inherited from the Witten complex structure in our application.

Assume  $A_0(h) = B(h)^* B(h)$  with

$$\begin{aligned} B(h) &: F^{(0)} \rightarrow F^{(1)} \quad \dim F^{(\ell)} = m_\ell \\ \text{and} \quad B(h) A_0(h) &= A_1(h) B(h). \\ &\quad \geq 0 \qquad \qquad \geq 0 \end{aligned}$$

Assume that it is possible to construct two almost orthonormal bases of  $(\varepsilon, h)$  dependent quasimodes :

$$\begin{aligned} \psi_k^{(0)} &= \psi_k^{(0)}(\varepsilon, h), \quad \langle \psi_k^{(0)} | \psi_{k'}^{(0)} \rangle = \delta_{k,k'} + O(e^{-\frac{\alpha}{h}}) \\ \psi_j^{(1)} &= \psi_j^{(1)}(\varepsilon, h), \quad \langle \psi_j^{(1)} | \psi_{j'}^{(1)} \rangle = \delta_{j,j'} + O(e^{-\frac{\alpha}{h}}), \\ k &\in \{1, \dots, m_0\} \quad j \in \{1, \dots, m_1\} , \end{aligned}$$

hold for any  $\varepsilon \in (0, \varepsilon_0)$ . Here and in the sequel,  $\alpha$  denotes a positive number which does not depend on  $\varepsilon \in (0, \varepsilon_0)$  (and  $h > 0$ ).

Assume additionally that there exists a injective map  $\{1, \dots, m_0\} \ni k \rightarrow j(k) \in \{1, \dots, m_1\}$  and a strictly decreasing sequence  $(\alpha_k)_{k \in \{1, \dots, m_0\}}$  such that

$$\begin{aligned} C_\varepsilon^{-1} e^{-\frac{\alpha_k + c\varepsilon}{h}} &\leq \left| \langle \psi_{j(k)}^{(1)} | B(h) \psi_k^{(0)} \rangle \right| \leq C_\varepsilon e^{-\frac{\alpha_k - c\varepsilon}{h}} \\ \forall j' \neq j(k), \quad &|\langle \psi_{j'}^{(1)} | B(h) \psi_k^{(0)} \rangle| \leq e^{-\frac{\alpha_k + \alpha}{h}} . \end{aligned}$$

**Result :** Under the above assumptions, the eigenvalues  $\lambda_1(h) < \dots < \lambda_{m_0}(h)$  of  $A_0(h)$  satisfy

$$\lambda_k(h) = \left| \langle \psi_{j(k)}^{(1)} | B(h) \psi_k^{(0)} \rangle \right|^2 (1 + O_\eta(e^{-\frac{\eta}{h}})) \quad (\eta > 0).$$

We next give the sketch of the proof. First observe that  $A_0(h) = B(h)^* B(h)$  implies that the eigenvalues of  $A_0(h)$  are the squares of the singular values of  $B(h)$  :

$$\lambda_k(h) = \mu_{m_0+1-k}(B(h))^2, \quad \mu_1(B(h)) = \|B(h)\| .$$

The singular values happen to be more flexible objects than the eigenvalues owing to the Fan inequality (see [Sim1] for example) :

$$\begin{aligned} \forall k \in \{1, \dots, m_0\} \quad &\mu_k(BC_0) \leq \|C_0\| \mu_k(B) \\ &\mu_k(C_1 B) \leq \|C_1\| \mu_k(B) . \end{aligned}$$

This yields the next property :

If  $\max \{ \|C_0\|, \|C_0^{-1}\|, \|C_1\|, \|C_1^{-1}\| \} \leq 1 + \rho$ ,  
then the inequalities

$$\frac{\mu_k(B)}{1 + \rho} \leq \mu_k(C_1 B C_0) \leq (1 + \rho) \mu_k(B).$$

hold for all  $k \in \{1, \dots, m_0\}$ .

Hence, a small change of bases induces a small relative variation of ALL singular values.

Again the first singular value  $\mu_1(h) = \sqrt{\lambda_{m_0}(h)} = \|B(h)\|$  is easy to identify :

$$\lambda_{m_0}(h) = \left| \langle \psi_{j(m_0)}^{(1)} | B(h) \psi_{m_0}^{(0)} \rangle \right|^2 (1 + O_\eta(e^{-\frac{\alpha'}{h}})) .$$

The spectral theorem and the min-max principle also give

$$\begin{aligned} \|\psi_{m_0}^{(0)} - 1_{\{\lambda_{m_0}(h)\}} \psi_{m_0}^{(0)}\| &= O(e^{-\frac{\alpha'}{h}}) \\ \text{and } \forall k < m_0, \quad \|\psi_k^{(0)} - 1_{[0, \lambda_{m_0}(h))} \psi_k^{(0)}\| &= O(e^{-\frac{\alpha'}{h}}) . \end{aligned}$$

We set

$$\begin{aligned} v_{m_0, m_0-1}^{(0)} &= \|1_{\{\lambda_{m_0}(h)\}} \psi_{m_0}^{(0)}\|^{-1} 1_{\{\lambda_{m_0}(h)\}} \psi_{m_0}^{(0)} \\ \text{and for } k < m_0 \quad v_{k, m_0-1}^{(0)} &= \|1_{[0, \lambda_{m_0}(h))} \psi_k^{(0)}\|^{-1} 1_{[0, \lambda_{m_0}(h))} \psi_k^{(0)} . \end{aligned}$$

In the space  $F^{(1)}$ , we take :

$$v_{j(m_0), m_0-1}^{(1)} = \left\| B(h) v_{m_0, m_0-1}^{(0)} \right\|^{-1} B(h) v_{m_0, m_0-1}^{(0)}$$

while for  $j \neq j(m_0)$   $v_{j, m_0-1}^{(1)}$  is the normalized image of  $\psi_j^{(1)}$  by the orthogonal projection  $\Pi_{\{v_{j(m_0), m_0-1}^{(1)}\}^\perp}$ . One can check for all  $j \in \{1, \dots, m_1\}$

$$\begin{aligned} \|v_{j, m_0-1}^{(1)} - \psi_j^{(1)}\| &= O(e^{-\frac{\alpha'}{h}}) \\ \text{and } \langle v_{j, m_0-1}^{(1)} | B(h) v_{k, m_0-1}^{(0)} \rangle &= \langle v_{j, m_0-1}^{(1)} | B(h) \psi_k^{(0)} \rangle . \end{aligned}$$

The last identity implies

$$\begin{aligned} \langle v_{j(k), m_0-1}^{(1)} | B(h) v_{k, m_0-1}^{(0)} \rangle &= \langle \psi_{j(k)}^{(1)} | B(h) \psi_k^{(0)} \rangle (1 + O(e^{-\frac{\alpha'}{h}})) \\ \text{and for } j' \neq j(k), \quad \langle v_{j', m_0-1}^{(1)} | B(h) v_{k, m_0-1}^{(0)} \rangle &= \langle \psi_{j(k)}^{(1)} | B(h) \psi_k^{(0)} \rangle O(e^{-\frac{\alpha'}{h}}) . \end{aligned}$$

By reverse induction from  $K = m_0$  down to  $K = 1$ , two  $K$ -sequences of bases  $(v_{k, K}^{(0)})_{k \in \{1, \dots, m_0\}}$  of  $F^{(0)}$  and  $(v_{j, K}^{(1)})_{j \in \{1, \dots, m_1\}}$  of  $F^{(1)}$  are constructed so that the next properties hold for  $\varepsilon \in (0, \varepsilon_0]$  and some  $\alpha > 0$  independent of  $\varepsilon$ .<sup>2</sup>

**1)** The systems  $(v_{k, K}^{(0)})_{K < k \leq m_0}$  and  $(v_{j(k), K}^{(1)})_{K < k \leq m_0}$  are orthonormal.

We then set

$$F_K^{(0)} = \text{Span} \left\{ v_{k, K}^{(0)}, K < k \leq m_0 \right\} \quad \text{and} \quad F_K^{(1)} = \text{Span} \left\{ v_{j(k), K}^{(1)}, K < k \leq m_0 \right\} .$$

---

<sup>2</sup>Indeed as it appears in the previous arguments, the constant  $\alpha > 0$  and the range  $[0, \varepsilon_0]$  has to be adapted at each step of the induction.

2) For  $1 \leq k \leq K$ ,  $v_{k,K}^{(0)}$  belongs to  $(F_K^{(0)})^\perp$  and for  $j \notin \{j(k), K < k \leq m_0\}$ ,  $v_{j,K}^{(1)}$  belongs to  $(F_K^{(1)})^\perp$ .

3) The estimates

$$\forall i \in \{1, \dots, m_\ell\}, \quad \|v_{i,K}^{(\ell)} - \psi_i^{(\ell)}\| = \mathcal{O}_\varepsilon(e^{-\alpha/h})$$

hold for  $\ell = 0, 1$ .

4) For  $K < k \leq m_0$ , the equality

$$B(h)v_{k,K}^{(0)} = \nu_k v_{j(k),K}^{(1)} \quad \text{and} \quad A_0(h)v_{k,K}^{(0)} = \nu_k^2 v_{k,K}^{(0)}$$

hold with

$$\nu_k = \langle \psi_{j(k)}^{(1)} | B(h)\psi_k^{(0)} \rangle (1 + \mathcal{O}_\varepsilon(e^{-\alpha/h})) .$$

They imply, observing also that  $\nu_k \neq 0$ ,

$$A_\ell(h)F_K^{(\ell)} \subset F_K^{(\ell)}, \quad \ell \in \{0, 1\} .$$

5) For all  $j \notin \{j(k), K < k \leq m_0\}$  and all  $k \in \{1, \dots, K\}$ , we have

$$\langle v_{j,K}^{(1)} | B(h)v_{k,K}^{(0)} \rangle = \langle v_{j,K}^{(1)} | B(h)\psi_k^{(0)} \rangle .$$

Since the smallest eigenvalue  $\lambda_1(h)$  is obtained in the last step of the induction, it is possible to include the case when  $\lambda_1(h) = 0$  ( $\alpha_1 = +\infty$ ) even if  $m_1 = m_0 - 1$ . In this last case one can simply increase by 1 the dimension of  $F^{(1)}$  by adding artificially a vector  $\psi_{j(1)}^{(1)}$  orthogonal to  $F^{(1)}$ .

### 3. Witten complex and main result.

#### 3.1. Witten complex.

Let  $(M, g)$   $n$ -dimensional Riemannian connected oriented compact<sup>3</sup> manifold. The function  $f \in \mathcal{C}^\infty(M)$  is assumed to be a Morse function. We call  $\mathcal{U}^{(p)} = \{U_1^{(p)}, \dots, U_{m_p}^{(p)}\}$  critical points with index  $p$ .

The Witten differential is the deformed differential

$$d_{f,h} = e^{-\frac{f(x)}{h}} (hd) e^{\frac{f(x)}{h}} ,$$

and the corresponding codifferential equals

$$d_{f,h}^* = e^{\frac{f(x)}{h}} (hd^*) e^{-\frac{f(x)}{h}} .$$

The Witten Laplacian is the associated Hodge Laplacian :

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

---

<sup>3</sup>This assumption can be relaxed in order to include the case  $M = \mathbb{R}^n$ .

Their restrictions to  $p$ -forms are indicated by the superscript  $^{(p)}$  and  $d \circ d = d^* \circ d^* = 0$  leads to

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

On 0-forms, one recovers the operator

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

Set  $F^{(p)} = \text{Ran } 1_{[0, h^{3/2})}(\Delta_{f,h}^{(p)})$  and  $\beta_{f,h}^{(p)} = d_{f,h}^{(p)}|_{F^{(p)}}$ . Then it is well known after Witten (see [Wit][CFKS][HelSj4]) that for  $h \in (0, h_0)$ , with  $h_0 > 0$  small enough, the dimension of the spectral subspace  $F^{(p)}$  exactly equals the number  $m_p$  of critical points with index  $p$ . Moreover the sequences

$$\begin{aligned} 0 \rightarrow F^{(0)} \xrightarrow{\beta_{f,h}^{(0)}} F^{(1)} \xrightarrow{\beta_{f,h}^{(1)}} \dots \xrightarrow{\beta_{f,h}^{(n-1)}} F^{(n)} \rightarrow 0 \\ 0 \leftarrow F^{(0)} \xleftarrow{\beta_{f,h}^{(0),*}} F^{(1)} \xleftarrow{\beta_{f,h}^{(1),*}} \dots \xleftarrow{\beta_{f,h}^{(n-1),*}} F^{(n)} \leftarrow 0 \end{aligned}$$

are exact. This provides an homotopy between the Morse theory ( $h \rightarrow 0$ ) and the standard Hodge theory ( $h \rightarrow +\infty$  which makes the  $f$  dependent term negligible) which leads to Morse inequalities.

In our present problem, we simply work with  $p = 0$  and  $p = 1$ . Essentially after applying the proper spectral projections to well chosen quasimodes, the question of finding the  $m_0$  first eigenvalues of  $\Delta_{f,h}^{(0)}$  reduces to the previously discussed finite dimensional problem with

$$\begin{aligned} A_0(h) &= \Delta_{f,h}^{(0)}|_{F^{(0)}} \\ A_1(h) &= \Delta_{f,h}^{(1)}|_{F^{(1)}} \\ B(h) &= \beta_{f,h}^{(0)} = d_{f,h}^{(0)}|_{F^{(0)}}. \end{aligned}$$

### 3.2. Main result

The next generic assumption simplifies the presentation of the labelling of local minima  $\{U_k^{(0)}, k \in \{1, \dots, m_0\}\}$  and of the mapping

$$\{2, \dots, m_0\} \ni k \rightarrow j(k) \in \{1, \dots, m_1\}.$$

A more general presentation, which also includes cases when  $j(1) \in \{1, \dots, m_1\}$  corresponding to  $e^{-\frac{f(x)}{h}} \notin L^2(M, dx)$  and  $\lambda_1(h) \neq 0$ , is given in the articles [HKN][HelNi3]. The generalization of this assumption is briefly discussed below.

**Simplified Assumption :** a) The critical values  $f(U_i^{(p)})$ ,  $p = 0, 1$  and  $1 \leq i \leq m_p$ , are distinct.

b) The differences  $f(U_j^{(1)}) - f(U_k^{(0)})$ ,  $1 \leq j \leq m_1$ ,  $1 \leq k \leq m_0$ , are distinct.

**Theorem 3.1.** *Under the above assumption, the  $m_0$  first eigenvalues of  $\Delta_{f,h}^{(0)}$  satisfy  $\lambda_1(h) = 0$  and*

$$\lambda_{k \geq 2}(h) = \frac{h}{\pi} |\hat{\lambda}_1(U_{j(k)}^{(1)})| \sqrt{\frac{|\det(\text{Hess } f(U_k^{(0)}))|}{|\det(\text{Hess } f(U_{j(k)}^{(1)}))|}} (1 + c_k(h)) \times \exp -\frac{2}{h} \left( f(U_{j(k)}^{(1)}) - f(U_k^{(0)}) \right)$$

with  $c_k(h) \sim \sum_{\ell=1} c_{k,\ell} h^\ell$ .

In [BoGayKl][BEGK], Bovier, Eckhoff, Gaynard and Klein obtained the remainder  $c_k(h) = O(h^{1/2} \log(h^{-1}))$  in the case  $M = \mathbb{R}^n$ . Their method which makes use of capacities in connection with potential theory, does not apply directly to the case of a general riemannian manifolds.

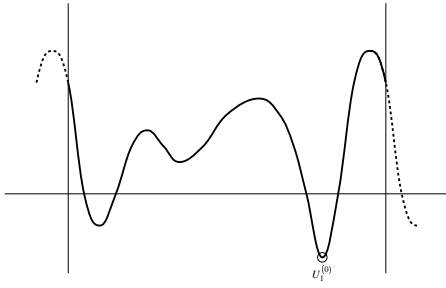
### 3.3. The mapping $k \rightarrow j(k)$ .

We explain here what is the mapping  $k \rightarrow j(k)$  introduced in Theorem 3.1. The process is as follows :

- 0) Take for  $U_1^{(0)}$  the global minimum of  $f$  (valid in our situation where  $M$  is compact). Consider the level set  $L(\lambda) = \{x \in M, f(x) < \lambda\}$ , starting from  $\lambda \sim +\infty$  with the convention  $f(U_{j(1)}^{(1)}) = +\infty$ .
- 1) When  $U_k^{(0)}$  and  $U_{j(k)}^{(1)}$  are defined for  $k = 1, \dots, K$ , decrease  $\lambda$  from  $\lambda = f(U_{j(K)}^{(1)})$  until the number of connected components of  $L(\lambda)$  is increased by 1.
- 2) The  $\lambda$ 's where the number of connected components increases have to be critical values of which the level curve meets a unique critical point with index 1. Denote by  $U_{j(K)}^{(1)}$  this new saddle point and by  $U_K^{(0)}$  the global minimum of the new connected component.
- 3) Iterate 1)-2) until all the local minima have been considered.

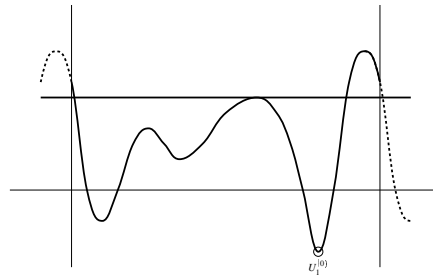
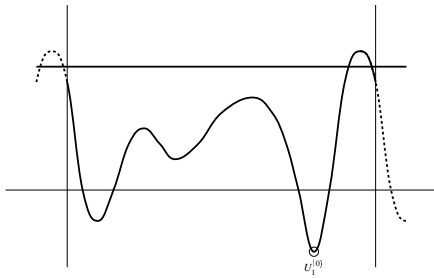
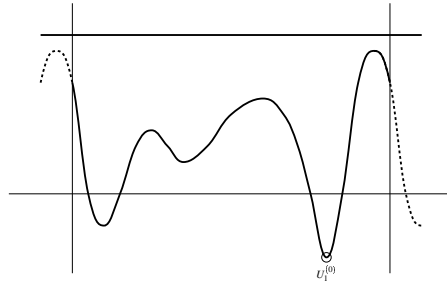
The next pictures provide a one dimensional example on  $M = S^1$ .



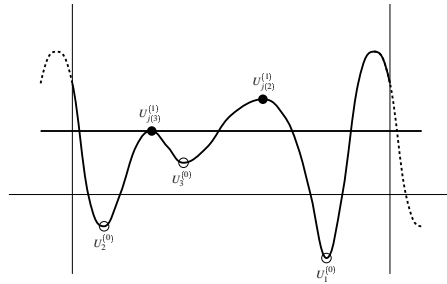
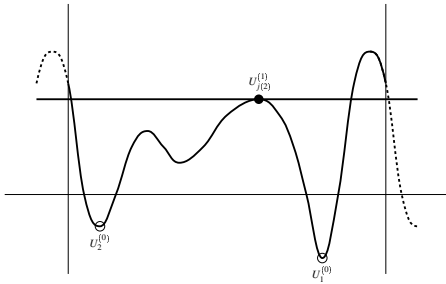


$U_1^{(0)}$  = Global minimum.

Consider the level set  $L(\lambda) = \{x \in M, f(x) < \lambda\}$ .



Decrease  $\lambda$  until the number of connected components  $L(\lambda)$  is increased by +1.



$U_2^{(0)}$ : new global minimum.

$U_{j(2)}^{(1)}$ : splitting point

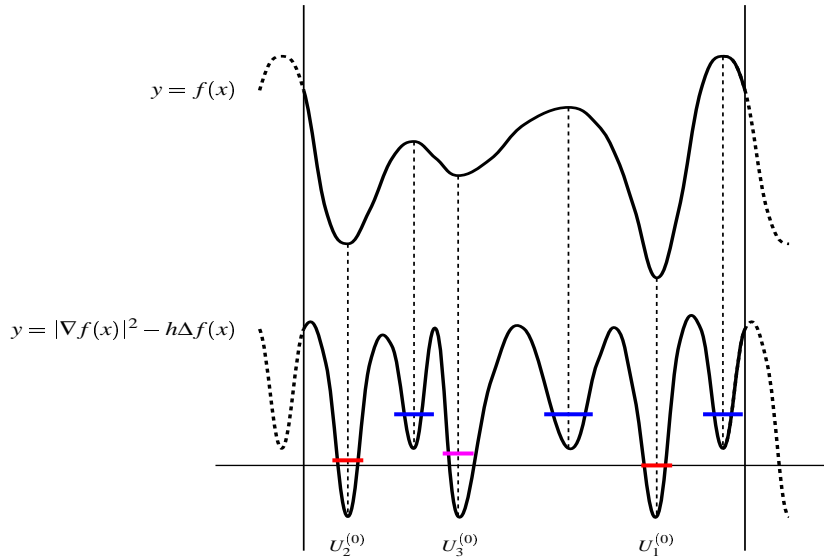
$f(U_{j(k)}^{(1)}) - f(U_k^{(0)})$  strictly decreasing.

### 3.4. Weakly resonant wells.

On the previous example on  $M = S^1$ , let us consider the subtle interaction between the wells of the potential  $|\nabla f(x)|^2 - h\Delta f(x)$  appearing in  $\Delta_{f,h}^{(0)}$ . At the level of the principal symbol, every critical point is a classical well, that is a minimum of  $|\nabla f(x)|^2$ . However the subprincipal term  $-h\Delta f(x)$  ensures (even in dimension  $> 1$ ) that the harmonic approximation at a critical point with index  $> 0$  is bounded from below by  $Ch$ ,  $C > 0$ . According to the denomination of Helffer-Sjöstrand in their work [HelSj2][HelSj3] devoted to molecular interaction, those critical points generates non resonant wells and do not affects the tunnel effect at exponentially small energies.

If one looks more accurately on the interaction between the wells corresponding to local minima, the exponentially small eigenvalues given in Theorem 3.1 occur in different exponential scales. Again according to the terminology of [HelSj2][HelSj3], we have to face the presence of weakly resonant wells. Those wells associated with local minima, lead to exponentially small eigenvalues but they do not affect the tunnel effect involved in (much) smaller eigenvalues.

Here is the picture for our example :



Here,  $U_3^{(0)}$  is a weakly resonant well. It does not affect the tunnel effect between  $U_2^{(0)}$  and  $U_1^{(0)}$ .

In the presence of an arbitrary number of local minima, the elimination of weakly resonant wells by induction can be quite complicated with the techniques of [HelSj2][HelSj3]. Fortunately here, the Witten complex structure, the properties of singular values which lead to a simple induction process for the linear algebra problem and the good choice of quasimodes permit to circumvent those difficulties.

### 3.5. Quasimodes.

Since the first localization of the low lying spectrum says  $\dim F^{(\ell)} = m_\ell$ , with  $F^{(\ell)} = 1_{[0, h^{3/2}]}(\Delta_{f,h}^{(\ell)})$ , it suffices to find  $m_0$  quasimodes attached to the local minima for  $\Delta_{f,h}^{(0)}$  and  $m_1$  quasimodes for  $\Delta_{f,h}^{(1)}$  attached to the critical points with index 1. Owing to the relation

$$d_{f,h}^{(0)}(\chi e^{-\frac{f(x)}{h}}) = e^{-\frac{f(x)}{h}}(d\chi)$$

it is quite easy to construct quadimodes for  $\Delta_{f,h}^{(0)}$  with an explicit global control. For  $\Delta_{f,h}^{(1)}$  we simply consider the first eigenmode of the Dirichlet realization  $\Delta_{f,h,j}^{D,(1)}$  in a small ball around the critical point  $U_j^{(1)}$ .

**Quasimodes for  $\Delta_{f,h}^{(0)}$  :** Take  $\psi_k(\varepsilon, h) = C(k, h)\chi_{k,\varepsilon}(x)e^{-\frac{f(x)-f(U_k^{(0)})}{h}}$ , where a full expansion of the normalization factor  $C(k, h)$  is given by the Laplace method. The cut-off  $\chi_{k,\varepsilon}$  is modelled on the connected component of  $U_k^{(0)}$  in  $\{f < f(U_{j(k)}^{(1)})\}$  with

$$\text{supp } \nabla \chi_{k,\varepsilon} \subset \left\{ \left| f(x) - f(U_{j(k)}^{(1)}) \right| \leq \varepsilon \right\}.$$

The parameter  $\varepsilon \in (0, \varepsilon_0)$  has to be adapted in every step of the final induction like it is suggested in the presentation of the linear algebra problem.

**Quasimodes for  $\Delta_{f,h}^{(1)}$  :** In a ball  $B(U_j^{(1)}, 2\varepsilon_1)$ ,  $\varepsilon_1 > 0$  small but independent of  $\varepsilon$ , consider the Dirichlet realization  $\Delta_{f,h}^{D,(1)}$  and its first normalized eigenvector  $u_j^{(1)}$ . Take then

$$\begin{aligned} \psi_j^{(1)}(h) &= \chi_j(x)u_j^{(1)} \\ \text{with } \chi_j &\in \mathcal{C}_0^\infty(B(U_j^{(1)}, 2\varepsilon_1)), \quad \chi_j \equiv 1 \quad \text{in } B(U_j^{(1)}, \frac{3}{2}\varepsilon_1). \end{aligned}$$

Let  $u_j^{wkb}$  denote a WKB approximation of  $u_j^{(1)}$  obtained after taking the solution  $\varphi(x) = d_{Agmon}(x, U_j^{(1)})$  to the eiconal equation  $|\nabla \varphi|^2 = |\nabla f|^2$  and all the transport equations around  $U_j^{(1)}$ . The next estimates

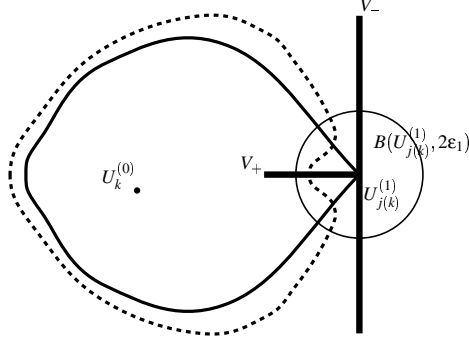
$$\begin{aligned} |\partial_x^\alpha \psi_j^{(1)}(x)| &= \tilde{O}(e^{-\frac{\varphi(x)}{h}}) \\ \left| \partial_x^\alpha (\psi_j^{(1)} - u_j^{wkb})(x) \right| &= O(h^\infty e^{-\frac{\varphi(x)}{h}}). \end{aligned}$$

hold for all  $x \in B(U_j^{(1)}, \varepsilon_1)$ . Note that the solution  $\varphi$  of the eiconal equation satisfies

$$\varphi(x) = d_{Agmon}(x, U_j^{(1)}) \geq \left| f(x) - f(U_j^{(1)}) \right|$$

with equality only along the stable manifold  $V_+$  (1D) and the unstable manifold  $V_-$  of  $\nabla f$ .

In order to have a computable interaction through  $d_{f,h}^{(0)}$  between the quasimodes  $\psi_k^{(0)}$  and  $\psi_{j(k)}^{(1)}$ , the cut-off function  $\chi_{k,\varepsilon}$  involved in the definition of  $\psi_k^{(0)}$  is taken so that its support does not meet the unstable manifold  $V_-$  around  $U_{j(k)}^{(1)}$ . All these conditions are summarized in the next picture.



The support of  $d\chi_{k,\varepsilon}$  is localized around the dashed curve.

### 3.6. Computation of $\langle \psi_j^{(1)}(h) \mid d_{f,h} \psi_k^{(0)}(\varepsilon, h) \rangle$ .

First of all we note that by taking  $\varepsilon_0 > 0$  and  $\varepsilon_1 > 0$  small enough

$$\langle \psi_j^{(1)}(h) \mid d_{f,h} \psi_k^{(0)}(\varepsilon, h) \rangle = 0$$

as soon as  $j \neq j(k)$ , because  $\psi_j^{(1)}$  and  $d_{f,h} \psi_k^{(0)}$  have disjoint support.

It remains to compute  $\langle \psi_{j(k)}^{(1)}(h) \mid d_{f,h} \psi_k^{(0)}(\varepsilon, h) \rangle$  (for  $k \geq 2$  here) : For a good choice of  $\chi_{k,\varepsilon}$ , we get

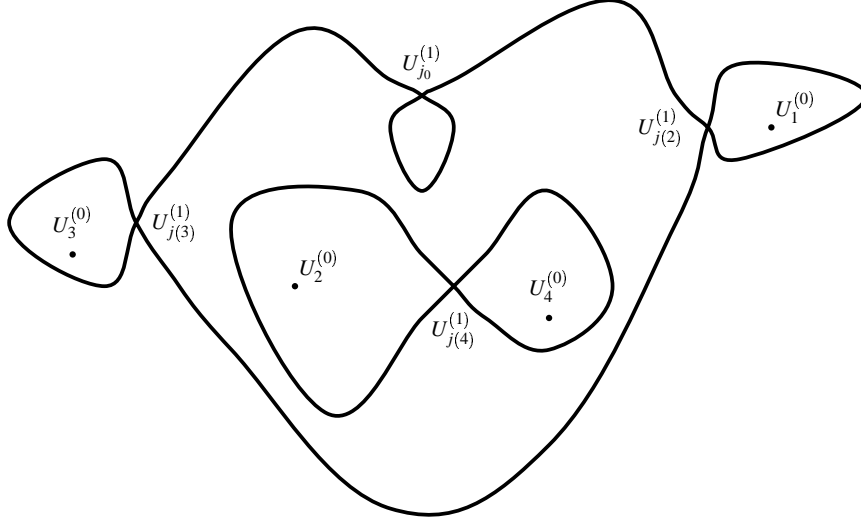
$$\begin{aligned} \langle \psi_j^{(1)}(h) \mid d_{f,h} \psi_k^{(0)}(\varepsilon, h) \rangle = \\ C_{k,h} \int_{B(0,\varepsilon_1)} \langle \psi_j^{(1)}(h) \mid h d\chi_{k,\varepsilon} \rangle(x) e^{-\frac{f(x) - f(U_k^{(0)})}{h}} dx + O(e^{-c\varepsilon/h}). \end{aligned}$$

In order to get an explicit approximation,  $\psi_j^{(1)}$  is replaced by  $u_j^{wkb}$  and the integration domain is reduced to a neighborhood of  $V_+$ .

Finally, the integration along  $V_+$  is done via Stokes Formula while the Laplace method is used for the integration transverse to  $V_+$ .

### 3.7. Weakened assumption.

Indeed the only important condition for Theorem 3.1 is that the sequence  $(f(U_{j(k)}^{(1)}) - f(U_k^{(0)}))_{k \geq 2}$  is strictly decreasing. This avoids multiple eigenvalues by separating all the exponential scales and eliminates pathologies concerned with weakly resonant wells. However this condition supposes that the mapping  $\{2, \dots, m_0\} \ni k \rightarrow j(k) \in \{1, \dots, m_1\}$  can be defined. Indeed it is possible to do it under a more general assumption which makes possible the equality  $f(U_j^{(1)}) = f(U_{j'}^{(1)})$  for  $j \neq j'$ . The construction of the mapping  $k \rightarrow j(k)$  is then a bit more involved since one has to choose the good saddle point associated with  $U_k^{(0)}$  among several critical points with index 1. We refer the reader to [HKN][HelNi3] for details. Here is a two dimensional example which is represented via the critical level curves of  $f$ .



$$f(U_1^{(1)}) < f(U_2^{(0)}) < f(U_3^{(0)}) = f(U_4^{(0)}) < f(U_{j(4)}^{(1)}) < f(U_{j(3)}^{(1)}) = f(U_{j(2)}^{(1)}) = f(U_{j0}^{(1)}).$$

#### 4. Case with boundary.

We end this summary by pointing out the new phenomena and the specific additional technical difficulties which occur in the case with boundary.

Now,  $(M, g)$  is a connected oriented compact riemaniann manifold with boundary  $\partial M$  and interior  $\dot{M} = M \setminus \partial M$ .

The function  $f \in \mathcal{C}^\infty(M)$  is Morse function on  $M$  with no critical points on  $\partial M$ . Moreover the restriction  $f|_{\partial M}$  is assumed to be Morse function. Those assumptions imply that the normal derivative  $\partial_n f(U)$  is not 0 when  $U$  is a critical point of  $f|_{\partial M}$ .

The first question which arises is about the proper self-adjoint realization of  $\Delta_{f,h}^{(p)}$  since it appears immediately that taking complete Dirichlet boundary conditions does not preserve the Witten complex structure. Up to the deformation it is a standard problem of Hodge theory with boundary and we refer to [Schw] for a general introduction. Note also the article [CL] of Chang and Liu who considered the first localization (up to  $O(h^{3/2})$ ) of the low lying spectrum of different realization of the Witten Laplacians, on a manifold with boundary.

We restricted our attention to the Dirichlet conditions, which can be imposed only partially for  $p > 0$ . The self-adjoint realization that we considered is  $\Delta_{f,h}^{DT}$  given by :

$$D(\Delta_{f,h}^{DT}) = \{ \omega \in \Lambda H^2(M); \quad \mathbf{t}\omega|_{\partial M} \equiv 0, \quad \mathbf{t}d_{f,h}^* \omega|_{\partial M} \equiv 0 \} .$$

It preserves the complex structure, in the sense that

$$d_{f,h}^{(p)}(1 + \Delta_{f,h}^{DT,(p)})^{-1}u = (1 + \Delta_{f,h}^{DT,(p+1)})^{-1}d_{f,h}^{(p)}u$$

holds for all  $u$  in the form domain of  $\Delta_{f,h}^{DT,(p)}$ .

Another property which must be taken into account is the presence of new saddle points, which generate small eigenvalues of  $\Delta_{f,h}^{DT,(1)}$  : the local minima  $U$  of  $f|_{\partial M}$  such that  $\partial_n f(U) > 0$ ,  $n$  outgoing normal vector.

This was already noticed in [CL] and if one considers the Neumann realization the condition  $\partial_n f(U) > 0$  is replaced by  $\partial_n f(U) < 0$ . Indeed it is rather elementary to understand this fact for the one dimensional problem. The construction of the mapping  $k \rightarrow j(k)$ , now defined for all  $k \in \{1, \dots, m_0\}$ , and the core of the proof follow the same lines as in the case without boundary by taking into account those new saddle points.

Indeed in the final result, the factor

$$\frac{h}{\pi} |\hat{\lambda}_1(U_{j(k)}^{(1)})| \sqrt{\frac{|\det(\text{Hess } f(U_k^{(0)}))|}{|\det(\text{Hess } f(U_{j(k)}^{(1)}))|}}$$

occurring in the expression of  $\lambda_k(h)$  has to be replaced by

$$\frac{2h^{1/2} |\nabla f(U_{j(k)}^{(1)})|}{\pi^{1/2}} \sqrt{\frac{|\det(\text{Hess } f(U_k^{(0)}))|}{|\det(\text{Hess } f|_{\partial\Omega}(U_{j(k)}^{(1)}))|}}$$

when  $U_{j(k)}^{(1)} \in \partial M$ .

Note the new technical points which have to be solved at the boundary for this problem :

**a)** Localization of the spectrum up to  $O(h^{3/2})$  : After considering the one-dimensional problem, a model half space quadratic problem is well solved by separation of variables (with  $f(x_n, x') = x_n + |x'|^2$  in an euclidean metric on  $\{x_n \leq 0\}$ ). However the reduction to this model problem is not completely obvious. The reason is that around a boundary point there are three given geometries : the boundary  $\partial M$ , the Morse function  $f$  and its level curves and the metric. With only two of them one can find suitable coordinates which simplify the analysis. In [CL], Chang and Liu choose freely the metric for the very good reason that they are only interested in (generalized) Morse inequalities. It is standard that Morse inequalities do not depend on the metric and therefore the best metric is the one which leads to the more direct calculations. However, in our case the metric is fixed from the beginning and the reduction to a simple one requires some care.

**b)** WKB estimates : The estimates of the form  $|u_j^{(1)} - u_j^{wkb}| = O(h^\infty e^{-\frac{\varphi(x)}{h}})$  can be understood (in an analytic framework) as a result of microhyperbolic propagation of regularity. An elliptic boundary value is first, after reduction to the boundary, an elliptic system on the boundary. Hence, the comparison between  $u_j^{(1)}$  and its WKB approximation has to be done in two steps when  $U_j^{(1)} \in \partial M$  :

- The propagation along the boundary  $\partial M$  for the reduced elliptic system.
- After this, the propagation from the boundary  $\partial M$  into the interior  $\dot{M}$ .

## References

- [Bis] J.M. Bismut. The Witten complex and the degenerate Morse inequalities. J. Differ. Geom. 23, 207-240 (1986).
- [BEGK] A. Bovier, M. Eckhoff, V. Gayrard, and M. Klein : Metastability in reversible diffusion processes I. Sharp asymptotics for capacities and exit times. Preprint 2002.
- [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.
- [Bur] D. Burghelea. Lectures on Witten-Helffer-Sjöstrand theory. Gen. Math. 5, 85-99 (1997).
- [CL] Kung Ching Chang, Jiaquan Liu. A cohomology complex for manifolds with boundary. Topological methods in non linear analysis. Volume 5, 1995, p. 325-340.
- [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).
- [DiSj] M. Dimassi, J. Sjöstrand. Spectral Asymptotics in the semi-classical limit. London Mathematical Society. Lecture Note Series 268. Cambridge University Press (1999).
- [Du] G.F.D. Duff. Differential forms in manifolds with boundary. Ann. of Math. 56 (1952), p. 115-127.
- [DS] G.F.D. Duff, D.C. Spencer. Harmonic tensors on Riemannian manifolds with boundary. Ann. of Math. 56 (1952), p. 128-156.
- [FrWe] M.I. Freidlin, A.D. Wentzell. Random perturbations of dynamical systems. Transl. from the Russian by Joseph Szuces. 2nd ed. Grundlehren der Mathematischen Wissenschaften. 260. New York (1998).
- [GoKr] I.C. Gohberg and M.G. Krejn. *Introduction à la théorie des opérateurs linéaires non auto-adjoints dans un espace hilbertien*. Monographies Universitaires de Mathématiques, No. 39. Dunod, Paris (1971).
- [Hel4] B. Helffer. *Introduction to the semi-classical Analysis for the Schrödinger operator and applications*. Springer Verlag. Lecture Notes in Math. n°1336 (1988).



- [Hel] 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 04-03, IRMAR, Univ. Rennes 1 (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).
- [HelNi3] B. Helffer and F. Nier. Quantitative analysis of metastability in reversible diffusion processes via a Witten complex approach : the case with boundary. In preparation.
- [HelSj1] B. Helffer and J. Sjöstrand. Multiple wells in the semi-classical limit I, *Comm. in PDE*, 9(4), p. 337-408, (1984).
- [HelSj2] B. Helffer and J. Sjöstrand. Puits multiples en limite semi-classique II -Interaction moléculaire-Symétries-Perturbations. Annales de l'IHP (section Physique théorique), Vol. 42, n<sup>o</sup>2, p. 127-212 (1985).
- [HelSj3] B. Helffer and J. Sjöstrand. Multiple wells in the semi-classical limit III. Math. Nachrichten 124, p. 263-313 (1985).
- [HelSj4] B. Helffer and J. Sjöstrand. Puits multiples en limite semi-classique IV -Etude du complexe de Witten -. *Comm. in PDE*, 10(3), p. 245-340 (1985).
- [HerNi] F. Hérau and F. Nier. Isotropic hypoellipticity and trend to the equilibrium for the Fokker-Planck equation with high degree potential. Arch. Ration. Mech. Anal. 171, n<sup>o</sup> 2, 151-218 (2004).
- [HolKusStr] R. Holley, S. Kusuoka, D. Stroock. Asymptotics of the spectral gap with applications to the theory of simulated annealing. J. Funct. Anal. 83, n<sup>o</sup> 2, 333-347 (1989).
- [Ko] 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).
- [Sim1] B. Simon. *Trace ideals and their applications*. Cambridge University Press IX, Lecture Notes Series vol. 35 (1979).
- [Sim2] B. Simon. Semi-classical analysis of low lying eigenvalues, I.. Nondegenerate minima: Asymptotic expansions. Ann. Inst. Poincaré, 38, p. 296-307 (1983).
- [Schw] G. Schwarz. Hodge decomposition. A method for Solving Boundary Value Problems. Lect. Notes in Mathematics 1607, Springer (1995).

- [Wit] E. Witten. Supersymmetry and Morse inequalities. J. Diff. Geom. 17, p. 661-692 (1982).
- [Zh] Weiping Zhang. Lectures on Chern-Weil theory and Witten deformations. Nankai Tracts in Mathematics. Vol. 4. World Scientific (2002).