Tunnel effect for semiclassical random walk

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Semiclassical random walk

Let $\phi \in C^\infty(\mathbb{R}^d)$ be a real function such that $d\mu_h = e^{-\phi(x)/h}dx$ is a probability measure. We are interested in the random-walk operator defined on the space $\mathcal{C}_0$ of continuous function going to 0 at infinity by

$$\mathbf{T}_h f(x) = \frac{1}{\mu_h(B_h(x))} \int_{B_h(x)} f(y) d\mu_h(y),$$

where $B_h(x) = B(x, h)$. By duality, this defines an operator $\mathbf{T}_h^\star$ on the set $\mathcal{M}_b$ of bounded Borel measures

$$\forall f \in \mathcal{C}_0, \forall \nu \in \mathcal{M}_b, \ \mathbf{T}_h^\star(\nu)(f) = \nu(\mathbf{T}_h f)$$

Invariant measure

Observe that if $d\nu$ has a density with respect to Lebesgue measure $d\nu = \rho(x)dx$,then

$$\mathbf{T}_h^\star(d\nu) = \left(\int_{|x-y|<h} \frac{1}{\mu_h(B_h(x))}\rho(x)dx\right) e^{-\phi(y)/h}dy$$

As a consequence, the measure

$$d\nu_{h,\infty} = \frac{\mu_h(B_h(x))e^{-\phi(x)/h}}{Z_h}dx := \mathcal{M}_h(x)dx$$

where Z_h is chosen so that $d\nu_{h,\infty}$ is a probability on $\mathbb{R}^d$ satisfies

$$\mathbf{T}_h^\star(d\nu_{h,\infty}) = d\nu_{h,\infty}.$$

We say that $d\nu_{h,\infty}$ is an invariant measure for $\mathbf{T}_h$ and $\mathcal{M}_h$ is sometimes called the Maxwellian.

Convergence to equilibrium

Question

For $d\nu \in \mathcal{M}_b$, what is the behavior of $(\mathbf{T}_h^\star)^n(d\nu)$ when $n \to \infty$?

Under suitable assumptions on ϕ we can easily prove the following :

Theorem

For any probability measure $d\nu$, we have

$$\lim_{n \to +\infty} (\mathbf{T}_h^\star)^n(d\nu) = d\nu_{h,\infty}$$

We are willing to compute the speed of convergence in the above limit. The answer is closely related to the spectral theory of $\mathbf{T}_h^\star$, at least when we restrict to a stable Hilbertian subspace of $\mathbf{T}_h^\star$ in $\mathcal{M}_b$.

Reduction and Some elementary properties

For the coming analysis, we restrict to the following Hilbertian subspace of measures (with density)

$$\mathcal{H}_h = L^2(\mathbb{R}^d, d\nu_{h,\infty}) \hookrightarrow \mathcal{M}_b : f \longrightarrow fd\nu_{h,\infty}$$

We denote again by $\mathbf{T}_h^*$ this restriction. We have the following elementary properties :

Proposition

The following hold true :

- $\mathbf{T}_h^*$ is bounded and self-adjoint on $\mathcal{H}_h$
- 1 is an eigenvalue of $\mathbf{T}_h^\star$ (Markov property)

Assumptions on ϕ

We make the following assumptions on ϕ :

- there exists $c, R > 0$ and some constants $C_\alpha > 0$, $\alpha \in \mathbb{N}^d$ such that :
$$\forall \alpha \in \mathbb{N}^d \setminus \{0\}, \forall x \in \mathbb{R}^d \, |\partial_x^\alpha \phi(x)| \leq C_\alpha$$
and
$$\forall |x| \geq R, \, |\nabla \phi(x)| \geq c \text{ and } \phi(x) \geq c|x|.$$
- ϕ is a Morse function (i.e. ϕ the critical points of ϕ are non-degenerate).
- We denote by $\mathcal{U}^{(k)}$ the set of critical points,of ϕ of index k, $n_k = \sharp\mathcal{U}^{(k)}, \mathcal{U}^{(0)} = \{\mathbf{m}_k, k = 1 \ldots n_0\}$ and for convenience $\mathcal{U}^{(1)} = \{\mathbf{s}_j, j = 1 \ldots n_1 + 1\}$ with $\mathbf{s}_1 = \infty$.
- We suppose that the values $\phi(\mathbf{s}_j) - \phi(\mathbf{m}_k)$, $\mathbf{s}_j \in \mathcal{U}^{(1)}$, $\mathbf{m}_k \in \mathcal{U}^{(0)}$ are distincts. (recall that the index of a critical point $\mathbf{c}$ is the number of negative eigenvalues of $Hess(\phi)(\mathbf{c})$).

Description of small eigenvalues

Theorem [Bony-Hérau-Michel]

Suppose that the previous assumptions are fullfilled. Then

- There exists $\kappa_0 > 0$ such that :
  - $\sigma_{ess}(\mathbf{T}_h^\star) \cap [1-\kappa_0, 1] = \emptyset$
  - $\sigma(\mathbf{T}_h^\star) \cap [-1, -1+\kappa_0] = \emptyset$
- There exists $\varepsilon > 0$ such that there are exactly n_0 eigenvalues of $\mathbf{T}_h^\star$ in the interval $[1-\varepsilon h, 1]$. One of them is 1 and the other enjoy the following asymptotic

$$\lambda_{k,h}^\star = 1 - \frac{h\theta_{k,0}}{2(d+2)} e^{-S_k/h}(1+\mathcal{O}(h))$$

where the coefficient θ_k, S_k are defined later.

Reformulation of the problem

Since we prefer to work in the standard $L^2(dx)$ space, we pose for the following

$$u = \mathcal{M}_h^{1/2} f \stackrel{\text{def}}{=} \mathbb{U}_h^{-1} f \quad \text{where} \quad \mathbb{U} : L^2(d\nu_{h,\infty}) \to L^2(dx) \text{ unitary}$$

and

$$T_h = \mathbb{U}_h^* \mathbf{T}_h^\star \mathbb{U}$$

which expression is

$$T_h f(x) = a_h(x) \frac{1}{\alpha_d h^d} \int_{|x-y|<h} a_h(y) f(y) dy$$

where

$$a_h(x)^{-2} = \frac{1}{\alpha_d h^d} \int_{|x-y|<h} e^{(\phi(x)-\phi(y))/h} dy.$$

We now have to study the spectral properties of the selfadjoint operator T_h on $L^2(dx)$

$$T_h u(x) = a_h(x) \frac{1}{\alpha_d h^d} \int_{|x-y|<h} a_h(y) u(y) dy$$

Observe that the operator $u \mapsto \frac{1}{\alpha_d h^d} \int_{|x-y|<h} u(y) dy$ is a fourier multiplier $G(hD_x)$ with

$$G(\xi) = \frac{1}{\alpha_d} \int_{|x|<1} e^{ix\cdot\xi} dx$$

We can then notice that

$$T_h = a_h G(hD_x) a_h \quad \text{and} \quad a_h^{-2} = e^{\phi/h} G(hD_x)(e^{-\phi/h})$$

In order to study the spectrum of T_h near 1, we can study the spectrum near 0 of

$$P_h \stackrel{\text{def}}{=} 1 - T_h = a_h (V_h(x) - G(hD_x)) a_h$$

where

$$V_h(x) = a_h^{-2}(x) = e^{\phi/h} G(hD_x)(e^{-\phi/h}).$$

Short heuristics

Let $u \in C_0^\infty(\mathbb{R}^d)$ be fixed, using the change of variable $y = x + hz$ and Taylor expansion for G in the expression of P_h, we show easily that

$$P_h u(x) = a_h \underbrace{(V_h(x) - G(hD_x))}_{\frac{1}{2(d+2)} P_h^W + \mathcal{O}(h^3)} a_h u(x)$$

where

$$P_h^W = -h^2\Delta + |\nabla\phi|^2 - h\Delta\phi$$

is the semiclassical Witten Lapacian. Here the term $\mathcal{O}(h^3)$ is not an error term from a spectral point of view. Anyway

questions

- P_h^W widely studied : can we benefit from this knowledge to compute the ev's of P_h ?
- Is there a supersymmetric structure for P_h as for P_h^W (recall $P_h(a_h^{-1} e^{-\phi/h}) = 0$) ?

Some biblio and known results

- The spectrum of semiclassical Witten laplacian has been analyzed by many authors : Witten 85, Helffer-Sjöstrand 85, Cycon-Froese-Kirch-Simon 87, Bovier-Gayrard-Klein 04, Helffer-Klein-Nier 04. In the last article, a complete asymptotic of exponentially small ones is given (under the above assumptions)
- The spectrum Metropolis operator has also been recently studied (using the connections with Witten). In bounded domains with Neumann conditions, Diaconis-Lebeau-Michel 12, and various geometries, Christianson-Guillarmou-Michel 13, Lebeau-Michel 10 (with an other scalling).
- No study of exponentially close to 1 spectrum for Metropolis (and "tunneling effect") so far...

Description of small eigenvalues

We recall some facts about $P_h^W = -h^2\Delta + |\nabla\phi|^2 - h\Delta\phi$.

- It is rather easy to show that P_h^W has $n_0 := \sharp\mathcal{U}^{(0)}$ eigenvalues $0 = \lambda_1 \leq \ldots \leq \lambda_{n_0}$, in the interval $[0, h^{3/2}]$.
- The most accurate result in [HKN04] gives an approximation of these eigenvalues (for $k \geq 2$) :

$$\lambda_k = h\theta_k(h)e^{-S_k/h} \quad \text{with} \quad \theta_k(h) = \sum_{l\geq 0} h^l\theta_{k,l},$$

- The quantities, $S_k, \theta_{k,0}$ can be computed : there exists a labelling of $\mathcal{U}^{(0)}$ and an application $j : \{1, \ldots, n_0\} \to \{1, \ldots, n_1 + 1\}$ such that (for $k \geq 2$) :

$$S_k = 2(\phi(\mathbf{s}_{j(k)}) - \phi(\mathbf{m}_k)) \quad \text{and} \quad \theta_{k,0} = \frac{|\hat{\lambda}_1(\mathbf{s}_{j(k)})|}{\pi}\sqrt{\frac{\det(\mathrm{Hess}\phi(\mathbf{m}_k))}{\det(\mathrm{Hess}\phi(\mathbf{s}_{j(k)}))}}$$

where $\hat{\lambda}_1(\mathbf{s}_{j(k)})$ is the negative eigenvalue of $\mathrm{Hess}\phi(\mathbf{s}_{j(k)})$.

Interaction matrix

The strategy of Helffer-Klein-Nier (see also Helffer-Sjostrand 84 and Hérau-Hitrik-Sjostrand 11 for Kramers-Fokker-Planck) is the following :

- Introduce
  - $F^{(0)}$ = eigenspace associated to the n_0 low lying eigenvalues on 0-forms
  - $\Pi^{(0)}$ = projector on $F^{(0)}$.
  - M = restriction of $\Delta_{\phi,h}$ to $F^{(0)}$.

  We have to compute the eigenvalues of M.
- We compute suitable quasimodes $f_k^{(0)}$, show that

$$e_k^{(0)} = \Pi^{(0)} f_k^{(0)} = f_k^{(0)} + error$$

  and compute the matrix of M in the base $e_k^{(0)}$.
- Doing that leads to error terms which are too big.
- In order to do that, use the supersymmetric structure.

Using Supersymmetry (I)

- For $p = 0, \dots, d-1$, denote $d^{(p)} : \Lambda^p\mathbb{R}^d \to \Lambda^{p+1}\mathbb{R}^d$ the exterior derivative and $d^{(p),*} : \Lambda^{p+1}\mathbb{R}^d \to \Lambda^p\mathbb{R}^d$ its formal adjoint. Then the Hodge Laplacian on p-form is defined by

$$-\Delta^{(p)} = d^{(p),*}d^{(p)} + d^{(p-1)}d^{(p-1),*}.$$

- The semiclassical Witten Laplacian (Witten, 1985) on p-form is defined by introducing the twisted exterior derivatives $d^{(p)}_{\phi,h} = e^{-\phi/h}(hd^{(p)})e^{\phi/h}$ and $d^{(p),*}_{\phi,h}$ its adjoint and by setting

$$P_h^{W,(p)} = d^{(p),*}_{\phi,h}d^{(p)}_{\phi,h} + d^{(p-1)}_{\phi,h}d^{(p-1),*}_{\phi,h}$$

- In particular, for $p = 0$, the Witten Laplacian on function is given by

$$P_h^W = P_h^{W,(0)} = d^{(0),*}_{\phi,h}d^{(0)}_{\phi,h} = -h^2\Delta + |\nabla\phi|^2 - h\Delta\phi.$$

Using Supersymmetry (II)

The fondamental remarks are the following :

- $P_h^{W,(p+1)} d_{\phi,h}^{(p)} = d_{\phi,h}^{(p)} P_h^{W,(p)}$ and $d_{\phi,h}^{(p),*} P_h^{W,(p+1)} = P_h^{W,(p)} d_{\phi,h}^{(p),*}$
- Denote $F^{(1)}$ the eigenspace associated to low lying eigenvalues on 1 forms, then $d_{\phi,h}^{(0)}(F^{(0)}) \subset F^{(1)}$ and $d_{\phi,h}^{(0),*}(F^{(1)}) \subset F^{(0)}$. Hence

$$M = L^* L$$

where L is the matrix of $d_{\phi,h}^{(0)} : F^{(0)} \to F^{(1)}$.

- The matrix $L = (L_{j,k})$ is very well approximated by

$$L_{j,k} = \langle f_j^{(1)}, d_{\phi,h}^{(0)} f_k^{(0)} \rangle + \mathcal{O}(e^{-(S_k+\alpha)/h}) \text{ with } L_{j(k),k} \sim e^{-S_k/h}$$

where $f_k^{(1)}$ are good localized quasimodes on 1-form.

- We can conclude by computing the singular values of L thanks to the structure ($k \longrightarrow S_k$ strictly decreasing) and the Ky fan inequalities.

Supersymmetry for Metropolis

Recall that $P_h^W = d_{\phi,h}^* d_{\phi,h}$. One fundamental step in our analysis is the following similar description of P_h :

Theorem [Bony-Hérau-Michel]

There exists a real valued symbol $q \in S^0(T^*\mathbb{R}^d, \partial\mathcal{A})$ such that

$$P_h = \frac{1}{2(d+2)} a_h d_\phi^* Q^* Q d_\phi a_h$$

with $Q = \mathrm{Op}_h^w(q)$. Moreover, the principal symbol q^0 of Q satisfies $q^0(x,\xi) = Id + \mathcal{O}((x-\mathbf{c},\xi)^2)$ near $(\mathbf{c},0)$ for any critical point $\mathbf{c} \in \mathcal{U}$. and Q is invertible in a similar class.

Here $\partial\mathcal{A} : T^*\mathbb{R}^d \to \mathcal{M}_d(\mathbb{R})$ is given by $\partial\mathcal{A}_{i,j}(x,\xi) = (\langle\xi_j\rangle)^{-1}$ and $q \in S^0(T^*\mathbb{R}^d, \mathcal{A})$ means $\partial_x^\alpha \partial_\xi^\beta q(x,\xi) = \mathcal{O}(\partial\mathcal{A}(x,\xi))$ component by component.

Random walks operator on (1)-forms

- Let us denote $L_\phi = Qd_\phi a_h$, then we have shown that (forgetting the prefactor $1/2(d+2)$)

$$P_h = L_\phi^* L_\phi \overset{\text{def}}{=} P_h^{(0)}$$

- We can then define an operator on (1)-forms with similar properties as the ones for the Witten Laplacian :

$$P_h^{(1)} = L_\phi L_\phi^* + (Q^*)^{-1} d_\phi^* M d_\phi Q^{-1}$$

where M is an operator acting on 2-form such that $P_h^{(1)}$ is elliptic.

- Observe that with this special choice the interwinning relations are still ok :

$$P_h^{(1)} L_\phi = L_\phi P_h^{(0)}$$

since

$$P_h^{(1)} L_\phi = L_\phi L_\phi^* L_\phi + (Q^*)^{-1} d_\phi^* M \underbrace{d_\phi Q^{-1} Q d_\phi}_{=d_\phi^2=0} a_h = L_\phi (L_\phi^* L_\phi)$$

More geometrical point of view

In fact denoting $G \stackrel{\text{def}}{=} Op(g_{j,k})_{j,k} = Q^*Q$, we can consider $a_h d_\phi^* G d_\phi a_h$ as a Hodge Witten Laplacian on (0)-form with pseudodifferential metric G^{-1}.
The corresponding Laplacian on (1) forms is therefore naturally given with

$$M = M_{(j,k),(a,b)} = \frac{1}{2} Op\left(a_h^2 \left(g_{j,a}g_{k,b} - g_{k,a}g_{j,b}\right)\right)$$

Here

$$M_{(j,k),(a,b)} \in \Psi^0\left(\langle\xi_j\rangle^{-1}\langle\xi_k\rangle^{-1}\langle\xi_a\rangle^{-1}\langle\xi_b\rangle^{-1}\right)$$

and

$$g_{j,k} \in \Psi^0(\langle\xi_j\rangle^{-1}\langle\xi_k\rangle^{-1})$$

Elements of proof of the Theorem (I)

We then can can follow similar arguments as in the Witten case

- $L_\phi = Qd_\phi a_h$ plays the role of the exterior derivative.
- minmax or IMS arguments imply that P_h has n_0 exponentially small eigenvalues and $P_h^{(1)}$ has n_1 exp. small eigenvalues.
- Denoting $F^{(0)}$ and $F^{(1)}$ the corresponding generalized eigenspaces, the interwinning relations give : $L_\phi^{(0)} : F^{(0)} \longrightarrow F^{(1)}$.
- The $f_k^{(0)} = \chi_k a_h^{(-1)} f_k^{W,(0)}$ are pretty good quasimodes for P_h, where $f_k^{W,(0)} \in F^{W,(0)}$ is well localized near $\mathbf{m}_k$ and close to $\mathbf{s}_{j(k)}$ (see HKN)
- The $f_j^{1)} = (Q^*)^{-1}\theta_j f_j^{W,(1)}$ are rather good quasimodes for $P_h^{(1)}$, where $f_j^{W,(1)} \in F^{W,(1)}$ is well localized near $\mathbf{s}_j$.
- If $e_k^{(0)} = \Pi^{(0)} f_k^{(0)}$ and $e_j^{(1)} = \Pi^{(1)} f_j^{(1)}$, then the families $\left\{e_k^{(0)}\right\}$ and $\left\{e_j^{(1)}\right\}$ are orthonormal families of $F^{(0)}$ and $F^{(1)}$ mod $\mathcal{O}(h)$.

Elements of proof of the Theorem (II)

- The matrix $L = L_{j,k}$ of $L_\phi^{(0)} : F^{(0)} \longrightarrow F^{(1)}$ with respect to these bases is well approximated by

$$
\begin{aligned}
L_{j,k} &= \left\langle f_j^{[1)}, L_\phi^{(0)} f_k^{(0)} \right\rangle + \mathcal{O}(e^{-(S_k+\alpha)/h}) \\
&= \left\langle (Q^*)^{-1}\theta_j f_j^{W,(1)}, Q d_\phi a_h a_h^{-1} \chi_k f_k^{W,(0)} \right\rangle + \mathcal{O}(e^{-(S_k+\alpha)/h}) \\
&= \left\langle \theta_j f_j^{W,(1)}, d_\phi \chi_k f_k^{W,(0)} \right\rangle + \mathcal{O}(e^{-(S_k+\alpha)/h}) \\
&= L_{j,k}^W + \mathcal{O}(e^{-(S_k+\alpha)/h}) \quad (\text{ recall } L_{j(k),k}^W \sim e^{-S_k/h})
\end{aligned}
$$

- of course the term $\mathcal{O}^{-(S_k+\alpha)/h}$ is fundamental, and relies on the crucial following fact :

$$
e_j^{(1)} - f_j^{(1)} = \mathcal{O}(h) \quad \text{but } L_\phi^*(e_j^{(1)} - f_j^{(1)}) = \mathcal{O}(e^{-\alpha/h})
$$

- We can conclude by computing the singular values of L thanks to the structure ($k \longrightarrow S_k$ strictly decreasing) and the Ky fan inequalities for which we only need $\mathcal{O}(h)$ approximate orthonormal basis

About the Factorization Lemma

We first recall some facts about pseudodifferential operators

- Let $\tau > 0$, we say that a symbol $p \in C^\infty(\mathbb{R}^{2d}, \mathbb{C})$ belongs to the class $\mathbb{S}^0_\tau(1)$ if
  - for all $x \in \mathbb{R}^d$, $\xi \mapsto p(x,\xi)$ is analtytic with respect to $\xi \in B_\tau = \{\xi \in \mathbb{C}^d,\ |\mathrm{Im}\,\xi| < \tau\}$
  - $\forall (x,\xi) \in \mathbb{R}^d \times B_\tau,\ |\partial_x^\alpha \partial_\xi^\beta p(x,\xi)| \leq C_{\alpha,\beta}$.
- We say that $p \in \mathbb{S}^0_\infty(1)$ if $p \in \mathbb{S}^0_\tau(1)$ for all $\tau > 0$.
- For $p \in \mathbb{S}^0_\tau(1)$, $\tau \in [0,\infty]$ we define the Weyl-quantization of p :

$$\mathrm{Op}_h^w(p)u(x) = (2\pi h)^{-d} \int_{\mathbb{R}^{2d}} e^{i(x-y)\xi/h} p(\frac{x+y}{2}, \xi) u(y) dy d\xi$$

for any $u \in \mathbb{S}(\mathbb{R}^d)$.

Let ϕ be as before. Let $p \in \mathbb{S}^0_\infty(1)$ and $P_h = \mathrm{Op}_h^w(p)$. Assume that the following assumptions hold true :

- p is real-valued (and hence P_h is self-adjoint).
- $P_h(e^{-\phi/h}) = 0$
- For all $x \in \mathbb{R}^d$, the function $\xi \in \mathbb{R}^d \mapsto p(x,\xi)$ is even.
- Near any critical points $U \in \mathcal{U}$ we have
$$p(x,\xi) = |\xi|^2 + |\nabla\phi(x)|^2 + \mathcal{O}(h + |(x-U,\xi)|^4).$$
- $\forall \delta > 0$, $\exists \alpha > 0, \forall (x,\xi) \in T^*\mathbb{R}^d$, $(d(x,\mathcal{U})^2 + |\xi|^2 \geq \delta \Longrightarrow p(x,\xi) \geq \alpha)$

Remark

The operator $G(hD) - V_h(x)$ entering in the formulation of P_h satisfies the above assumptions since G is the fourier transform of $1\!\mathrm{l}_{|z|<1}$.

Let us that $D_\phi = h\nabla_x + \nabla\phi(x)$ and $\partial\mathcal{A} : T^*\mathbb{R}^d \to \mathcal{M}_d(\mathbb{R})$ given by $\partial\mathcal{A}_{i,j}(x,\xi) = (\langle\xi_j\rangle)^{-1}$.

Theorem

Under the above assumptions, there exists $\tau > 0$ and a real valued symbol $q \in \mathbb{S}^0_\tau(T^*\mathbb{R}^d, \mathcal{A})$ such that

$$P_h = D_\phi^* Q^* Q D_\phi$$

with $Q = \mathrm{Op}_h^w(q)$. Moreover, the principal symbol q^0 of Q satisfies $q^0(x,\xi) = Id + \mathcal{O}((x - \mathbf{c}, \xi)^2)$ near $(\mathbf{c}, 0)$ for any critical point $\mathbf{c} \in \mathcal{U}$.

A shorter proof !

As we saw before, the links between The Witten Laplacian and the Random walk operator are strong. Indeed we showed before that (exponentially close to 1)

$$\lambda_{k,h}^{\star} = 1 - \frac{1}{2(d+2)}\lambda_{k,h}^{W}(1+\mathcal{O}(h))$$

where the $\lambda_{k,h}^{\star}$ are the eigenvalues for the Metropolis operator $\mathbf{T}_h^{\star}$ and $\lambda_{k,h}^{W}$ the ones for the Witten Laplacian.
In fact using the minmax principle and a more direct comparison between the 2 we are able to show that

$$\lambda_{k,h}^{\star} = 1 - \frac{1}{2(d+2)}\lambda_{k,h}^{W}(1+o(1))$$

Perspectives

- Asymptotic in $\mathcal{O}(h^\infty)$ / More intrinsic supersymmetric structure
- Analysis on manifolds and with boundary
- "Non-selfadjoint" case : walk with random velocity (equivalent of the Fokker-Planck case w.r.t. the Witten one)