Semiclassical methods for Langevin dynamics at low temperature

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Advances in Computational Statistical Physics
CIRM, September 2018

Plan

Langevin equations

Let ϕ be a potential landscape on $\mathbb{R}^d$. Consider the Langevin equation describing the movement of a particle under a deterministic force $-\nabla\phi(x_t)$ and a random force given by the derivative of the Brownian motion B_t

$$\begin{cases} \dot{x}_t = m^{-1} v_t \\ \dot{v}_t = \nabla\phi(x_t) - \gamma\dot{x}_t + \sqrt{\gamma/\beta}\,\dot{B}_t \end{cases} \tag{1}$$

where $m =$ mass of the particle, $\gamma =$ friction coefficient, $\beta^{-1} =$ temperature of the system.
For massless particle we obtain the overdamped Langevin equation

$$\dot{x}_t = -\gamma^{-1}\nabla\phi(x_t) + \sqrt{1/(\gamma\beta)}\,\dot{B}_t \tag{2}$$

Macroscopic point of view

Let u be the probability density of presence of particle satisfying the Langevin equations. It satisfies the Fokker-Planck equation

$$h\partial_t u = \mathscr{L} u$$

- Langevin equation $\rightsquigarrow$ Kramers-Fokker-Planck operator

$$\mathscr{L} = \mathscr{L}_{KFP} := -vh\partial_x + \nabla\phi(x)h\partial_v - h\partial_v \circ (h\partial_v + 2v)$$

- Overdamped Langevin equation $\rightsquigarrow$ Kramers-Smoluchovski operaror

$$\mathscr{L} = \mathscr{L}_{KS} := h\partial_x \circ (h\partial_x + 2\nabla\phi(x))$$

where h is a rescaled parameter proportional to the temperature.

Assumptions on ϕ

In the sequel we assume that

- $\phi : \mathbb{R}^d \to \mathbb{R}$ is a smooth Morse function.
- there exists $C > 0$ and a compact $K \subset \mathbb{R}^d$ such that for all $x \in \mathbb{R}^d \setminus K$, one has

$$|\nabla\phi(x)| \geq \frac{1}{C}, \ |\mathrm{Hess}(\phi(x))| \leq C|\nabla\phi|^2, \ \text{and } \phi(x) \geq C|x|.$$

These Fokker-Planck equations admit a global equilibrium $\mathcal{M}$:

- Kramers-Fokker-Planck $\rightsquigarrow \mathcal{M}(x,v) = \frac{1}{C} e^{-2(\phi(x)+v^2/2)/h}$
- Kramers-Smoluchovski $\rightsquigarrow \mathcal{M}(x) = \frac{1}{C} e^{-2\phi(x)/h}$

In other words

$$\mathscr{L}(\mathcal{M}) = 0$$

Under the preceding assumptions, $\mathcal{M} \in L^p$ for any $p \geq 1$ and one can chose C such that $\mathcal{M}$ is a probability density. Under some spectral gap assumption any initial distribution u_0, converges to equilibrium

$$e^{-t\mathscr{L}} u_0 \to \mathcal{M}, \text{ when } t \to \infty$$

Question

What is the speed of convergence in the above limit ?

Eyring Kramers law

In a seminal paper, Kramers [1940] computed the average transition rate for a double well potential in 1D :

$$\tau_\phi \sim a_\phi e^{2S/h}$$

with

- $S =$ the highest height a particle has to jump in order to reach the absolute minimum of ϕ
- a_ϕ explicit in terms of derivative of ϕ

Conjugation by the Maxwellian

We look at the evolution of initial densities of the form

$$u_0 = \tilde{u}_0 \mathcal{M}^{1/2}$$

with $\tilde{u}_0 \in L^2(dx)$. The natural Hilbert space to study this question is $L^2(\mathcal{M}(x)^{-1}dx)$. Let

$$\begin{aligned} U_{\mathcal{M}} : L^2(\mathcal{M}(x)^{-1}dx) \to L^2(dx) \\ u \mapsto \mathcal{M}^{-\frac{1}{2}} u \end{aligned} \tag{3}$$

then $U_{\mathcal{M}}$ is an isometry.

For any $u_0 \in L^2(\mathcal{M}(x)^{-1}dx)$ we have

$$e^{-t\mathscr{L}} u_0 = U_{\mathcal{M}}^* e^{-tP} U_{\mathcal{M}} u_0$$

the operators $P_\bullet := U_{\mathcal{M}} \mathscr{L}_\bullet U_{\mathcal{M}}^*$ are given by

$$P_{KS} = -h^2\Delta + |\nabla\phi|^2 - h\Delta\phi$$

and

$$P_{KFP} = -vh\partial_x + \partial_x\phi h\partial_v + (-h^2\Delta_v + v^2 - hd)$$

As a consequence for any probability density $u_0 = \mathcal{M}^{\frac{1}{2}}\tilde{u}_0$ with $\tilde{u}_0 \in L^2(dx)$ we have

$$\|e^{-t\mathscr{L}} u_0 - \mathcal{M}\|_{L^2(\mathcal{M}^{-1}dx)} = \|e^{-tP}\tilde{u}_0 - \langle \tilde{u}_0, \mathcal{M}^{\frac{1}{2}}\rangle \mathcal{M}^{\frac{1}{2}}\|_{L^2(dx)}$$

Some remarks on the generator P

- The operator P_{KS} is self-adjoint on $L^2(dx)$. It is the celebrated Witten Laplacian associated to ϕ.
- The operator P_{KFP} is not self-adjoint on $L^2(dxdv)$. This leads to serious complications
- In both cases, we will study the spectrum of P in order to get some information on the speed of return to equilibrium.

Preliminary results on Witten Laplacians

Consider the semiclassical Witten Laplacian associated to ϕ :

$$\Delta_\phi = -h^2\Delta + |\nabla\phi|^2 - h\Delta\phi = (-h\partial_x + \partial\phi) \circ (h\partial_x + \partial\phi)$$

where $h \in]0,1]$ denotes the semiclassical parameter. Under the preceding assumptions, one has the following properties on Δ_ϕ.

- Δ_ϕ is essentially self-adjoint on $\mathcal{C}_c^\infty(\mathbb{R}^d)$.
- $\Delta_\phi \geq 0$
- there exists $C_0, h_0 > 0$ such that for all $0 < h < h_0$

$$\sigma_{ess}(\Delta_\phi) \subset [C_0, \infty[$$

- 0 is an eigenvalue of Δ_ϕ associated to the eigenstate $e^{-\phi/h}$.

Goal :

Study the small eigenvalues of Δ_ϕ.

Rough localization result

Theorem [Helffer-Sjöstrand-Witten, 80's]

Let $\mathcal{U}^{(0)}$ denote the set of minima of ϕ and $n_0 = \sharp\mathcal{U}^{(0)}$. There exists $\epsilon_0 > 0$ such that for $h > 0$ small enough :

- $\sigma(\Delta_\phi) \cap [0, \epsilon_0 h]$ has n_0 elements.
- these n_0 "small" eigenvalues are $\mathcal{O}(e^{-C/h})$.

Proof.

- Consider the quasimodes

$$f_{\mathbf{m}}^{(0)}(x) = h^{-\frac{d}{4}}\chi_{\mathbf{m}}(x)e^{-(\phi(x)-\phi(\mathbf{m}))/h}, \ \mathbf{m} \in \mathcal{U}^{(0)}$$

  for some cut-off functions $\chi_{\mathbf{m}}$ localized around $\mathbf{m}$.
- Compute

$$\Delta_\phi f_{\mathbf{m}}^{(0)} = h^{-\frac{d}{4}}[h^2\Delta, \chi_{\mathbf{m}}]e^{-(\phi(x)-\phi(\mathbf{m}))/h} = \mathcal{O}(e^{-C/h})$$

- Use self-adjointness of Δ_ϕ to conclude (min-max).

Exponentially small eigenvalues : log-limit

Denote $0 = \lambda_1(h) < \lambda_2(h) \leq \ldots \leq \lambda_{n_0}(h)$ the small eigenvalues of Δ_ϕ.

- Freidlin-Wentzell compute the limit of $h \log(\lambda_j(h))$ as $h \to 0$ (large deviations approach)
- On compact manifolds, Holley-Kusuoka-Stroock [89] proved (by functional inequalities approach) that

$$C_1 h e^{-2S/h} \leq \lambda_2(h) \leq C_2 h e^{-2S/h}$$

  with $S =$ highest height a particle has to jump in order to reach the absolute minimum of ϕ
- Mathieu [95], Miclo [95] generalized this result to λ_j, $j \geq 3$ (functional inequalities)

Remark

One aims to compute the exact prefactors. This is important

- from a mathematical point of view
- for applications : accelerated dynamics algorithms use these prefactors, see Voter [97,98].

Exponentially small eigenvalues : sharp result

Theorem

There exists a function $S : \mathcal{U}^{(0)} \to \mathbb{R}_+^*$ such that the n_0 small eigenvalues $(\lambda_{\mathbf{m}}(h))_{\mathbf{m}\in\mathcal{U}^{(0)}}$ satisfy

$$\lambda_{\mathbf{m}}(h) = h\zeta(\mathbf{m}, h)e^{-2S(\mathbf{m})/h}$$

where $\zeta(\mathbf{m}, h) \sim \sum_{r=0}^{\infty} h^r\zeta_r(\mathbf{m})$ and $\zeta_0(\mathbf{m})$ is explicit.

This theorem was proved by

- Bovier-Gayrard-Klein [04], potential theory approach. Non degeneracy assumption on the family of heights $(S(\mathbf{m}))_{\mathbf{m}\in\mathcal{U}^{(0)}}$.
- Helffer-Klein-Nier [04] by semiclassical methods. Non degeneracy assumption.
- Michel [17] in the full general case.

The labelling procedure I

Let $\mathcal{U}^{(1)}$ denote the set saddle points of ϕ. For any $\mathbf{s} \in \mathcal{U}^{(1)}$ and $r > 0$ small enough, the set

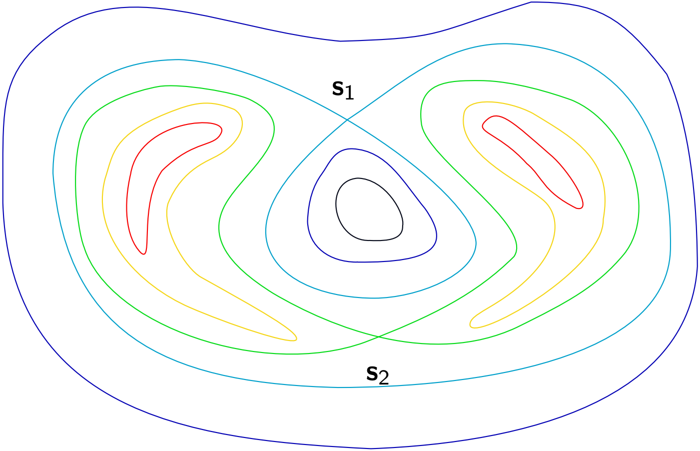
$$B(\mathbf{s}, r) \cap \{x \in X,\ \phi(x) < \phi(\mathbf{s})\}$$

has exactly two connected components $C_j(\mathbf{s}, r)$, $j = 1, 2$.

Definition (Hérau-Hitrik-Sjöstrand, 2011)

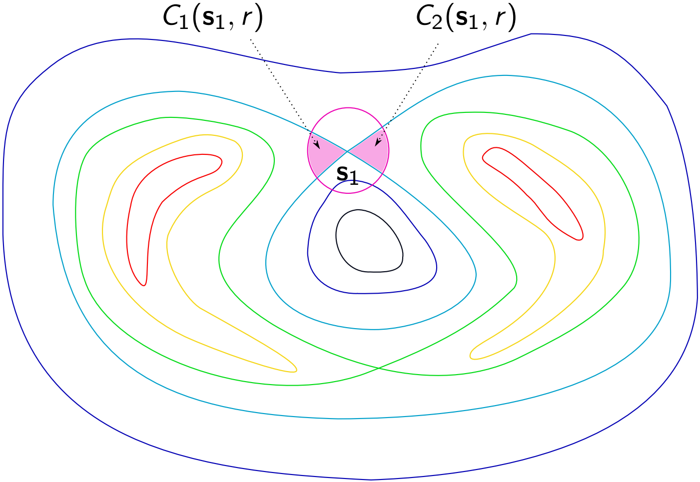
- $\mathbf{s} \in \mathcal{U}^{(1)}$ is a separating saddle point (ssp) iff $C_1(\mathbf{s}, r)$ and $C_2(\mathbf{s}, r)$ are contained in two different connected components of $\{x \in X,\ \phi(x) < \phi(\mathbf{s})\}$. We denote by $\mathcal{V}^{(1)}$ the set of ssp.
- $\sigma \in \mathbb{R}$ is a separating saddle value (ssv) if it is of the form $\sigma = \phi(\mathbf{s})$ with $\mathbf{s} \in \mathcal{V}^{('1)}$. We denote $\underline{\Sigma} = \phi(\mathcal{V}^{(1)}) = \{\sigma_2 > \sigma_3 > \ldots > \sigma_N\}$.

Example of SSP I

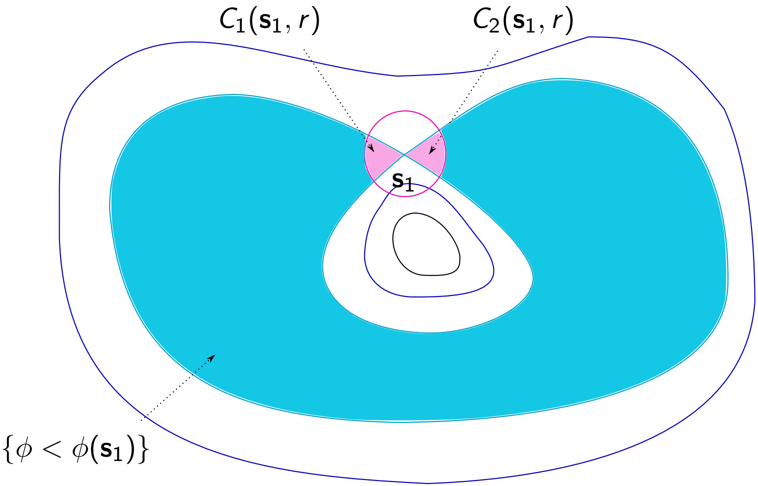


Level set of a potential with 2 minima, 2 saddle points and 1 maximum

Example of SSP II

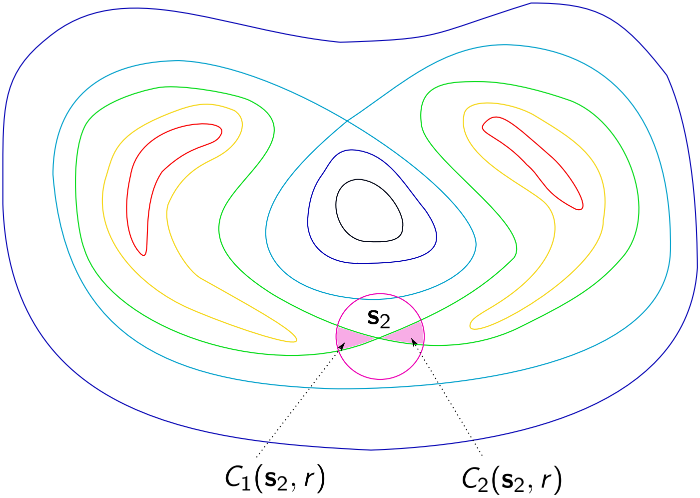


Example of SSP II

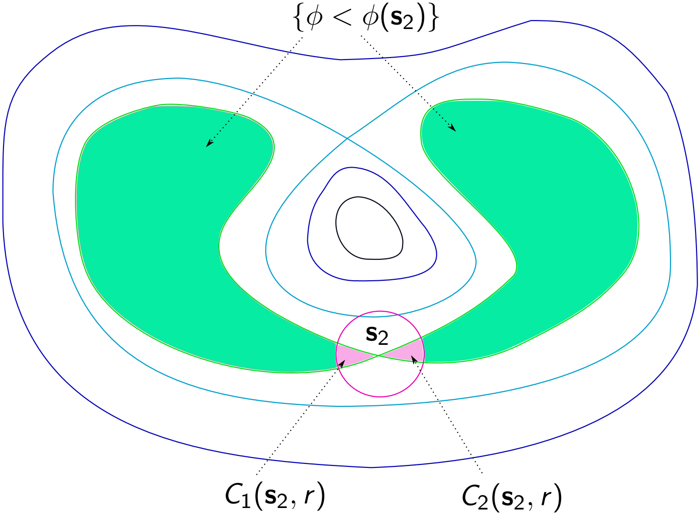


$\mathbf{s}_1$ is not separating

Example of SSP III



Example of SSP III



$\mathbf{s}_2$ is separating

The labelling procedure II

Add a fictive infinite saddle value $\sigma_1 = +\infty$ to $\underline{\Sigma}$ and let

$$\Sigma = \{\sigma_1\} \cup \underline{\Sigma} = \{\sigma_1 > \sigma_2 > \ldots > \sigma_N\}$$

- To $\sigma_1 = +\infty$ associate the unique connected component $E_{1,1} = \mathbb{R}^d$ of $\{\phi < \sigma_1\}$. In $E_{1,1}$, pick up $m_{1,1}$ one (non necessarily unique) minimum of $\phi_{|E_{1,1}}$.
- The set $\{\phi < \sigma_2\}$ has finitely many connected components. One of them contains $m_{1,1}$. The others are denoted $E_{2,1}, \ldots, E_{2,N_2}$. In each of these CC, one choses one absolute minimum $m_{2,j}$ of $\phi_{|E_{2,j}}$.
- The set $\{\phi < \sigma_k\}$ has finitely many CC. One denotes by $E_{k,1}, \ldots, E_{k,N_k}$ those of these CC which do not contain any $m_{i,j}$, $i < k$. In each $E_{k,j}$ one choses one absolute minimum $m_{k,j}$ of $\phi_{|E_{k,j}}$.

The labelling procedure III

Let $\mathcal{O}(X)$ denote the connected open subsets of X. Using the preceding labelling one constructs the following applications :

- $\boldsymbol{\sigma} : \mathcal{U}^{(0)} \to \Sigma$, defined by $\boldsymbol{\sigma}(\mathbf{m}_{i,j}) = \sigma_i$.
- $E : \mathcal{U}^{(0)} \to \mathcal{O}(X)$, defined by $E(\mathbf{m}_{i,j}) = E_{i,j}$.
- $S = \boldsymbol{\sigma} - \phi$

The Generic case I

The following hypothesis introduced by Hérau-Hitrik-Sjöstrand (2011) is a generalization of Helffer-Klein-Nier assumption (2004).

Generic Assumption (GA) :

For all $\mathbf{m} \in \mathcal{U}^{(0)}$, the following hold true :

i) $\phi_{|E(\mathbf{m})}$ has a unique point of minimum

ii) for any connected component E of $\{\phi < \sigma(\mathbf{m})\}$

$$E \cap \mathcal{V}^{(1)} \neq \emptyset \Longrightarrow \exists! \, \mathbf{s} \in \mathcal{V}^{(1)}, \; \phi(\mathbf{s}) = \sup \phi(E \cap \mathcal{V}^{(1)})$$

This assumption yields a bijection

$$\mathbf{s} : \mathcal{U}^{(0)} \to \mathcal{V}^{(1)} \cup \{\infty\}$$

We let

$$S(\mathbf{m}) = \phi(\mathbf{s}(\mathbf{m})) - \phi(\mathbf{m})$$

with the convention $\phi(\infty) = \infty$.

The Generic case II

Let us write $\lambda(\mathbf{m}, h)$, $\mathbf{m} \in \mathcal{U}^{(0)}$ the n_0 small eigenvalues of Δ_ϕ.

Theorem (Helffer-Klein-Nier 2004, Hérau-Hitrik-Sjöstrand 2011)

Suppose the the Generic Assumption is satisfied. Then the n_0 small eigenvalues of Δ_ϕ satisfy

$$\lambda(\mathbf{m}, h) = h\zeta(\mathbf{m}, h)e^{-2S(\mathbf{m})/h}$$

where $\zeta(\mathbf{m}, h) \sim \sum_{r=0}^{\infty} h^r \zeta_r(\mathbf{m})$ and

$$\zeta_0(\mathbf{m}) = \pi^{-1}|\mu(\mathbf{s}(\mathbf{m}))|\sqrt{\frac{|\det \phi''(\mathbf{m})|}{|\det \phi''(\mathbf{s}(\mathbf{m}))|}}$$

where $\mu(\mathbf{s})$ is the unique negative eigenvalue of ϕ'' in $\mathbf{s}$.

A simple example

Suppose that the following hypothesis are verified :

- The set of minimal values is reduced to one point :
  $\exists c_0,\ \forall \mathbf{m} \in \mathcal{U}^{(0)},\ \phi(\mathbf{m}) = c_0$
- The set of saddle values is reduced to one point :
  $\exists c_1,\ \forall \mathbf{m} \in \mathcal{U}^{(1)},\ \phi(\mathbf{m}) = c_1$

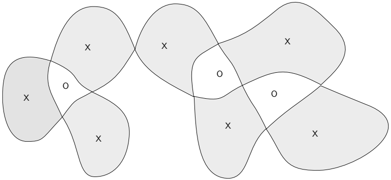


FIGURE – The sublevel set $\{\varphi < \sigma\}$ (dashed region) associated to a potential φ satisfying the assumptions. The x's represent local minima, the o's, local maxima.

Theorem (Michel 2017)

The n_0 small eigenvalues of Δ_ϕ satisfy $\lambda_1 = 0$ and for all $k = 2, \dots n_0$,

$$\lambda_k(h) = h\zeta_k(h)e^{-2S/h}$$

where $S = c_1 - c_0$ and

$$\zeta_k(h) \sim \sum_{r=0}^{\infty} h^r \zeta_{k,r}$$

and $\zeta_{k,0}$ are the non zero eigenvalues of the weighted graph $\mathcal{G}$ defined by

- The vertices of the graph are the minima $\mathbf{m} \in \mathcal{U}^{(0)}$.
- The edges between two vertices $\mathbf{m}$, $\mathbf{m}'$ are the saddle points $\mathbf{s} \in \mathcal{V}^{(1)}$ such that $\mathbf{s} \in \overline{E}(\mathbf{m}) \cap \overline{E}(\mathbf{m}')$.
- The weights explicitly depend on the values of ϕ'' on $\mathcal{U}^{(0)}$ and $\mathcal{U}^{(1)}$.

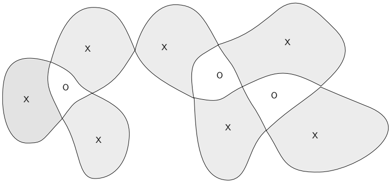


FIGURE – The sublevel set $\{\varphi < \sigma\}$ (dashed region) associated to a potential φ satisfying the assumptions. The x's represent local minima, the o's, local maxima.

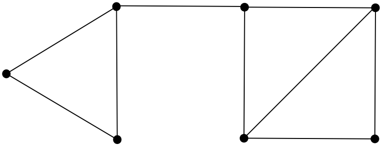


FIGURE – The graph associated to the potential represented in Figure 2

Finite dimensional reduction

The general strategy of Helffer-Klein-Nier 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 Δ_ϕ to $F^{(0)}$.

  We have to compute the eigenvalues of M.
- We compute suitable BKW approximated eigenfunctions $f_{\mathbf{m}}^{(0)}$ indexed by $\mathbf{m} \in \mathcal{U}^{(0)}$, and show that

$$\Pi^{(0)} f_{\mathbf{m}}^{(0)} = f_{\mathbf{m}}^{(0)} + error$$

  and compute the matrix of M in the base $\Pi^{(0)} f_{\mathbf{m}}^{(0)}$.
- Doing that leads to error terms which are too big.
- In order to overcome this difficulty, they use the supersymmetric structure.

Supersymmetric structure

- For $0 \leq p \leq d$, let Ω^pdenote the space of p-differential forms on $\mathbb{R}^d$ and let $d : \Omega^p \to \Omega^{p+1}$ denote the exterior derivative.
- Introduce the twisted semiclassical derivative

$$d_\phi = e^{-\phi/h} \circ hd \circ e^{\phi/h} = hd + \partial\phi\wedge$$

- the semiclassical Witten Laplacian on p forms is

$$\Delta_\phi^{(p)} = d_\phi^* \circ d_\phi + d_\phi \circ d_\phi^*$$

- for $p = 0$, we recover

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

The Witten Laplacian on 1-forms

The operator $\Delta_\phi^{(1)}$ is essentially self-adjoint on $\mathcal{C}_c^\infty(\Omega^1)$ and non negative. Morever, one has

$$\Delta_\phi^{(1)} = \Delta_\phi^{(0)} \otimes \mathrm{Id} + h\,\mathrm{Hess}(\phi)$$

- there exists $C_0, h_0 > 0$ such that for all $0 < h < h_0$

$$\sigma_{ess}(\Delta_\phi^{(1)}) \subset [C_0, \infty[$$

- $\sigma(\Delta_\phi^{(1)}) \cap [0, \epsilon_0 h]$ has n_1 elements.
- the eigenfunctions associated to the n_1 small eigenvalues of $\Delta_\phi^{(1)}$ are exponentially localized near the saddle points $\mathbf{s} \in \mathcal{U}^{(1)}$ (Agmon estimates).

Using Supersymmetry

The fondamental remarks are the following :

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

$$M = L^* L$$

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

- The matrix L is well approximated $L = (1 + \mathcal{O}(e^{-\alpha/h}))\mathcal{L}$ with

$$\mathcal{L} := (\langle d_\phi^{(0)} f_{\mathbf{m}}^{(0)}, f_{\mathbf{s}}^{(1)} \rangle)_{,\mathbf{s} \in \mathcal{U}^{(1)} \mathbf{m} \in \mathcal{U}^{(0)}}$$

where $f_{\mathbf{s}}^{(1)}$ are BKW approximated eigenfunctions on 1-form.

Singular values analysis

- The eigenvalues of M are the singular values of $L = (1 + \mathcal{O}(e^{-\alpha/h}))\mathcal{L}$
- The fondamental point is that the error terms induced by change of basis, etc. result in multiplicative errors thanks to the following

Lemma (Fan inequalities)

Let A, B be two matrices and denote by μ_n the singular values of any matrix. Then

$$\mu_n(AB) \leq \|B\|\mu_n(A)$$

$$\mu_n(AB) \leq \|A\|\mu_n(B)$$

where $\|C\|$ denotes the norm of $C : \mathbb{R}^p \to \mathbb{R}^q$ with $\mathbb{R}^\bullet$ endowed with ℓ^2 norms.

Exit event from a domain

Let Ω be a basin of attraction for the deterministic dynamic $\dot{x} = -2\nabla\phi(x)$ and let $\mathcal{D} \subset \Omega$. Let (X_t) be driven by overdamped Langevin equation with X_0 distributed according to the stationary measure of $\mathcal{D}$. We want to compute

- the mean first exit time from $\mathcal{D}$ for the dynamic (X_t)
- the law of the first exit point

Let (λ_1, u_1) be the first eigenpair of the infinitesimal generator $\mathscr{L}_{KS}$ with Dirichlet boundary conditions on $\partial\mathcal{D}$:

$$\begin{cases} -2\nabla\phi \cdot h\nabla u_1 + h^2\Delta u_1 = -\lambda_1 u_1 \text{ on } \mathcal{D}, \\ u_1 = 0 \text{ on } \partial\mathcal{D}. \end{cases}$$

Then

- mean exit time $= \lambda_1$
- the law of the first exit point is proportional to $-\partial_n u_1 d\sigma_{\partial\mathcal{D}}$.

Some results

After conjugation by $e^{-\phi/h}$, we are lead to consider the Witten Laplacian with boundary conditions.

- Helffer-Nier [06] : Small eigenvalues for Dirichlet boundary cond.
- Le Peutrec [10] : Small eigenvalues for Neumann BC
- di Gesu-Lelièvre-Le Peutrec-Nectoux [17] : computation of $\partial_n u_1$ up to the boundary

Kramers-Fokker-Planck equations

Consider the Kramers-Fokker-Planck operator acting on $L^2(\mathbb{R}^d_x \times \mathbb{R}^d_v)$

$$P = -vh\partial_x + \partial_x\phi h\partial_v + (-h^2\Delta_v + v^2 - hd)$$

This operator is (look at the x variable)

- non elliptic
- non self-adjoint

This has serious consequences. We don't know

- what is the nature of the spectrum of P.
- how to go from quasimodes to eigenfunctions.

Hypoellipticity

- One has
$$P = X_0 + b^* b$$
with $X_0 = -vh\partial_x + \partial_x\phi h\partial_v$ and $b = h\partial_v + v$. We have the following relations
$$[b, X_0] = a, \; [[b, X_0], X_0] = [a, X_0] = -\operatorname{Hess}(\phi) b$$
with $a = h\partial_x + \partial_x\phi$. This implies
$$[a^* b, X_0] = a^* a - hb^* \operatorname{Hess}(V) b$$
- One wants to use these relations in the spirit of Hörmander's hypoellipticity theorem.

Consider the operator Λ defined by

$$\begin{aligned}\Lambda^2 &:= 1 + a^* a + b^* b \\ &= 1 + \Delta_\phi + \Delta_{\frac{v^2}{2}}\end{aligned}$$

Theorem (Hérau-Nier [04])

There exists $C > 0$ such that for any $u \in \mathcal{C}_c^\infty(\mathbb{R}^d)$ we have

$$\|\Lambda^{\frac{2}{3}} u\|^2 \leq C(\|Pu\|^2 + \|u\|^2)$$

Corollary

Assume that $\nabla\phi$ grows sufficiently fast at infinity, then P has compact resolvent.

Resolvant estimate

Theorem (Hérau-Nier [04])

Let $\epsilon = \min(\frac{1}{8}, \frac{1}{8d-4})$. There exists some constants $c, C, C' > 0$ such that the following holds true :

i) The spectrum of P is contained in the infinite cusp $S \cap \{\mathrm{Re}\, z \geq 0\}$ with

$$S = \{z \in \mathbb{C},\ \mathrm{Re}\, z \geq c|z|^{\epsilon} \text{ or } |z| \leq C\}$$

ii) For any $z \notin S$ we have

$$\|(P - z)^{-1}\|_{L^2 \to L^2} \leq C'|z|^{-\epsilon}$$

Return to equilibrium

In the following, we denote by Π_0 the orthogonal projector (in $L^2(\mathbb{R}^{2d})$on the vector space generated by the half-Maxwellian $\mathcal{M}(x,v)^{\frac{1}{2}}$.

Theorem (Hérau-Nier [04])

Under the preceding assumptions, there exists $C, \alpha_1 > 0$ such that

$$\|e^{-tP}u_0 - \Pi_0 u_0\| \leq Ce^{-\alpha_1 t}\|u_0\|$$

for all $u_0 \in L^2(\mathbb{R}^{2d})$.

Contour integral

- Write

$$e^{-tP} = \frac{1}{2i\pi}\int_{\partial S} e^{-tz}(P-z)^{-1}dz$$

where the integral converges in L^2 sense thanks to the cusp shape of S and the resolvent estimate.

- Modify the integration contour

$$e^{-tP} = \frac{1}{2i\pi}\int_{|z|=C} e^{-tz}(P-z)^{-1}dz + \frac{1}{2i\pi}\int_{\partial S'} e^{-tz}(P-z)^{-1}dz$$

$$= \Pi_0 + \frac{1}{2i\pi}\int_{\partial S'} e^{-tz}(P-z)^{-1}dz = \Pi_0 + \mathcal{O}_{L^2}(e^{-\alpha_1 t})$$

since $S' \subset \{\mathrm{Re}\, z \geq \alpha_1\}$ for some $\alpha_1 > 0$.

Remark

To find the best α_1 we need to compute the small eigenvalues of P.

Small eigenvalues of Kramers-Fokker-Plank operators

Theorem (Hérau-Hitrik-Sjöstrand [08-11])

Suppose that ϕ is a Morse function satisfying theGeneric Assumption. Then

- There exists $\epsilon_0, h_0 > 0$ such that for any $0 < h < h_0$, P has exactly n_0 eigenvalues in $\{0 \leq \mathrm{Re}\, z \leq \epsilon_0 h\}$.
- These n_0 small eigenvalues satisfy $\lambda(\mathbf{m}, h) = h\zeta(\mathbf{m}, h)e^{-2S(\mathbf{m})/h}$ where $\zeta(\mathbf{m}, h) \sim \sum_{r=0}^{\infty} h^r \zeta_r(\mathbf{m})$ and

$$\zeta_0(\mathbf{m}) = \pi^{-1}|\mu(\mathbf{s}(\mathbf{m}))|\sqrt{\frac{|\det \phi''(\mathbf{m})|}{|\det \phi''(\mathbf{s}(\mathbf{m}))|}}$$

where $\mu(\mathbf{s})$ is the unique negative eigenvalue of the matrix $\begin{pmatrix} 0 & \mathrm{Id} \\ \mathrm{Hess}\,\phi(\mathbf{s}) & \mathrm{Id} \end{pmatrix}$.

Supersymmetry for KFP

Let $f(x,v) = \phi(x) + \frac{v^2}{2}$ and introduce the twisted exterior derivatives $d_{f,h}$ mapping 0-forms to 1-forms on $\mathbb{R}^{2d}_{x,v}$. Using the basis of 1-forms $dx_1, \ldots, dx_d, dv_1, \ldots, dv_d$ this reads

$$d_{f,h} = \begin{pmatrix} h\partial_x + \partial_x V \\ h\partial_v + v \end{pmatrix}$$

The KFP operator enjoys a supersymmetric structure

$$P = d_{f,h}^{A,*} \circ d_{f,h}$$

where $d_{f,h}^{A,*}$ denotes the adjoint of $d_{f,h}$ for the non symmetric skew-product

$$\langle u, v \rangle_A = \langle Au, v \rangle$$

for any $u, v \in \Omega^1(\mathbb{R}^{2d})$ with

$$A = \begin{pmatrix} 0 & -\operatorname{Id} \\ \operatorname{Id} & \frac{1}{2}\operatorname{Id} \end{pmatrix}$$

Sketch of proof

- Introduce a natural operator on 1-forms

$$P^{(1),A} := d_{f,h}^{A,*} \circ d_{f,h} + d_{f,h} \circ d_{f,h}^{A,*}$$

- Study the spectral theory of $P^{(1),A}$.
  - Resolvent estimates
  - Quasimodes
- Perform a "singular value analysis" in the spirit of Witten Laplacian. Compute

$$L := \langle d_{f,h} f_{\mathbf{m}}^{(0)}, f_{\mathbf{s}}^{(1)} \rangle_A$$

- Problem : the skew product $\langle , \rangle_A$ is not symmetric.
  $\rightsquigarrow$ Solution : Use extra symmetry (PT symmetry) :

$$U^* P U = P^*$$

with $Uf(x,v) = f(x,-v)$.

Non-local Fokker-Planck equations

- Consider the Fokker-Planck equation $\partial_t u = P_Q u$ with

$$P_Q u = vh\partial_x - \nabla\phi(x)h\partial_v + Q(v) \tag{4}$$

where the collision operator is a pseudodifferential operator $Q(u) := \mathrm{Op}_h^w(q)(u)$ such that $Q(\mathcal{M}) = 0$.

- A typical example is linear relaxation kernel

$$Q(u) := u - \langle u, \phi_0\rangle\phi_0$$

with $\phi_0(v) = (2\pi h)^{-d/2} e^{-v^2/(2h)}$.

Goals

1) Prove exponential return to equilibrium. 2) Compute the optimal rate.

Some partial results

- Resolvent estimates for P_Q and rough localization of eigenvalues (V. Robbe 2015)
- Construction of pseudodifferential supersymmetric structure for P_Q (Hérau-Michel 2018)
- Resolvant estimates for the operator $P_Q^{(1)}$ acting on 1-forms (Hérau-Michel 2018)

Work in progress : Agmon estimates, small eigenvalues analysis.