Semiclassical methods for the analysis of reversible and non reversible metastable processes

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Analysis and simulations of metastable systems

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Plan

Motivations

Consider a time homogenous Langevin processes

$$dX_t = \xi(X_t) + \sqrt{2h}\sigma(X_t)dB_t$$

where

- $(B_t) =$ Brownian motion on $M = \mathbb{R}^d$ or a compact manifold.
- $\xi : M \to TM =$ vector field
- the matrix σ is the diffusion coefficient
- h is proportional to the temperature of the system.

Metastability (process point of view)

Denote $X^* = \{\xi = 0\}$ the set of stationary points of ξ.

- Assume $x_* \in X^*$ is asymptotically stable for the deterministic flow $h = 0$: for $x \simeq x_*$, $X_t(x)$ remains close to x_* and converges to x_* when $t \to +\infty$.
- If $0 < h << 1$, X_t may stay close to x_* during long time (depending on h) until it escapes and converges to another stationary point
- One aims to quantify this discrete dynamic on the set of critical points

The exit problem from a fixed domain

Let $\Omega \subset M$ be a smooth bounded open set. Given $x \in \Omega$ denote

$$\tau_{\Omega^c}^x = \inf\{t \geqslant 0,\ X_t^x \notin \Omega\}$$

where X_t^x denotes the process with initial condition $X_{t=0}^x = x$.

Questions

- compute $\mathbb{E}(\tau_{\Omega^c}^x)$?
- compute the distribution of the exit point $X_{\tau_{\Omega^c}^x}^x$
- links with the spectrum of the associated generator
- Hitting time problem: given two equilibrum point x_*, y_*, compute $\mathbb{E}(\tau_{B(y_*,h)}^{x_*})$

- Freidlin-Wentzell 70's, Day 80's, DiGesu-Lelievre-Le Peutrec-Nectoux 10 's, Bovier-Eckhoff-Gayrard-Klein (00's)
- See the review by [Berglund 13].

Fokker-Planck equations

The generator of the process (X_t) is

$$\mathcal{L} = -h\sum_{i,j} a_{i,j}\partial_{x_i}\partial_{x_j} - \sum_k \xi_k \partial_{x_k}$$

with $a = (a_{i,j}) = \sigma\sigma^t$. We shall denote $\mathcal{L}^\dagger$ the formal adjoint of $\mathcal{L}$

- Given any test function φ, let $u(t,x) = \mathbb{E}(\varphi(X_t^x))$. Then u solves the Fokker-Planck equation

$$\partial_t u + \mathcal{L}u = 0,\ u_{|t=0} = \varphi$$

- Denote by $\mu(t,x)$ the law of the process (X_t) with initial distribution μ_0. Then μ solves the

$$\partial_t u + \mathcal{L}^\dagger \mu = 0,\ \mu_{|t=0} = \mu_0$$

Stationary measure

We will often assume the following

Assumption Gibbs

There exists a smooth function $f : \mathbb{R}^d \to \mathbb{R}$ such that $\mathcal{L}^\dagger(e^{-f/h}) = 0$.

Question

- Solving the equation in adapted functional spaces.
- Long time behavior of the solutions? Return to equilibrium? Eyring-Kramers law?
- Resolvent estimates
- Spectral asymptotics?

Summary of some questions of interrest

- Reversible processes (self-adjoint generator)
  - Boundaryless case
    - topological questions
    - construct sharp quasimodes
  - Boundary case
    - relation between spectrum and exit time
    - exit event
    - construction of quasimodes
- Non-reversible processes (non self-adjoint generator)
  - Resolvent estimates
    - Elliptic situation
    - Hypoelliptic situation
  - Quasimode construction
  - Eigenvalue expansion (return to equilibrium)
  - Boundary value problems

Questions discussed in this lecture

- Reversible processes (self-adjoint generator)
  - Boundaryless case
    - topological questions $\surd$
    - construct sharp quasimodes $\surd$
  - Boundary case
    - relation between spectrum and exit time $\surd$
    - exit event $\surd$
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- Non-reversible processes (non self-adjoint generator)
  - Resolvent estimates
    - Elliptic situation $\surd$
    - Hypoelliptic situation $\surd$
  - Quasimode construction $\surd$
  - Eigenvalue expansion (return to equilibrium) $\surd$
  - Boundary value problems $\surd$

Recalls on unbounded operators

Let H be a Hilbert space and $A : D(A) \to H$ be un unbounded operator with dense domain $D(A)$.

- A is said to be closed if its graph is closed.
- The spectrum $\sigma(A)$ of a closed operator A is defined by

$$\sigma(A)^c = \{z \in \mathbb{C},\ (A - z) \text{ is invertible } \}$$

  If $z \notin \sigma(A)$, then $(A - z)^{-1}$ is bounded.
- The adjoint A^* of A has domain

$$D(A^*) = \{v \in H,\ \exists C_v > 0,\ \forall u \in D(A),\ |\langle Au, v\rangle| \leqslant C\|u\|\}$$

- We say that A is symmetric if $D(A) \subset D(A^*)$ and for all $u, v \in D(A)$, $\langle Au, v\rangle = \langle u, Av\rangle$
- We say that A is self-adjoint if A is symmetric and $D(A) = D(A^*)$.
- We say that A is essentially self-adjoint if it admits a unique self-adjoint extension.

Functionnal calculus of self-adjoint operators

- Let $A : D(A) \to H$ be self-adjoint. Denote $\mathcal{B}_b(\mathbb{R}^d)$ the space bounded Borel functions. There exists an application $f \mapsto f(A)$ defined on $\mathcal{B}_b(\mathbb{R}^d)$ such that
  - $(f+g)(A) = f(A) + g(A)$, $(fg)(A) = f(A)g(A)$
  - $\|f(A)\| = \sup_{\lambda\in\sigma(A)} |f(\lambda)|$
  - if $f \geqslant 0$, then $f(A) \geqslant 0$
- Given a Borel set $\Omega \subset \mathbb{R}$, denote $P_\Omega = 1_\Omega(A)$.
- For any $\psi \in H$, $\Omega \mapsto \langle P_\Omega\psi, \psi\rangle$ is a Borel measure denoted by $d\langle P_\lambda\psi, \psi\rangle$. One has

$$\langle f(A)\psi, \psi\rangle = \int_{\sigma(A)} f(\lambda) d\langle P_\lambda\psi, \psi\rangle$$

  or more shortly

$$f(A) = \int_{\sigma(A)} f(\lambda) dP_\lambda$$

- the above formula can be generalized to unbounded function f for ψ in suitable domains.

Applications of functional calculus

- One has the resolvent estimate for self-adjoint operators

$$\forall z \in \mathbb{C}\backslash\sigma(A),\ \|(A-z)^{-1}\|_{H\to H} \leqslant \frac{1}{\operatorname{dist}(z,\sigma(A))}.$$

- Assume A is a non-negative self-adjoint operator. Let $u_0 \in D(A)$ and let $u(t) = e^{-tA}u_0$. Then u solves the heat equation

$$\partial_t u + Au = 0, \quad u_{|t=0} = u_0.$$

- Assume A has compact resolvent and denote $\lambda_k,\ k \geqslant 1$ the increasing sequence of eigenvalues and Π_K the associated orthogonal projector. Then $f(A) = \sum_{k\geqslant 1} f(\lambda_k)\Pi_k$. In particular for any $K \geqslant 1$

$$e^{-tA} = \sum_{k=1}^{K-1} e^{-t\lambda_k}\Pi_k + O_H(e^{-t\lambda_K})$$

Spectrum of self-adjoint operators

Theorem (Weyl criterion)

Let $A : D(A) \to H$ be a self-adjoint operator and let $\lambda \in \mathbb{C}$. Then $\lambda \in \sigma(A)$ iff there exists a normalized sequence (f_n) such that $(A - \lambda)f_n \to 0$ as $n \to \infty$.

Definition-Proposition

- The essential spectrum of A (denoted by $\sigma_{ess}(A)$) is the set of $\lambda \in \mathbb{C}$ such that there exists an infinite orthonormalized sequence (f_n) such that $(A - \lambda)f_n \to 0$ as $n \to \infty$.
- The discrete spectrum of A (denoted by $\sigma_{disc}(A)$) is the set of eigenvalues of A which are isolated with finite multiplicity.

One has $\sigma(A) = \sigma_{disc}(A) \sqcup \sigma_{ess}(A)$.

Maxi-min principle

Proposition (Maximin principle)

Let $A : D(A) \to H$ be a self-adjoint operator bounded from below. Assume A admits an increasing sequence of eigenvalues $(\lambda_k)_{k \geqslant 1}$ such that $\lambda_k \leqslant \inf \sigma_{ess}(A)$. Then one has

$$\lambda_k = \max_{\psi_1,\dots,\psi_{n-1} \in H} \; \min_{u \in D(A), u \perp \psi_1,\dots,\psi_{n-1}} \langle Au, u \rangle.$$

Corollary

Let F be a finite dimensional subspace of H.

- Assume $\dim F = k$ and $A \geqslant a$ on $D(A) \cap F^{\perp}$, then $\lambda_{k+1} \geqslant a$
- Assume $F \subset D(A)$, $\dim F = k$ and $A \leqslant a$ on F, then $\lambda_k \leqslant a$

Schrödinger operators

Consider a semiclassical Schrödinger operator on $L^2(\mathbb{R}^d)$

$$P = -h^2\Delta + V$$

- Assume $V \in C^0(\mathbb{R}^d, \mathbb{R})$ bounded from below, $V \geqslant -m$, then P is essentially self-adjoint on $C_c^\infty(\mathbb{R}^d)$.
- If $\lim_{|x|\to+\infty} V(x) = +\infty$, then P has compact resolvent

$$\sigma(P) = \{eigenvalues\ going\ to + \infty\}$$

- If $\liminf_{|x|\to+\infty} V(x) = c_0 > 0$, then

$$\sigma_{ess}(P) \subset [c_0 + \infty[$$

and

$$\sigma(P)\cap]-\infty, c_0[= \sigma_{disc}(P) = \{finite\ multiplicity\ eigenvalues\}$$

- Using functional calculus one has

$$e^{-tP} = \sum_{k=1}^{K-1} e^{-t\lambda_k}\Pi_k + O(e^{-t\lambda_K})$$

where $\lambda_1 \leqslant \ldots \leqslant \lambda_k \leqslant \ldots$ denote the sequence of eigenvalues below the essential spectrum.

- One aims at computing the eigenvalues of P when $h \to 0$. This leads to
  - Harmonic approximation
  - WKB methods

The harmonic oscillator

Let A be a symmetric positive definite matrix and let

$$N_A(h) = -h^2\Delta + \langle Ax, x\rangle$$

acting on $L^2(\mathbb{R}^d)$. Then

- $N_A(h)$ has compact resolvent
- One has

$$\sigma(N_A(h)) = \{h\nu_k,\ k \in \mathbb{N}^d\}$$

  where $\nu_k = \sum_{j=1}^d \sqrt{\mu_j}(2k_j + 1)$ and the μ_j are the eigenvalues of A.
- $h\nu_0$ has multiplicity 1 associated to $e^{-\langle A^{\frac{1}{2}}x,x\rangle/h}$.
- eigenfunctions= Hermite functions are $O(e^{-|x|^2/ch})$ for some $c > 0$.

Proof

- Using unitary transformation U such that $U^t AU$ is diagonal we can assume $d = 1$. We study

$$N = -h^2 \frac{d^2}{dx^2} + a^2 x^2$$

  on the line.
- We make the change of variable $x \mapsto (\frac{h}{a})^{\frac{1}{2}} x$, then $N \rightsquigarrow haQ$ with

$$Q = -\frac{d^2}{dx^2} + x^2 = b^* b + 1$$

  with $b = \partial_x + x$.
- observe that $b(e^{-x^2/2}) = 0$ gives the ground state
- use

$$Qb^* u = b^* Q + 2b^*$$

  to generate the other eigenvalues

Single well potential

Let $P = -h^2\Delta + V$ with V a smooth confining potential with only one local minimum (in x_0) which is non degenerate. Then

Theorem [Helffer-Sjöstrand, Simon 80's]

$\sigma(P)$ is made of eigenvalues of finite multiplicity $(E_k(h))_{k\in\mathbb{N}^d}$ and for all $k \in \mathbb{Z}^d$,

$$E_k(h) = V(x_0) + \nu_k h + O(h^{\frac{6}{5}})$$

where ν_k are the eigenvalues of $N_A(1)$ with $A = \frac{1}{2}\,\mathrm{Hess}(V)(x_0)$. In particular the bottom of the spectrum is

$$E_0(h) = V(x_0) + h\sum_{j=1}^{d}(\frac{\lambda_j}{2})^{\frac{1}{2}} + O(h^{\frac{6}{5}})$$

where λ_j are the eigenvalues of $\mathrm{Hess}(V)(x_0)$.

Harmonic approximation

We can assume $x_0 = 0$ and $V(x_0) = 0$. Assume to simplify the numerology $d = 1$. Let $(f_k(h))_{k\in\mathbb{N}^d}$ be the Hermite function associated to the eigenvalue $\nu_k h$ of $N_A(h)$. Recall

$$f_k = O(e^{-|x|^2/Ch}).$$

Let $\chi \in C_c^\infty(\mathbb{R}^d)$ equal to 1 near 0.

- Introduce the quasimodes $g_k(h) = \chi(h^{-\frac{2}{5}}x)f_k(x)$
- For $k \geqslant 0$, let

$$F_k = \text{span}\{g_1, \dots, g_k\}$$

  with the convention $F_0 = \emptyset$.

Observe that $g_k - f_k = O(e^{-ch^{-\frac{1}{5}}})$ in any Sobolev norm.

Upper bound on λ_k.

Denote $N_A = N_A(h)$. Recall that

$$P = -h^2\Delta + \frac{1}{2}\langle Ax, x > +O(|x|^3) = N_A + O(|x|^3)$$

Moreover $|x|^3 = O(h^{\frac{6}{5}})$ on $\mathrm{supp}(\chi_h)$. Hence, for any $j \leqslant k$, one has

$$\langle Pg_j, g_j\rangle = \langle N_A g_j, g_j\rangle + \langle O(x^3)g_j, g_j\rangle = \langle N_A g_j, g_j\rangle + O(h^{\frac{6}{5}})\|f_j\|^2$$

Moreover

$$N_A g_j = N_A f_j - N_A((1-\chi_h)f_j) = h\nu_j g_j + O(e^{-ch^{-\frac{1}{5}}})$$

hence for all $j \leqslant k$

$$\langle Pg_j, g_j\rangle = h\nu_j\|g_j\|^2 + O(h^{\frac{6}{5}})\|g_j\|^2$$

which shows that, $\lambda_k \leqslant h\nu_k + O(h^{\frac{6}{5}})$.

Lower bound on λ_k.

Assume $u \in F_{k-1}^{\perp}$. Then $\chi_h u$ is orthogonal to span$\{f_j,\ j \leqslant k-1\}$. Hence,

$$\langle P\chi_h u, \chi_h u\rangle = \langle N_A \chi_h u, \chi_h u\rangle + O(h^{\frac{6}{5}})\|\chi_h u\|^2 \geqslant (h\nu_k + O(h^{\frac{6}{5}}))\|\chi_h u\|^2$$

and

$$\begin{aligned}\langle P(1-\chi_h)u, (1-\chi_h)u\rangle &\geqslant \langle V(1-\chi_h)u, (1-\chi_h)u\rangle \\ &\geqslant C\langle x^2(1-\chi_h)u, (1-\chi_h)u\rangle \\ &\geqslant h^{\frac{4}{5}}\|(1-\chi_h)u\|^2\end{aligned}$$

and hence

$$\langle Pu, u\rangle \geqslant (h\nu_k + O(h^{\frac{6}{5}}))\|u\|^2$$

which shows that $\lambda_{k+1} \geqslant h\nu_k - O(h^{\frac{6}{5}})$.

Generalization

Let $P = -h^2\Delta + V + hW$ with:

- V a smooth confining potential with only one local minimum in 0
- $\mathrm{Hess}(V)(0)$ invertible
- W a smooth bounded potential

Theorem [Helffer-Sjöstrand, Simon 80's]

$\sigma(P)$ is made of eigenvalues of finite multiplicity $(E_k(h))_{k\in\mathbb{N}^d}$ and for all $k \in \mathbb{Z}^d$,

$$E_k(h) = V(0) + h(\nu_k + W(0)) + O(h^{\frac{6}{5}})$$

where ν_k are the eigenvalues of $N_A(1)$ with $A = \frac{1}{2}\,\mathrm{Hess}(V)(0)$. In particular the bottom of the spectrum is

$$E_0(h) = V(0) + h\Big(W(0) + \sum_{j=1}^{d}\big(\frac{\lambda_j}{2}\big)^{\frac{1}{2}}\Big) + O(h^{\frac{6}{5}})$$

Semiclassical anzats

Goal

Prove more precise spectral asymptotics

Suppose $V(0) = 0$. One looks for $(E(h), u_h)$ under the form

$$E(h) \sim h \sum_{j \geqslant 0} h^j E_j, \quad u_h(x) \sim e^{-\phi(x)/h} \sum_{j \geqslant 0} h^j a_j(x)$$

Plug this into the equation $(-h^2\Delta + V - E(h))u_h = 0$, we get

- Eikonal equation

$$|\nabla \phi(x)|^2 = V(x)$$

- Transport equations

$$(\mathcal{L} - E_0)a_j = \frac{1}{2}\Delta a_{j-1} + \sum_{k=0}^{j-1} E_{j-k} a_k$$

with $\mathcal{L} = \nabla\phi \cdot \nabla + \frac{1}{2}\Delta\phi$ and the convention $a_k = 0$ for $k < 0$.

Positive solutions of the Eikonal equation

One aims to solve near 0

$$|\nabla\phi(x)|^2 = V(x)$$
$$\mathrm{Hess}(\phi) > 0$$

If $V(x) = \langle Ax, x\rangle$ with $A = \frac{1}{2}\mathrm{Hess}(V)(0)$, take $\phi(x) = \langle A^{\frac{1}{2}}x, x\rangle$.
In the general case, we can use symplectic geometry

- Let $q(x,\xi) = |\xi|^2 - V(x)$ and the associated Hamiltonian vector field $H_q = \partial_\xi q \partial_x - \partial_x q \partial_\xi$.
- Observe that q is constant along the flow $\exp(tH_q)$
- apply the stable/instable manifold theorem to the H_q flow in $(0,0)$ gives stable manifold $\Lambda_+ \subset \mathbb{R}^{2d}$
- one has $\Lambda_+ \subset \{q = 0\}$
- since $\mathrm{Hess}(V)(0) > 0$ then $\dim(\Lambda_+) = d$
- Λ_+ is Lagragian, $\Lambda_+ = \{\xi = \nabla\phi_+(x)\}$ for some smooth function ϕ_+
- $\mathrm{Hess}\,\phi_+(0)$ is positive definite

Solving the transport equations

- Equation on a_j:
$$(\mathcal{L} - E_0)a_j = R_j$$
with $\mathcal{L} = \nabla\phi \cdot \nabla + \frac{1}{2}\Delta\phi$.
- Consider the vector field $\Gamma = \nabla\phi \cdot \nabla$ and let $k = \frac{1}{2}\Delta\phi - E_0$. We look for non trivial solutions u of
$$\Gamma u + ku = g$$
by characteristic method.
- Let γ_x be the integral curve of Γ such that $\gamma_x(0) = x$. Then
$$(\frac{d}{dt} + k(\gamma_x))u \circ \gamma_x = g(\gamma_x)$$

- Integrate between $-\infty$ and 0 gives

$$u(x) = u(0)e^{-\int_{-\infty}^{0} k(\gamma_x(s))ds} + \int_{-\infty}^{0} e^{\int_0^t k(\gamma_x(s))ds} g(\gamma_x(t))dt$$

  which is well defined and smooth as soon as
  - $k(0) = 0$
  - g vanishes at infinite order in 0.
- Consequently, we first solve the transport equation modulo $O(x^\infty)$

Approximate solution of the transport equations

- We look for solutions u of

$$\Gamma u + ku = g.$$

in formal power expansion $u = \sum_{m \geqslant 0} u_m$ with $u_m \in \mathscr{P}^m_{hom}$ homogenous polynomial of degree m.

- Denote $H = \mathrm{Hess}(\phi)(0)$, then $\Gamma = Hx \cdot \partial_x + O(x^2)\partial_x$. Then

$$(Hx \cdot \partial_x + k(0))u_0 = g_0 \tag{T0}$$

and for $m \geqslant 1$

$$(Hx \cdot \partial_x + k(0))u_m = v_m \tag{T$\geqslant$}$$

where v_m depends on $g_m, u_0, \dots, u_{m-1}$.

- To simplify consider the first transport equation, then $g_0 = 0$.
- Since $Hx \cdot \partial_x = 0$ on $\mathscr{P}^0_{hom}$ solving (T0) is possible as soon as $k(0) = 0$. This is equivalent to choose $E_0 = \frac{1}{2}\Delta\phi(0)$.
- Since H is definite positive, then for $m \geqslant 1$, $Hx \cdot \partial_x$ is invertible on $\mathscr{P}^m_{hom}$ which permits to solve (T$\geqslant$).
- Using a Borel procedure, we obtain solution $\tilde{u}$ such that

$$\Gamma \tilde{u} + k\tilde{u} = O(x^\infty)$$

- We look for solution u under the form $u = \tilde{u} + v$ with $v = O(x^\infty)$. Then v solves

$$\Gamma v + kv = g \tag{1}$$

  for some $g = O(x^\infty)$ depending on $\tilde{u}$.
- Conclude with characteristic method.

Accurate asymptotics

Using the previous construction we get the following

Theorem [Helffer-Sjöstrand 80's]

For any $k \geqslant 1$, there exists a formal serie $E_k(h) \sim h\sum_{j\geqslant 0} h^j E_{k,j}$ and a symbol $a_k(x,h) \sim \sum_{j\geqslant 0} h^j a_j(x)$ such that near $x = 0$, one has

$$(P - E_k(h))(a_k e^{-\phi/h}) = O(h^\infty)e^{-\phi/h}$$

with $E_{k,0} \neq 0$ equal to the k-th eigenvalue of the harmonic approximation of P and $a_0 = 1$.

As a corollary, we get the following

Theorem [Helffer-Sjöstrand 80's]

For any $k \in \mathbb{N}$, the eigenvalues $\lambda_k(h)$ admits a power expansion $\lambda_k(h) \sim h\sum_{j\geqslant 0} E_{k,j} h^j$

Proof

Let $f_k = \chi a_k e^{-\phi/h}$ for some cut-off function χ. Then

$$\langle Pf_k, f_k \rangle = E_k(h)\|f_k\|^2 + O(h^\infty)$$

hence by maxi-min principle, $\lambda_k \leqslant E_k + O(h^\infty)$. Conversely, assume by contradiction there exists $M \in \mathbb{N}$ such that $\lambda_k \leqslant E_k(h) - Ch^M$ and let $N \geqslant M + 1$. Hence the Riesz projector

$$\tilde{\Pi}_k := \frac{1}{2i\pi} \int_{\partial D(E_k(h), h^N)} (z - P)^{-1} dz = 0.$$

Since $\lambda_{k+1} \geqslant E_k(h) + Ch$ then for all $z \in \partial D(E_k(h), h^N)$, one has $(P - z)^{-1} = O(h^{-M})$ and since $(P - E_k(h))f_k = O(h^\infty)$, then

$$(z - P)^{-1} f_k = (z - E_k)^{-1} f_k + O(h^\infty).$$

This implies $\tilde{\Pi}_k f_k = f_k + O(h^\infty)$ which is a contradiction. $\square$

Keywords to go further

- multiple well setting
- degenerate situations (non-resonant wells, submanifolds critical sets)
- exponential estimates of eigenfunctions (Agmon estimates)
- tunnel effect
- resonance theory
- non-selfadjoint operators

Bibliography

- M. Reed and B. Simon, Methods of modern mathematical physics. I. Functional analysis.
- C. Cheverry and N. Raymond, A guide to spectral theory, 2021
- B. Helffer, Spectral theory and its applications, 2013
- H. Cycon, R. Froese, W. Kirch, B. Simon, Schrödinger operators with application to quantum mechanics and global geometry, 1987
- B. Helffer, Semiclassical analysis for the Schrödinger operator and application, 1988
- M. Dimassi and J. Sjöstrand, Spectral asymptotics in the semiclassical limit, 1999

Overdamped Langevin equation

Consider the overdamped Langevin process

$$dX_t = -2\nabla f(X_t) + \sqrt{2h}dB_t$$

The generator of this process is

$$\mathcal{L} = h\Delta - 2\nabla f \cdot \nabla.$$

We consider this operator on $L^2(\mathbb{R}^d, e^{-2f/h}dx)$. Let $\Omega\psi = e^{f/h}\psi$, then

$$\Omega^{-1}L\Omega = -\frac{1}{h}\Delta_{f,h}$$

where $\Delta_{f,h} = -h^2\Delta + |\nabla f|^2 - h\Delta f$ is the semiclassical Witten Laplacian associated to f.

Witten Laplacian I

Assumption (Confin)

There exists $C > 0$ and a compact $K \subset \mathbb{R}^d$ such that for all $x \in \mathbb{R}^d \backslash K$, one has

$$|\nabla f(x)| \geqslant \frac{1}{C}, \ |\mathrm{Hess}(f(x))| \leqslant C|\nabla f|^2, \ \text{and} \ f(x) \geqslant C|x|.$$

Under this assumption, one has the following properties

- Δ_f is essentially self-adjoint on $\mathcal{C}_c^\infty(X)$.
- $\Delta_f \geqslant 0$
- there exists $C_0, h_0 > 0$ such that for all $0 < h < h_0$

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

- 0 is an eigenvalue of Δ_f associated to the eigenstate $e^{-f/h}$.

Witten Laplacian II

Assumption (Morse)

We assume f is a Morse function. We denote

- $\mathcal{U}$ = critical points of f
- $\mathcal{U}^{(p)}$= critical points of f of index p
- $n_p = \sharp\mathcal{U}^{(p)} < \infty$

Theorem [Witten 82, Simon 84, Helffer-Sjöstrand 84]

There exists $C, \epsilon_0, h_0 > 0$ such that for all $0 < h < h_0$ one has

$$\sharp\sigma(\Delta_f) \cap [0, \epsilon_0 h] = n_0.$$

Moreover

$$\sigma(\Delta_f) \cap [0, \epsilon_0 h] \subset [0, e^{-C/h}].$$

Proof

- Apply previous result to $P = -h^2\Delta + V + hW$ with
$$V = |\nabla f|^2 \text{ and } W = -\Delta f$$
- The minima of V are all the critical points of f denoted by $\mathcal{U}$.
- In any point $\mathbf{u} \in \mathcal{U}$, one has
$$\operatorname{Hess}(V) = 2\operatorname{Hess}(f)^2 \quad \text{and} \quad W = -\operatorname{tr}\operatorname{Hess}(f)$$
In particular the eigenvalues of $\operatorname{Hess}(V)$ are $\tilde{\lambda}_j = 2\lambda_j^2$, where $\lambda_j =$ eigenvalues of $\operatorname{Hess}(f)$.
- Apply harmonic approximation in $x_0 \in \mathcal{U}$. The associated first eigenvalue is
$$E_0 = h\Big(\sum_{j=1}^{d}\Big(\frac{\tilde{\lambda}_j}{2}\Big)^{\frac{1}{2}} + W(0)\Big) + O(h^{\frac{6}{5}})$$
$$= h\Big(\sum_{j=1}^{d}|\lambda_j| - \sum_{j=1}^{d}\lambda_j\Big) + O(h^{\frac{6}{5}})$$

- **First case: x_0 is a minimum of f.** Then all the λ_j are positive, hence

$$\sum_{j=1}^{d} |\lambda_j| - \sum_{j=1}^{d} \lambda_j = 0$$

which implies

$$E_0 = O(h^{\frac{6}{5}})$$

- **Second case: x_0 is a critical points of index $j \geqslant 1$.** Then one of the λ_j is negative and hence

$$\sum_{j=1}^{d} |\lambda_j| - \sum_{j=1}^{d} \lambda_j > 0$$

which implies

$$E_0 \geqslant c_0 h$$

for some $c_0 > 0$

- Let $\mathbf{m} \in \mathcal{U}^{(0)}$ and let $\chi \in C_c^\infty(\mathbb{R}^d)$ be equal to 1 near 0. For $r > 0$ small, let

$$\psi_{\mathbf{m},r}(x) = Z_{\mathbf{m},h}\chi(\frac{x-\mathbf{m}}{r})e^{-(f-f(\mathbf{m}))/h}$$

with $Z_{\mathbf{m},h} > 0$ such that $\|\Psi_{\mathbf{m},r}\|_{L^2} = 1$. By Laplace method, one has

$$Z_{\mathbf{m},h} = h^{-\frac{d}{4}}\frac{\det \mathrm{Hess}(f)^{\frac{1}{4}}}{\pi^{\frac{d}{4}}}.$$

- Since $\Delta_f e^{-f/h} = 0$, then

$$\Delta_f \psi_{\mathbf{m},r} = h^2 Z_{\mathbf{m},h}[\chi, \Delta]e^{-(f-f(\mathbf{m}))/h}$$

- Since $f - f(\mathbf{m}) \geqslant c > 0$ on $\mathrm{supp}([\chi, \Delta])$ then

$$\Delta_f \psi_{\mathbf{m},r} = O(e^{-c/h})$$

Exponentially small eigenvalues: log-limit

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

- On compact manifolds, [Holley-Kusuoka-Stroock 89] proved (by functional inequalities approach) that

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

  with S = highest height a particle has to jump in order to reach the absolute minimum of f

- [Mathieu 95], [Miclo 95] generalized this result to λ_j, $j \geqslant 3$ (functional inequalities)
- Breackthrough in understanding the interraction between wells by [Bovier-Eckhoff-Gayrard-Klein 04].

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

Theorem [Bovier-Gayrard-Klein 04], [Helffer-Klein-Nier 04]

Suppose (Confin), (Morse) and a non-degeneracy assumption (NonDegen) are satisfied. Then, there exists a map

$$\mathbf{j} : \mathcal{U}^{(0)} \to \mathcal{P}(\mathcal{U}^{(1)})$$

such that f is constant on $\mathbf{j}(\mathbf{m})$ and for all $\mathbf{m} \in \mathcal{U}^{(0)}$ and h small enough

$$\lambda(\mathbf{m}, h) = h\zeta(\mathbf{m}, h)e^{-2\frac{f(\mathbf{j}(\mathbf{m}))-f(\mathbf{m})}{h}}$$

where $\zeta(\underline{\mathbf{m}}, h) = 0$ and for all $\mathbf{m} \neq \underline{\mathbf{m}}$, ζ admits a classical expansion $\zeta \sim \sum_k h^k \zeta_k$ with

$$\zeta_0(\mathbf{m}) = \frac{(\det \operatorname{Hess} f(\mathbf{m}))^{\frac{1}{2}}}{2\pi}\Big(\sum_{\mathbf{s}\in\mathbf{j}(\mathbf{m})} \frac{|\mu(\mathbf{s})|}{|\det \operatorname{Hess} f(\mathbf{s})|^{\frac{1}{2}}}\Big)$$

The labelling procedure I

For any $\mathbf{s} \in \mathcal{U}^{(1)}$ and $r > 0$ small enough, the set

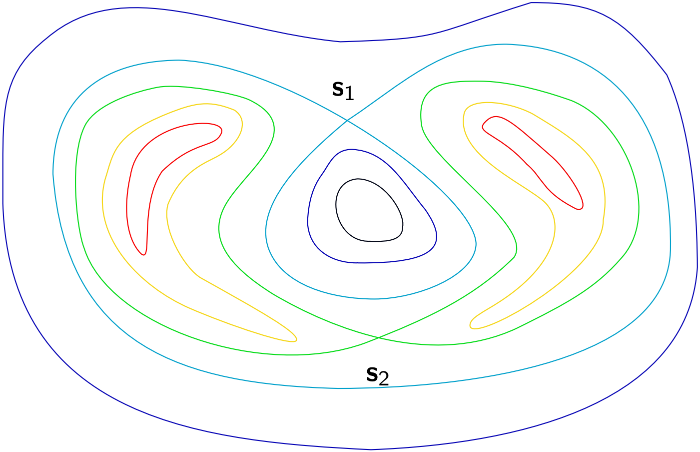
$$B(\mathbf{s}, r) \cap \{x \in \mathbb{R}^d,\ f(x) < f(\mathbf{s})\}$$

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

Definition [Hérau-Hitrik-Sjöstrand 11]

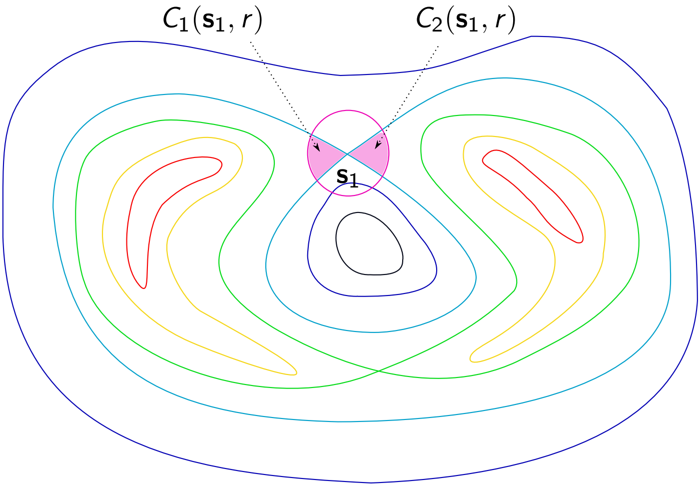
- $\mathbf{s} \in \mathcal{U}^{(1)}$ is a separating saddle point (ssp) iff $C_1(\mathbf{s}, r)$ and $C_2(\mathbf{s}, r)$ are contained in two different connected components of $\{x \in \mathbb{R}^d,\ f(x) < f(\mathbf{s})\}$. We denote by $\mathcal{V}^{(1)}$ the set of ssp.
- $\sigma \in \mathbb{R}$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

Example of SSP I

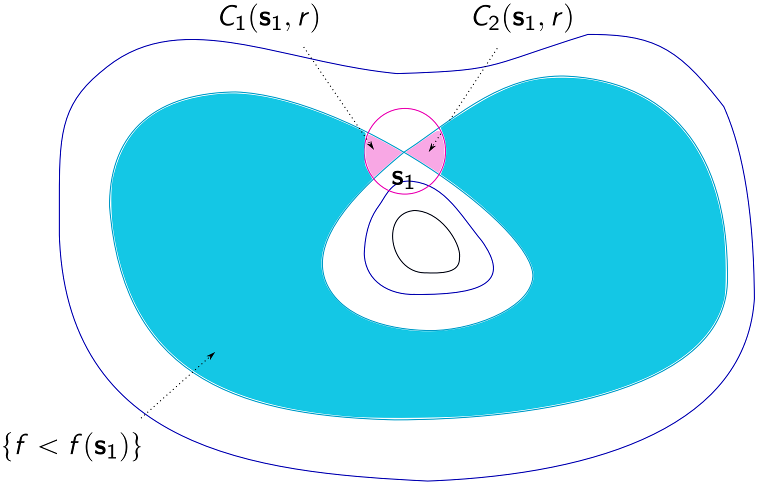


Level set of a potential with 2 minima, 2 saddle points and 1 maximum

Example of SSP II

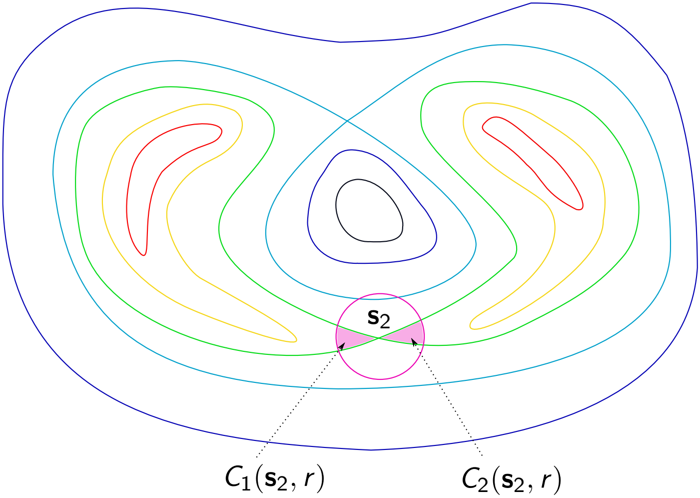


Example of SSP II

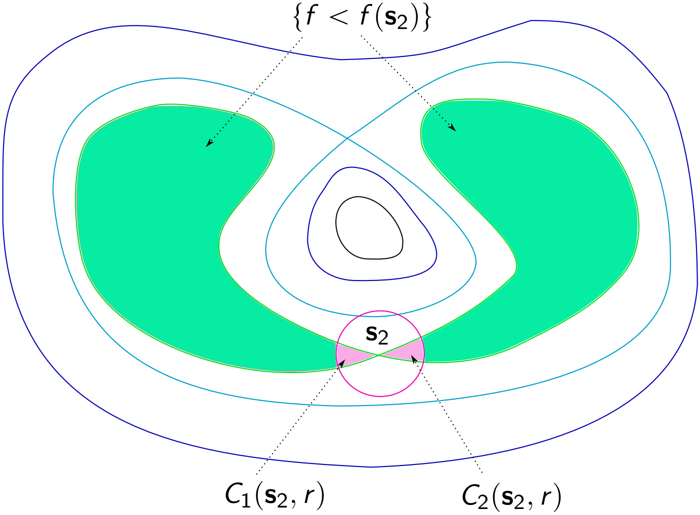


$\mathbf{s}_1$ is not separating

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 $\{f < \sigma_1\}$. In $E_{1,1}$, pick up $m_{1,1}$ one (non necessarily unique) minimum of $f_{|E_{1,1}}$.
- The set $\{f < \sigma_2\}$ 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 $f_{|E_{2,j}}$.
- The set $\{f < \sigma_k\}$ 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 $f_{|E_{k,j}}$.

The labelling procedure III

- Denote $\underline{\mathbf{m}} = \mathbf{m}_{1,1}$ the absolute minimum of f that was chosen at the first step of the labelling procedure.
- Let $\mathcal{O}(\mathbb{R}^d)$ denote the connected open subsets of $\mathbb{R}^d$. Using the preceding labelling one constructs the following applications:
  - $\boldsymbol{\sigma} : \mathcal{U}^{(0)} \to \Sigma$, defined by $\boldsymbol{\sigma}(\mathbf{m}_{i,j}) = \sigma_i$.
  - $E : \mathcal{U}^{(0)} \to \mathcal{O}(\mathbb{R}^d)$, defined by $E(\mathbf{m}_{i,j}) = E_{i,j}$. That is $E(\mathbf{m})$ is the CC of $\{f < f(\sigma(\mathbf{m}))\}$ that contains $\mathbf{m}$.
  - $$\mathbf{j} : \mathcal{U}^{(0)} \to \mathcal{P}(\mathcal{V}^{(1)})$$
    defined by $\mathbf{j}(\mathbf{m}) = \partial E(\mathbf{m}) \cap \mathcal{V}^{(1)}$.

The non degeneracy Assumption

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

Non Degeneracy Assumption (NonDegen):

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

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

ii) for any $\mathbf{m} \neq \mathbf{m}'$, $\mathbf{j}(\mathbf{m}) \cap \mathbf{j}(\mathbf{m}') = \emptyset$

Proof: Finite dimensional reduction

The general strategy:

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

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

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

- Compute the matrix of M in the base $\Pi^{(0)} \varphi_{\mathbf{m}}^{(0)}$.
- Compute the eigenvalues of M by complex analysis methods

Construction of Gaussian quasimodes

- To simplify consider the double-well case with 2 minima $\mathbf{m}_1$ and $\mathbf{m}_2$ and one saddle point $\mathbf{s} = 0$. Assume also $f(\mathbf{m}_1) < f(\mathbf{m}_2) = 0$.
- Inspired by [Bovier etal 04], [Di Gesu Le Peutrec 17], [Le Peutrec-Michel 20], we consider the quasimodes

$$\varphi_{\mathbf{m}_1} = Z_1 e^{-(f-f(\mathbf{m}_1))/h}$$

and

$$\varphi_{\mathbf{m}_2} = Z_2 \chi_2 \theta_2 e^{-(f-f(\mathbf{m}_2))/h}$$

with χ_2 and θ_2 suitable cut-off functions

Definition of θ_2

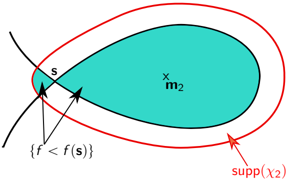
Look for $\theta = \theta_2$ under the form

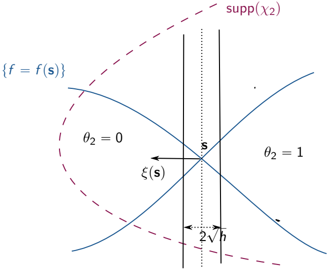
$$\theta(x,h) = 1 + \frac{1}{c_h}\int_0^{\ell(x,h)} e^{-s^2/2h} ds \qquad (2)$$

with

- ℓ smooth, $\ell(x,h) \sim \sum_{j\geqslant 0} h^j \ell_j(x)$ and $\ell_0 \neq 0$.
- Think $\ell(x,h)$ as a linear coordinate function nears $\mathbf{s}$, $\ell(x,h) \sim (x-\mathbf{s})\cdot\xi(\mathbf{s})$
- c_h normalization coeff. such that $v = -1$ for $\ell >> 1$ and $v = 1$ for $\ell << -1$

Cut-off functions





Action of the operator on the quasimodes

Lemma

One has

$$P(\theta e^{-f/h}) = (w + r)e^{-(f+\frac{\ell^2}{2})/h},$$

where

$$w = h\big(2\nabla f \cdot \nabla \ell + |\nabla \ell|^2 \ell\big) - h^2 \Delta \ell$$

the function r and all its derivatives are (locally) bounded, uniformly with respect to h, and $\operatorname{supp}(r) \subset \{|\ell| \geqslant \tau\}$.

Equations on ℓ

- We look for ℓ so that

$$w = O(h^\infty)$$

- Using the expansion $\ell(x,h) \sim \sum_{j\geqslant 0} h^j \ell_j(x)$ and identifying the powers of h, we get the
  - "Eikonal" equation on ℓ_0

$$2\nabla f \cdot \nabla \ell_0 + |\nabla \ell_0|^2 \ell_0 = 0$$

  - Transport equations on the ℓ_j, $j \geqslant 1$

$$2\nabla f \cdot \nabla \ell_j + 2\ell_0 \nabla \ell_0 \cdot \nabla \ell_j + |\nabla \ell_0|^2 \ell_j = -R_j(x, \ell_0, \ldots, \ell_{j-1}),$$

  with R_j depending only on $\ell_0, \ldots, \ell_{j-1}$.

Resolution of the "Eikonal" equation

- Let ϕ_+ be "the definite positive" solution of

$$|\nabla \phi_+|^2 = |\nabla f|^2.$$

- One can show that

$$\phi_+ - f = \frac{1}{2}\ell_0^2$$

  for some smooth function ℓ_0
- ℓ_0 solves the "Eikonal" equation.
- Let $\xi(\mathbf{s}) = \nabla \ell_0(\mathbf{s})$. Then $\xi(\mathbf{s})$ is an eigenvector of $\mathrm{Hess}(f)(\mathbf{s})$ associated to its unique negative eigenvalue $\mu(\mathbf{s})$ and $|\xi(\mathbf{s})|^2 = -\mu$.
- Observe in particular that $f + \frac{1}{2}\ell_0^2$ is positive definite.

End of the proof

Denote $S_2 = f(\mathbf{s}) - f(\mathbf{m}_2)$ and let $\zeta(h) \sim \sum_{r=0}^{\infty} h^r \zeta_r$ with $\zeta_0 \neq 0$.

Proposition

Assume (Morse) and (Confin) and that there exists $L^2(\Omega)$-normalized functions $\varphi_{2,h} \in D(P_h)$ such that:

- $\langle P_h \varphi_{2,h}, \varphi_{2,h} \rangle_{L^2} = \zeta(h) e^{-2S_2/h}$,
- $\| P_h \varphi_{2,h} \|_{L^2}^2 = O(h^\infty) \langle P_h \varphi_{2,h}, \varphi_{2,h} \rangle_{L^2}$,

then

$$\lambda(\mathbf{m}_2, h) = h\zeta(h) e^{-2S_2/h}$$

Remarks

- The original semiclassical proof by Helffer-Klein-Nier uses supersymmetry properties of the Witten Laplacian. This requires
  - introduce the Witten Laplacian $\Delta_f^{(1)}$ on 1-forms
  - use Helffer-Sjostrand's BKW constructions for $\Delta_f^{(1)}$
- The gaussian quasimodes construction is more robust and can be generalized to
  - Non-reversible settings [Le Peutrec-Michel 20], [Bony-Le Peutrec-Michel 22]
  - pseudodifferential settings [Normand 23]

Extensions

- General Morse functions [Michel 19]
- Small eigenvalues of Witten Laplacian on p-forms [Le Peutrec-Nier-Viterbo 2013]
- More general critical sets
  - Arhenius law for general functions [Le Peutrec-Nier-Viterbo, to appear]
  - submanifold critical sets [Assal-Bony-Michel 23]
- Problems with boundary
  - Dirichlet BC [Helffer-Nier 2006]
  - Neumann BC [Le Peutrec 2010]
  - First exit point from a domain [Di Gesu-Le Peutrec-Lelièvre-Nectoux 2010's]

Bibliography

- H. Cycon, R. Froese, W. Kirch, B. Simon, Schrödinger operators with application to quantum mechanics and global geometry, 1987
- B. Helffer and J. Sjöstrand, Puits multiples en mécanique semi-classique IV, 1985
- B. Helffer, M. Klein and F. Nier, Quantitative analysis of metastability via Witten complex approach, 2004
- F. Hérau, M. Hitrik and J. Sjöstrand, Tunnel effect for Kramers-Fokker-Planck type operators, 2008
- D. Le Peutrec and L. Michel, Sharp asymptotics for non-reversible metastable diffusion processes, 2020

General framework

We consider a semiclassical second order differential operator

$$P = -h \operatorname{div} \circ A \circ h\nabla + \frac{1}{2}(b \cdot h\nabla + h \operatorname{div} \circ b) + c$$

where the symmetric matrix $A = (a_{ij})$, the vector field $b = (b_k)$ and the function c depend smoothly on $x \in \mathbb{R}^d$. Throughout, we assume

$$\begin{aligned} &\forall |\alpha| \geqslant 0, \quad \partial_x^\alpha a_{i,j}(x,h) = \mathcal{O}(1), \\ &\forall |\alpha| \geqslant 1, \quad \partial_x^\alpha b_j(x,h) = \mathcal{O}(1), \\ &\forall |\alpha| \geqslant 2, \quad \partial_x^\alpha c(x,h) = \mathcal{O}(1). \end{aligned}$$

General framework

We assume that for any $e \in \{a_{ij}, b_j, c\}$, one has the classical expansion

$$\forall \alpha \in \mathbb{N}^d,\ \forall K \geqslant 0,\ \partial_x^\alpha (e - \sum_{k=0}^{K} h^k e^k) = O(h^{K+1})$$

We also assume that

$$c^0(x) \geqslant 0\,, \quad \text{and} \quad A(x,h) = (a_{i,j}(x,h))_{i,j} \text{ is positive semidefinite.}$$

Theorem [Hérau-Hitrik-Sjöstrand 2008]

Under the above assumption the operator P initially defined on $\mathscr{S}(\mathbb{R}^d)$ admits a unique maximal accretive extension.

Some examples

- Witten Laplacian: Take $A = \mathrm{Id}$, $b = 0$ and $c(x) = |\nabla f(x)|^2 - h\Delta f(x)$, then
$$P = -h^2\Delta + |\nabla f|^2 - h\Delta f := \Delta_f$$
- Non reversible diffusion: take $A = \mathrm{Id}$, $c(x) = |\nabla f(x)|^2 - h\Delta f(x)$ and $b(x) \perp \nabla f(x)$ on $\mathbb{R}^d$, then
$$P = \Delta_f + b \cdot h\partial_x$$
- Generalized Kramers-Fokker-Planck operators: take $A = \begin{pmatrix} 0 & 0 \\ 0 & \mathrm{Id} \end{pmatrix}$, $b(x, v) = \begin{pmatrix} \partial_v W(v) \\ -\partial_x V(x) \end{pmatrix}$ $c(x, v) = |\partial_v W(v)|^2 - h\Delta_v W(v)$. Then
$$P = \partial_v W \cdot h\partial_x - \partial_x V \cdot h\partial_v + \Delta_W$$
where Δ_W = Witten Laplacian in variable v associated to $W(v)$.

Resolvent estimate in non selfadjoint setting

- For selfadjoint operators one has

$$\|(A - z)^{-1}\| = \frac{1}{\mathrm{dist}(z, \sigma(A))}$$

- For non selfadjoint operators, the above estimate fails to be true:

$$A = \begin{pmatrix} 0 & 1 \\ 0 & 0 \end{pmatrix} \Longrightarrow (A + z)^{-1} = \begin{pmatrix} 1/z & -1/z^2 \\ 0 & 1/z \end{pmatrix}$$

- link between spectrum and resolvent estimate leads to the notion of pseudospectrum
- intensive area of research in the early 2000's, see references in
  - B. Davies, Linear operators and their spectra, 2007
  - J. Sjöstrand, Non selfadjoint differential operators, 2019

Elliptic models

Consider the non reversible elliptic model

$$P = \Delta_f + \nu \cdot h\nabla$$

with vector field ν such that for all $x \in \mathbb{R}^d$,

$$|\nu(x)| \leqslant C(1 + |\nabla f(x)|)$$

and

$$\nu(x) \cdot \nabla f(x) = 0 \quad \text{and} \quad \operatorname{div}(\nu) = 0$$

This model was studied by Bouchet-Reygner 2016, Landim-Mariani-Seo 2019 (hitting time), Landim-Seo 2019 (1D periodic result without the decomposition of b)

Theorem [Le Peutrec-Michel, 2020]

The following hold true:

- There exists $C, \Lambda_0 > 0$ such that $\sigma(P) \subset \Gamma_{\Lambda_0}$ where

$$\Gamma_{\Lambda_0} = \{z \in \mathbb{C},\ \operatorname{Re}(z) \geqslant 0, |\operatorname{Im} z| \leqslant \Lambda_0(\operatorname{Re}(z) + \sqrt{\operatorname{Re}(z)}\}$$

- One has

$$\|(P-z)^{-1}\|_{L^2 \to L^2} \leqslant \frac{C}{\operatorname{Re}(z)}$$

  for all $z \in \Gamma_{\Lambda_0}^c \cap \{\operatorname{Re}(z) \geqslant 0\}$.

- There exists $c_1 > 0$ and $h_0 > 0$ such that for all $0 < h < h_0$ the map $z \mapsto (P-z)^{-1}$ is meromorphic in $\{\operatorname{Re}(z) < c_1\}$ with finite rank residues.

First spectral localization

Assume f is a Morse function with n_0 minima.

Theorem [Le Peutrec-Michel, 2020]

There exists $\epsilon_0 > 0$ and $h_0 > 0$ such that for all $h \in]0, h_0]$, $\sigma(P) \cap \{\mathrm{Re}(z) \leqslant \epsilon_0 h\}$ is finite and

$$\sharp\sigma(P) \cap \{\mathrm{Re}(z) \leqslant \epsilon_0 h\} = n_0$$

Moreover , one has

$$\sigma(P) \cap \{\mathrm{Re}(z) \leqslant \epsilon_0 h\} \subset B(0, C' e^{-C/h})$$

for some $C, C' > 0$. Eventually, for any $0 < \epsilon < \epsilon_0$, one has

$$(P - z)^{-1} = \mathcal{O}(h^{-1})$$

uniformly with respect to z such that $|z| \geqslant \epsilon h$ and $\mathrm{Re}(z) < \epsilon_0 h$.

One idea of Proof

- Observe

$$\mathrm{Re}\langle Pu, u\rangle = \langle \Delta_f u, u\rangle = \|\nabla_f u\|^2 \geqslant 0$$

and

$$|\,\mathrm{Im}\langle Pu, u\rangle| \leqslant C(\|\nabla_f u\|^2 + \|u\|\|\nabla_f u\|)$$

Then write

$$2|\langle (P-z)u, u\rangle| \geqslant |\,\mathrm{Re}\langle (P-z)u, u\rangle| + |\,\mathrm{Im}\langle (P-z)u, u\rangle| \\ \geqslant \|\nabla_f u\|^2 - \mathrm{Re}(z)\|u\|^2 + |\,\mathrm{Im}(z)|\|u\|^2 - |\,\mathrm{Im}\langle Pu, u\rangle|$$

- Localization of small eigenvalues is proved by using a Grushin problem associated to the eigenvectors of small eigenvalues of the Witten laplacian $e_1, \dots, e_{n_0}$ and observing that
  - $\Delta_f \geqslant Ch$ on $\{e_1, \dots, e_{n_0}\}^\perp$
  - $\nu \cdot h\partial_x e_j = \nu \cdot (h\partial_x + \nabla_x f)e_j = O(e^{-c/h})$

The semiclassical hypocoercivity approach for KFP

Let

$$P = vh\partial_x - \partial_x V h\partial_v - h^2\Delta_v + |v|^2 - hd$$

acting on $L^2(\mathbb{R}^{2d})$. Throughout we denote

$$X = vh\partial_x - \partial_x V h\partial_v \text{ and } N = -h^2\Delta_v + |v|^2 - hd.$$

Proposition

The operator P initially defined on $C_c^\infty(\mathbb{R}^{2d})$ admits a unique maximal accretive extension that we still denote by $(P, D(P))$.

Assumption (Confin)

There exist $C > 0$ and a compact set $K \subset \mathbb{R}^d$ such that

$$V \geqslant -C, \quad |\nabla V(x)| \geqslant \frac{1}{C} \quad \text{and} \quad |\operatorname{Hess} V(x)| \leqslant C|\nabla V(x)|^2 .$$

for all $x \in \mathbb{R}^d \backslash K$.

We denote

$$f(x, v) = \frac{|v|^2}{2} + V(x)$$

and $\mu(x, v) = e^{-f/h}$.

Lemma

Suppose that Assumption (Confin) holds true. One has $\mu \in D(P)$ and

$$X(\mu) = Y(\mu) = N(\mu) = 0$$

Assumption (Morse)

The function V is a Morse function.

Under this assumption, the Witten laplacian Δ_V in the x variable acting on $L^2(\mathbb{R}^d)$ admits $n_0 = \sharp\mathcal{U}^{(0)}$ exponentially small eigenvalues. Denote by $(\lambda(\mathbf{m}), \phi_{\mathbf{m}})_{\mathbf{m}\in\mathcal{U}^{(0)}}$ the associated eigenpairs. One has

- $\|\delta_x\phi_{\mathbf{m}}\| = O(e^{-c/h})$ where $\delta_x = h\nabla_x + \nabla_x V$
- for all $u \in \text{span}\{\phi_{\mathbf{m}}, \mathbf{m} \in \mathcal{U}^{(0)}\}^\perp$, $\langle \Delta_V u, u\rangle \geqslant Ch\|u\|^2$

For any $\mathbf{m}$, define $g_{\mathbf{m}}(x, v) = \phi_{\mathbf{m}}(x)e^{-\frac{|v|^2}{2h}}$. The g_m are orthogonal and hence the vector space

$$G_h = \text{span}\{g_{\mathbf{m}},\ \mathbf{m} \in \mathcal{U}^{(0)}\}$$

has dimension n_0. Throughout, for $t \in \mathbb{R}$, we denote

$$\Sigma_t = \{z \in \mathbb{C},\ \text{Re}(z) < t\}.$$

Resolvent estimate on a finite codimension space

Theorem

Suppose that Assumptions (Confin) and (Morse) are satisfied. There exists $h_0 > 0$, $\epsilon_0 > 0$ and $c_1 > 0$ such that for all $h \in]0, h_0]$, and all $u \in D(P) \cap G_h^\perp$, one has

$$\|(P - z)u\|_{L^2} \geqslant c_1 h \|u\|_{L^2}$$

uniformly with respect to $z \in \Sigma_{\epsilon_0 h}$.

- Hérau, 2006 (Boltzmann)
- Dolbeault-Mouhot-Schmeiser 2009, Villani 2009 (general setting)
- Robbe 2016 (semiclassical Boltzmann)
- Guillin-Nectoux 2020 (semiclassical PDMP)

Proof of hypocoercive estimates

We introduce the function $\rho(v) = \left(\frac{\pi}{h}\right)^{\frac{d}{4}} e^{-\frac{|v|^2}{2h}}$ and the projector defined on $L^2(\mathbb{R}^{2d})$ by

$$\Pi_\rho u(x,v) = \int_{\mathbb{R}^d} u(x,v)\rho(w)dw\rho(v).$$

We define an auxiliary operator

$$A = \left(h + (\alpha h)^{-1}(X\Pi_\rho)^*(X\Pi_\rho)\right)^{-1}(X\Pi_\rho)^*$$

where $\alpha = \int_{\mathbb{R}^d} |v|^2 e^{-|v|^2} dv$.

Lemma

The operator A is bounded on $L^2(\mathbb{R}^{2d})$, it satisfies $A = \Pi_\rho A$ and one has the estimate

$$\|A\|_{L^2\to L^2} \leqslant \frac{\sqrt{\alpha}}{2}$$

Proposition

There exists $c_0, \delta_0, h_0 > 0$ such that for all $h \in]0, h_0]$ and for all $u \in D(P) \cap G_h^{\perp}$, one has

$$\mathrm{Re}\,\left\langle Pu, (1+\delta_0(A+A^*))u\right\rangle_{L^2} \geqslant c_0 h\|u\|_{L^2}^2$$

Application to the proof of the theorem. For $\epsilon_0 = \frac{c_0}{2+\delta_0\sqrt{\alpha}}$ and $\mathrm{Re}\, z < \epsilon_0 h$ we have

$$\mathrm{Re}\langle (P-z)u, (1+\delta_0(A+A^*)u\rangle \geqslant \frac{c_0}{2} h\|u\|^2.$$

Using Cauchy-Schwartz and the boundedness of A, it follows that

$$\|(P-z)u\| \geqslant c_1 h\|u\|$$

for some $c_1 > 0$.

Proof of the Proposition

Recall $\Delta_V = -h^2\Delta + |\nabla V|^2 - h\Delta V = \delta_x^*\delta_x$, $\delta_x = h\nabla_x + \nabla_x V$.

Lemma

One has

$$(X\Pi_\rho)^*(X\Pi_\rho) = h\alpha_d \Delta_V \circ \Pi_\rho$$

where $\alpha_d = \int_{\mathbb{R}^d} |v|^2 e^{-|v|^2} dv = \frac{d}{2}\pi^{\frac{d}{2}}$. As a consequence, one has

$$A = (h + \Delta_V)^{-1}(X\Pi_\rho)^*$$

Proof. Write $\Pi_\rho f(x,v) = f_\rho(x) e^{-v^2/(2h)}$ and observe

$$(vh\partial_x - \partial_x V h\partial_v)(f_\rho(x)e^{-v^2/(2h)}) = v \cdot \delta_x f_\rho(x) e^{-v^2/(2h)}$$

and

$$\langle (X\Pi_\rho)^*(X\Pi_\rho)f, g\rangle_{L^2(\mathbb{R}^{2d}_{x,v})} = \int_{\mathbb{R}^d} \langle \delta_x f_\rho, \delta_x g_\rho\rangle_{L^2(\mathbb{R}^d_x)} |v|^2 e^{-\frac{|v|^2}{h}} dv$$

For all $\delta > 0$, let us define

$$I_\delta = \mathrm{Re}\left\langle Pu, (1 + \delta(A + A^*)u\right\rangle_{L^2}$$

Using the decomposition $P = X + N$, and the skew-adjointness of X, one gets

$$I_\delta = \langle Nu, u\rangle + \delta\langle Pu, (A + A^*)u\rangle$$

Since $N \geqslant h(1 - \Pi_\rho)$, it follows that

$$\begin{aligned} I_\delta &\geqslant h\|(1 - \Pi_\rho)u\|^2 + \delta\langle Pu, (A + A^*)u\rangle. \\ &\geqslant h\|(1 - \Pi_\rho)u\|^2 + \delta(\langle AXu, u\rangle + \langle ANu, u\rangle \\ &\qquad + \langle Xu, Au\rangle + \langle Nu, Au\rangle) \end{aligned}$$

and since $A = \Pi_\rho A$ and $\Pi_\rho N = 0$ it follows that

$$I_\delta \geqslant h\|(1 - \Pi_\rho)u\|^2 + \delta\langle AX\Pi_\rho u, \Pi_\rho u\rangle + \delta J$$

with

$$J = \langle AX(1 - \Pi_\rho)u, u\rangle + \langle ANu, u\rangle + \langle Xu, Au\rangle.$$

$$I_\delta \geqslant h\|(1-\Pi_\rho)u\|^2 + \delta\langle AX\Pi_\rho u, \Pi_\rho u\rangle + \delta J$$

Recall

$$AX\Pi_\rho = (h+\Delta_V)^{-1}\Pi_\rho(X\Pi_\rho)^* X\Pi_\rho = h\alpha(h+\Delta_V)^{-1}\Delta_V\,\Pi_\rho$$

Lemma

There exists $c_0, h_0 > 0$ such that for all $h \in]0, h_0]$ and $u \in G_h^\perp$, one has

$$\langle AX \circ \Pi_\rho u, u\rangle \geqslant c_0 h\|\Pi_\rho u\|^2$$

Proof.

- Observe that $u \in G_h^\perp \Longrightarrow \Pi_\rho u \in \mathrm{span}\{\phi_{\mathbf{m}},\ \mathbf{m} \in \mathcal{U}^{(0)}\}^\perp$.
- Hence, on $G_h^\perp$, $\Delta_V \Pi_\rho \geqslant ch$ and by functionnal calculus

$$(h+\Delta_V)^{-1}\Delta_V\,\Pi_\rho \geqslant \frac{c}{1+c}\Pi_\rho$$

- We deduce

$$I_\delta \geqslant h\|(1-\Pi_\rho)u\|^2 + \delta c_0 h\|\Pi_\rho u\|^2 + \delta J$$

- We want to estimate the error term $J = \langle AX(1-\Pi_\rho)u, u\rangle + \langle ANu, u\rangle + \langle Xu, Au\rangle$

Lemma

There exists $C, h_0 > 0$ such that for all $h \in]0, h_0]$ and for all $u \in G_h^\perp$, one has

$$|\langle AX(1-\Pi_\rho)u, u\rangle| \leqslant Ch\|\Pi_\rho u\| \, \|(1-\Pi_\rho)u\|$$

$$|\langle ANu, u\rangle| \leqslant Ch\|\Pi_\rho u\| \, \|(1-\Pi_\rho)u\|$$

$$|\langle Xu, Au\rangle| \leqslant Ch\|(1-\Pi_\rho)u\|^2$$

End of the proof

It follows that

$$
\begin{aligned}
I_\delta &\geqslant h(1 - C\delta)\|(1-\Pi_\rho)u\|^2 + c_0\delta h\|\Pi_\rho u\|^2 \\
&\qquad\qquad\qquad - C\delta h\|\Pi_\rho u\| \, \|(1-\Pi_\rho)u\| \\
&\geqslant h(1 - C\delta - C\delta R)\|(1-\Pi_\rho)u\|^2 + \delta h(C - \frac{C}{R})\|\Pi_\rho u\|^2 \\
&\geqslant Ch\|u\|^2
\end{aligned}
$$

by taking R large first and then $\delta > 0$ small and then $h > 0$ small.

Resolvent estimate away from the small "spectrum"

Theorem

Suppose that Assumptions (Confin) and (Morse) are satisfied. There exists $h_0 > 0$, $\epsilon_0 > 0$ and $c > 0$ such that for all $h \in]0, h_0]$, $\sharp\sigma(P) \cap \Sigma_{\epsilon_0 h} = n_0$ counted with multiplicity. Moreover, there exists $C > 0$ such that

$$\sigma(P) \cap \Sigma_{\epsilon_0 h} \subset \{|z| \leqslant e^{-C/h})\}$$

and for all $0 < \epsilon_1 < \epsilon_0$, and all $h \in]0, h_0]$, one has

$$\|(P - z)^{-1}\|_{L^2 \to L^2} = O(h^{-1})$$

uniformly with respect to $z \in \Sigma_{\epsilon_0 h} \backslash B(0, \epsilon_1 h)$.

- Let $\mathbb{P}$ denote the orthogonal projection on G_h and let $z \in \Sigma_{\epsilon_0 h} \backslash B(0, \epsilon_1 h)$.
- For all $u \in D(P)$, one has $P\mathbb{P}u = O(e^{-c/h}\|u\|)$ and $P^*\mathbb{P}u = O(e^{-c/h}\|u\|)$ which implies

$$\begin{aligned}\|(P-z)u\|^2 &= \|(P-z)\mathbb{P}u\|^2 + \|(P-z)(1-\mathbb{P})u\|^2 \\ &\qquad + 2\,\mathrm{Re}\langle (P-z)(1-\mathbb{P})u, (P-z)\mathbb{P}u\rangle \\ &\geqslant |z|^2\|\mathbb{P}u\|^2 + (\epsilon_0-\epsilon_1)^2h^2\|(1-\mathbb{P})u\|^2 + O(e^{-c/h})\|u\|^2 \\ &\geqslant ch^2\|u\|^2\end{aligned}$$

  for $h > 0$ small enough.
- One has the same estimate for $(P^* - z)$.
- This shows:
  - $\sigma(P) \cap \{\mathrm{Re}(z) < \epsilon_0 h\} \subset \{|z| < \epsilon_1 h\}$
  - the resolvent estimate

Consider the Riesz projector

$$\Pi_0 = \frac{1}{2i\pi}\int_{|z|=\epsilon_1 h}(z-P)^{-1}dz.$$

Let us prove that $d_0 := \dim \operatorname{Ran} \Pi_0 = n_0$.

- First $d_0 \leqslant n_0$ since $\|P\Pi_0\| \leqslant C\epsilon_1 h$ and $P \geqslant \epsilon_0 h$ on $G_h^\perp$ and $\dim G_h = n_0$.
- Conversely, for $\mathbf{m} \in \mathcal{U}^{(0)}$, denote $\tilde{g}_{\mathbf{m}} = \Pi_0 g_{\mathbf{m}}$. One has

$$\begin{aligned}\tilde{g}_{\mathbf{m}} - g_{\mathbf{m}} &= \frac{1}{2i\pi}\int_{|z|=\epsilon_1 h}((z-P)^{-1} - z^{-1})g_m dz \\ &= -\frac{1}{2i\pi}\int_{|z|=\epsilon_1 h} z^{-1}(z-P)^{-1}Pg_m dz = O(e^{-C/h})\end{aligned}$$

thanks to the resolvent estimate.

- Since $(g_{\mathbf{m}})$ is orthonormal then $(\tilde{g}_{\mathbf{m}})$ quasi-orthonormal family of $\operatorname{Ran}\Pi_0$.
- Using Gram-Schmidt procedure it can be orthonormalized in a family $\bar{g}_{\mathbf{m}}$ such that $g_{\mathbf{m}} - \bar{g}_{\mathbf{m}} = O(e^{-c/h})$.
- This proves that $d_0 \geqslant n_0$. Moreover for any $u \in \operatorname{Ran}\Pi_0$, one has $u = \sum_{\mathbf{m}} \langle u, \bar{g}_{\mathbf{m}} \rangle \bar{g}_{\mathbf{m}}$, hence

$$Pu = \sum_{\mathbf{m}} \langle u, \bar{g}_{\mathbf{m}} \rangle P \bar{g}_{\mathbf{m}} = O(e^{-c/h}).$$

Hence $P_{| \operatorname{Ran}\Pi_0} = O(e^{-c/h})$

Remarks on the method

- Robust method that can be generalized to many situations
  - Boltzmann equations [Robbe 16], [Normand 23]
  - PDMP [Guillin-Nectoux 20]
  - degenerate KFP [Delande, 23]
- requires a Gibbs state and separation of variables

Hérau-Hitrik-Sjöstrand theory: Assumptions

Let $p(x,\xi,h)$ denote the semiclassical Weyl symbol of P.

- One has $p = p^0 + O(h)$, where $p^0 = p_2^0 + ip_1^0 + p_0^0$ with

$$p_2^0(x,\xi) = \xi \cdot A^0(x)\xi,\ p_1^0(x,\xi) = b^0(x)\cdot\xi,\ p_0^0(x) = c^0(x)$$

- We define the symbol $\widetilde{p}(x,\xi) = p_0^0(x) + \frac{p_2^0(x,\xi)}{\langle\xi\rangle^2}$ and given $T > 0$

$$\langle\widetilde{p}\rangle_T = \frac{1}{2T}\int_{-T}^{T} \widetilde{p} \circ e^{tH_{p_1^0}}\,dt.$$

- Introduce the critical set

$$\mathcal{C} = \{(x,0) \in T^*\mathbb{R}^d;\ b^0(x) = 0 \text{ and } c^0(x) = 0\}.$$

Hérau-Hitrik-Sjöstrand theory: Assumptions

Denote $\rho = (x, \xi)$. We assume that $\mathcal{C} = \{\rho_1, \dots, \rho_N\}$ is finite and

- for any neighborhood U of $\pi_x \mathcal{C}$, there exists $C > 0$ such that

$$\text{meas}\left\{t \in [-T, T];\ c^0\left(e^{tb^0\cdot\nabla}(x)\right) \geqslant \frac{1}{C}\right\} \geqslant \frac{1}{C}. \qquad \text{(Ell)}$$

- for some fixed $T > 0$ there exists some constant $C > 0$ such that that

$$\text{for } \rho \text{ near any } \rho_j, \text{ we have } \langle \widetilde{p} \rangle_T(\rho) \geqslant \frac{1}{C}|\rho - \rho_j|^2 \qquad \text{(Harmo)}$$

Hérau-Hitrik-Sjöstrand theory: results

Theorem (Hérau-Hitrik-Sjöstrand 2008)

Assume (Ell) and (Harmo) hold true. For any $B > 0$, there exists $C > 0$ such that for h small enough,

- the operator P has no spectrum in
$$\{z \in \mathbb{C};\ \operatorname{Re} z < Bh \text{ and } |\operatorname{Im} z| > Ch\},$$
- the spectrum of P in $D(0, Bh)$ is discrete and
$$\|(P - z)^{-1}\| \leqslant \frac{C}{h},$$
uniformly on $\{z \in \mathbb{C},\ \operatorname{Re} z < Bh,\ dist(z, \sigma(P)) \geqslant h/B\}$.

Hérau-Hitrik-Sjöstrand theory: results

Theorem (Hérau-Hitrik-Sjöstrand 2008)

The spectrum of P in $D(0, Bh)$ is made eigenvalues of the form

$$\mu_{\rho,k}(h) = h(\mu^0_{\rho,k} + \mathcal{O}(h^\alpha)),$$

where $\alpha > 0$ and

$$\mu^0_{\rho,k} = \frac{1}{i}\sum_{\ell=1}^{d} \nu_{\rho,k,\ell}\lambda_{\rho,\ell} + \frac{1}{2}\widetilde{tr}(p,\rho),$$

with $\nu_{\rho,k,\ell} \in \mathbb{N}$ and $\lambda_{\rho,\ell}$, $\widetilde{tr}(p,\rho)$ constants depending on the quadratic approximation of P.

Our assumptions

We assume that

- there exists $f : \mathbb{R}^d \to \mathbb{R}$ such that $e^{-f/h}$ belongs to $L^2(\mathbb{R}^d)$ and

$$P(e^{-f/h}) = 0 \qquad \text{and} \qquad P^\dagger(e^{-f/h}) = 0, \qquad \text{(Gibbs)}$$

  where $P^\dagger$ denotes the formal adjoint of P.

- $$f \text{ is a Morse fct with finite numb. of crit. pts.} \qquad \text{(Morse)}$$

  From now, we denote $\mathcal{U}$ the set of critical points of f, $\mathcal{U}^{(j)}$ the critical points of index j.

As an immediate consequence, we have the indentities

$$b^0(x) \cdot \nabla f(x) = 0 \quad \text{and} \quad c^0(x) = A^0(x) \nabla f(x) \cdot \nabla f(x)$$

Remark on the hypo-elliptic assumption

Lemma (Kalman criterion)

Let us assume (Gibbs) and (Morse). Then, the condition (Harmo) is satisfied if and only if, for every $\mathbf{u} \in \mathcal{U}$,

$$\bigcap_{n=0}^{d-1} \ker\left(A^0 (B^t)^n\right) = \{0\}.$$

where $A^0 = A^0(\mathbf{u})$ and $B = db^0(\mathbf{u})$.

Lemma

Suppose that assumptions (Harmo), (Gibbs) and (Morse) hold true. Then $\mathcal{C} = \mathcal{U} \times \{0\}$.

Proof. Recall $\mathcal{C} = \{(x,0) \in T^*\mathbb{R}^d;\ b^0(x) = 0 \text{ and } c^0(x) = 0\}$.

- Let $\mathbf{u} \in \mathcal{U}$, then $c^0(\mathbf{u}) = 0$ and $\nabla f(x) = H(x - \mathbf{u}) + O((x - \mathbf{u})^2)$ with H invertible. Hence

$$b^0(x) \cdot H(x - \mathbf{u}) = O((x - \mathbf{u})^2))$$

  which proves $b^0(\mathbf{u}) = 0$ and $\mathcal{U} \times \{0\} \subset \mathcal{C}$.

- Conversely, assume $(\mathbf{u}, 0) \in \mathcal{C}$ and denote $\eta = \nabla f(\mathbf{u})$. Then

$$0 = c^0(\mathbf{u}) = A^0(\mathbf{u})\eta \cdot \eta$$

  Hence $\eta \in \ker(A^0)$. Moreover, one can prove $\eta \in \ker B^t$. Hence $\eta = 0$.

Rough Asymptotics

Proposition

Assume the above assumptions. There exist $\varepsilon_* > 0$ and $h_0 > 0$ such that for $h \in]0, h_0]$, P has exactly $n_0 = \sharp\mathcal{U}^{(0)}$ eigenvalues in $\{\mathrm{Re}(z) < \varepsilon_* h\}$ and these eigenvalues are $\mathcal{O}(h^{1+\alpha})$ with $\alpha > 0$.

Notation

- We denote $\lambda(\mathbf{m}, h)$, $\mathbf{m} \in \mathcal{U}^{(0)}$ these small eigenvalues.
- We chose $\underline{\mathbf{m}}$ and absolute minimum of f.

A geometrical Lemma

Notations

$B(\mathbf{u}) = db^0(\mathbf{u})$
$H(\mathbf{u}) = \mathrm{Hess}(f)(\mathbf{u})$

Lemma

Let $k \in \{0, \dots, d\}$. Let $\mathbf{u} \in \mathcal{U}^{(k)}$ be a critical point of index k. Then, $i)$ the matrix

$$\Lambda(\mathbf{u}) := 2H(\mathbf{u})A^0(\mathbf{u}) + B^t(\mathbf{u})$$

admits exactly k eigenvalues in $\mathbb{C}_-$ and $d - k$ eigenvalues in $\mathbb{C}_+$.
$ii)$ if $k = 1$, then the unique eigenvalue $\mu(\mathbf{u})$ in $\mathbb{C}_-$ is real (and thus $\mu(\mathbf{u}) < 0$).

Similar Lemma was proved by [Landim-Mariani-Seo 2019] and [Le Peutrec-Michel 2020] for elliptic operators.

Proof of the geometric Lemma

- Linearizing the equation $b^0(x) \cdot \nabla f(x) = 0$, we get $B^t H = \tilde{J}$ with $\tilde{J}$ antisymetric, hence $B^t = HJ$ with J antisymetric, and we get
$$\Lambda := H(2A^0 + J).$$
- Consider the matrix $\Lambda_r = r\Lambda + (1-r)H$
- Show that Λ_r has no eigenvalue on $\mathrm{Re}(z) = 0$. Indeed, if $\Lambda_r u = zv$ with $\mathrm{Re}(z) = 0$, then
$$0 = \mathrm{Re}\langle \Lambda_r v, H^{-1} v\rangle = 2r\langle A^0 v, v\rangle + (1-r)\|v\|^2$$
- Use continuity argument with respect to $r \in [0, 1]$.

Sharp asymptotics of small spectral values

Theorem [Bony-Le Peutrec-Michel]

Suppose that the above assumptions hold true. Under a non degeneracy assumption on the minima of f, there exists a map $\mathbf{j} : \mathcal{U}^{(0)} \to \mathcal{P}(\mathcal{U}^{(1)})$ such that f is constant on $\mathbf{j}(\mathbf{m})$ and for all $\mathbf{m} \in \mathcal{U}^{(0)}$ and h small enough

$$\lambda(\mathbf{m}, h) = h\zeta(\mathbf{m}, h)e^{-2\frac{f(\mathbf{j}(\mathbf{m}))-f(\mathbf{m})}{h}}$$

where $\zeta(\underline{\mathbf{m}}, h) = 0$ and for all $\mathbf{m} \neq \underline{\mathbf{m}}$, ζ admits a classical expansion $\zeta \sim \sum_k h^k \zeta_k$ with

$$\zeta_0(\mathbf{m}) = \frac{(\det \mathrm{Hess}\, f(\mathbf{m}))^{\frac{1}{2}}}{2\pi}\Big(\sum_{\mathbf{s}\in\mathbf{j}(\mathbf{m})} \frac{|\mu(\mathbf{s})|}{|\det \mathrm{Hess}\, f(\mathbf{s})|^{\frac{1}{2}}}\Big)$$

Remarks

- This theorem recovers previous results
  - Elliptic reversible case: Bovier-Gayrard-Klein 04, Helffer-Klein-Nier 04
  - Elliptic Non reversible case: Le Peutrec-Michel 20
  - Fokker-Planck type operators with symmetries (supersymmetry and PT-symmetry) Hérau-Hitrik-Sjöstrand 08-11 (operators of the form

$$P = d_f^* \circ G \circ d_f$$

    with d_f twisted derivative and G invertible matrix.)
- there exists operators satisfying our assumptions which are not supersymmetric
- We can get rid of the Non-Degeneracy assumption a deal with all Morse functions
- this theorem gives all the small eigenvalues, that is the whole metastable time scales

Strategy of proof

Let

$$\Pi_h = \frac{1}{2i\pi} \int_{|z|=\epsilon h} (P - z)^{-1} dz$$

and $E_h = \operatorname{Ran} \Pi_h$. Then $\dim E_h = n_0$ and $P : E_h \to E_h$.

Goal

Compute the spectrum of the restriction of P to E_h. This is a problem in finite dimension.

The general strategy is the following:

1) Construct suitable approximated eigenfunctions $\varphi_{\mathbf{m}}$, $\mathbf{m} \in \mathcal{U}^{(0)}$ of the operator P
2) Project these eigenfunctions on E_h, $e_{\mathbf{m}} = \Pi_h \varphi_{\mathbf{m}}$ and estimate the difference $e_{\mathbf{m}} - \varphi_{\mathbf{m}}$.
3) Compute the matrix M of P in the base $(e_{\mathbf{m}}, \mathbf{m} \in \mathcal{U}^{(0)})$
4) Compute the spectrum of M

Details on steps 2,3,4

- Step 2 uses the resolvent estimate via the formula

$$e_{\mathbf{m}} - \varphi_{\mathbf{m}} = \Pi_h \varphi_m - \varphi_m = \frac{1}{2i\pi} \int_{|z|=\epsilon h} ((P-z)^{-1} - z^{-1}) \varphi_{\mathbf{m}} dz$$
$$= \frac{-1}{2i\pi} \int_{|z|=\epsilon h} (P-z)^{-1} z^{-1} P \varphi_{\mathbf{m}} dz = O(h^{-1} \| P \varphi_{\mathbf{m}} \|)$$

- Step 3 consists in application of Laplace's method
- Step 4 consists in computing the spectrum of a non self-adjoint matrix. We replace maxi-min principle by Schur complement method

Gaussian cut-off

Given $\mathbf{s} \in \mathcal{U}^{(1)}$, we look for an approximate solution of $Pu = 0$ near $\mathbf{s}$ under the form

$$u(x) = (1 + v(x,h))e^{-f(x)/h},$$

with a function v of the form

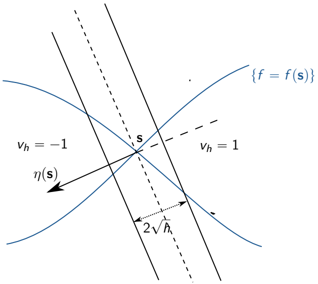
$$v(x,h) = \frac{1}{c_h}\int_0^{\ell(x,h)} e^{-s^2/2h} ds \quad (3)$$

with

- ℓ smooth, $\ell(x,h) \sim \sum_{j\geqslant 0} h^j \ell_j(x)$ and $\ell_0 \neq 0.$ and $\tau > 0$ is a small parameter
- c_h = normalization coeff.

Construction inspired from [Bovier-Gayrard-Klein 04, Di Gesu-Le Peutrec 17 , Le Peutrec-Michel 20]

- Think $\ell(x,h)$ as a linear coordinate function nears $\mathbf{s}$, $\ell(x,h) \sim (x-\mathbf{s})\cdot\eta(\mathbf{s})$
- c_h is such that $v=-1$ for $\ell >> 1$ and $v=1$ for $\ell << -1$



Action of the operator on the quasimodes

Lemma

One has

$$P(ve^{-f/h}) = (w + r)e^{-(f+\frac{\ell^2}{2})/h},$$

where

$$w = h\Big((2A\nabla f + b)\cdot\nabla\ell + (A\nabla\ell\cdot\nabla\ell)\ell\Big) - h^2\,\mathrm{div}(A\nabla\ell),$$

the function r and all its derivatives are (locally) bounded, uniformly with respect to h, and $\mathrm{supp}(r) \subset \{|\ell| \geqslant \tau\}$.

Equations on ℓ

Using the expansion $\ell(x,h) \sim \sum_{j\geqslant 0} h^j \ell_j(x)$ and identifying the powers of h, we get the

- Eikonal equation on ℓ_0

$$(2A^0\nabla f + b^0)\cdot\nabla\ell_0 + (A^0\nabla\ell_0\cdot\nabla\ell_0)\ell_0 = 0 \qquad \text{(Eik)}$$

- Transport equations on the ℓ_j, $j\geqslant 1$

$$(2A^0\nabla f + 2\ell^0 A^0\nabla\ell^0 + b^0)\cdot\nabla\ell_j + (A^0\nabla\ell_0\cdot\nabla\ell_0)\ell_j = -R_j \qquad \text{(Transp)}$$

with R_j depending only on $\ell_0,\dots,\ell_{j-1}$.

Resolution of the Eikonal equation

Lemma (Hérau-Hitrik-Sjöstrand, Bony-Le Peutrec-Michel)

Let $\mathbf{s} \in \mathcal{U}^{(1)}$. There exists a function ℓ_0 solving (Eik) in a neighborhood of $\mathbf{s}$ and such that

- the vector $\eta(\mathbf{s}) := \nabla \ell_0(\mathbf{s})$ is an eigenvector of the matrix
  $$\Lambda(\mathbf{s}) = 2H(\mathbf{s})A^0(\mathbf{s}) + B^t(\mathbf{s})$$
  associated to its negative eigenvalue $\mu(\mathbf{s})$.
- $$\det \mathrm{Hess}\left(f + \frac{1}{2}\ell_0^2\right)(\mathbf{s}) = -\det \mathrm{Hess}(f)(\mathbf{s}).$$

Recall on Hille-Yosida Theorem

Theorem (Hile-Yosida)

Let E be a Banach space and $A : D(A) \to E$ be an unbounded operator with dense domain. Then the following are equivalent

i) A generates a semigroup of contraction $S(t) = e^{-tA}$

ii) for all $\lambda \in]-\infty, 0[$, $A - \lambda$ is invertible and one has the estimate

$$\|(A-\lambda)^{-1}\|_{E\to E} \leqslant -\frac{1}{\lambda}$$

Remark

The constant 1 in the RHS of the resolvent is crucial.

Corollary

Assume there exists $\omega \in \mathbb{R}_+$ such that

$$\forall \lambda < \omega, \; \|(A-\lambda)^{-1}\|_{E\to E} \leqslant \frac{1}{\omega-\lambda}$$

Then

$$\|S(t)\|_{E\to E} \leqslant e^{-\omega t}$$

Application to eigenvalue expansion: first try

- Suppose $P : D(P) \to L^2$ is a KFP operator. Then P is maximal accretive hence $\|e^{-tP}\| \leqslant 1$
- Assume we are in the situation where $\sigma(P) \cap \{\mathrm{Re}(z) < \epsilon\} = \{\lambda_1, \dots, \lambda_{n_0}\}$ and let Π be the associated Riesz projector. Then

$$e^{-tP} = e^{-tP}\Pi + e^{-tP}(1 - \Pi)$$

- the term $e^{-tP}\Pi$ can be computed if one knows the λ_k
- one aims at estimating $e^{-tP}(1 - \Pi) = e^{-t\hat{P}}$ where $\hat{P} = \hat{\Pi}P\hat{\Pi}$ with $\hat{\Pi} = 1 - \Pi$.
- By definition, $\sigma(\hat{P}) \subset \{\mathrm{Re}(z) \geqslant \epsilon\}$

- If P is self-adjoint, then for all $\lambda < \epsilon$

$$\|(\hat{P} - \lambda)^{-1}\| \leqslant \frac{1}{dist(z, \sigma(\hat{P}))} \leqslant \frac{1}{\epsilon - \lambda}$$

  This implies that

$$\|e^{-tP}(1 - \Pi)\| \leqslant e^{-\epsilon t} << \|e^{-tP}\Pi\|$$

  by Hille-Yosida corollary

- in the general case, $(\hat{P} - \lambda)^{-1}$ is not better than $-\frac{1}{\lambda}$ for $\lambda < 0$.

Case of sectorial operators

Let $P : D(P) \to E$ be maximal accretive and assume that P is sectorial, that is there exists $\theta > 0$ such that

$$\sigma(P) \subset \Lambda_\theta := \{|\operatorname{Im}(z)| \leqslant \theta \operatorname{Re}(z)\}$$

and for any $\theta' > \theta$, there exists $C > 0$ such that for all $z \in \mathbb{C} \backslash \Lambda_{\theta'}$, one has

$$\|(P - z)^{-1}\|_{E \to E} \leqslant C|z|^{-1}$$

- Let $\Gamma = \Gamma_+ \cup \Gamma_-$ with $\Gamma_\pm = \{-1 + x(1 \pm i\theta),\ \pm x \geqslant 0\}$
- Then one has the Dunford representation formula

$$e^{-tP} = \int_\Gamma e^{-tz}(P - z)^{-1} dz$$

- Under the same localization assumption on the spectrum of P as above, one has

$$e^{-tP} = e^{-tP}\Pi + \int_{\tilde{\Gamma}} e^{-tz}(P-z)^{-1}dz$$

where $\tilde{\Gamma} = \ldots.$

- Using the resolvent estimate, this yields

$$e^{-tP} = e^{-tP}\Pi + O(e^{-\epsilon t}).$$

- This approach can be used to deal with non reversible diffusions
$$P = \Delta_f + b \cdot h\nabla$$
- In non semiclassical setting, a similar approach is used in Hérau-Nier (04) (with parabolic integration contour) to deal with KFP operator
- For semiclassical KFP operator, we do not have uniform resolvent estimate away from the spectrum

Gearhardt-Prüss Theorem

Theorem (Gearhardt-Prüss)

Let $P : D(P) \to E$ be a densely defined closed operator generating a continuous semigroup $U(t)$. Assume there exists $\omega > 0$ such that $(P - z)^{-1}$ is bounded uniformly with respect to $z \in \{\mathrm{Re}(z) < \omega\}$. Then there exists a constant $M > 0$ such that

$$\forall t \geqslant 0, \ \|U(t)\|_{E \to E} \leqslant Me^{-\omega t} \qquad (P(M, \omega))$$

- We want to apply this result to $P(1 - \Pi)$
- When P depends on h we need a control of M with respect to h.

Quantitative Gearhardt-Prüss Theorem

Theorem (Helffer-Sjöstrand)

Let $P : D(P) \to E$ be a densely defined closed operator generating a continuous semigroup $U(t)$. Assume that

- there exists $\hat{M} > 0$ and $\hat{\omega} \in \mathbb{R}$ such that
$$\forall t \geqslant 0, \ \|U(t)\| \leqslant \hat{M} e^{-\hat{\omega} t}$$
- there exists $\omega > \hat{\omega}$ and $r(\omega) > 0$ s.t. $\sigma(P) \subset \{\mathrm{Re}(z) > \omega\}$ and
$$\forall \, \mathrm{Re}(z) \leqslant \omega, \ \|(P - z)^{-1}\| \leqslant \frac{1}{r(\omega)}$$

Then

$$\forall t \geqslant 0, \ \|U(t)\|_{E \to E} \leqslant \hat{M}\left(1 + \frac{2\hat{M}(\omega - \hat{\omega})}{r(\omega)}\right) e^{-\omega t}$$

Application to Fokker-Planck equations

Let $P = P(h)$ be semiclassical Fokker Plank operator as above. Assume that the assumption (Harmo), (Ell), (Gibbs), (Morse) are satisfied. Then we proved

- P is maximal accretive
- There exists $\epsilon_0 > 0$ such that for all r, ϵ such that $0 < r < \epsilon < \epsilon_0$, one has

$$\sigma(P) \cap \{\mathrm{Re}(z) \leqslant \epsilon_0 h\} = \{\lambda_{\mathbf{m}},\ \mathbf{m} \in \mathcal{U}^{(0)}\}$$

and

$$\forall z \in \{\mathrm{Re}(z) \leqslant \epsilon h\} \backslash B(0, rh),\ \|(P - z)^{-1}\| \leqslant Ch^{-1}$$

for some $C > 0$ depending on ϵ, h.

Let

$$\Pi_h = \frac{1}{2i\pi} \int_{|z|=\frac{\epsilon}{2}h} (z-P)^{-1} dz$$

and $Q := P(1-\Pi_h)$ with domain $D(Q) = (1-\Pi_h)D(P)$. Then

- there exists $C > 0$ such that $\|\Pi_h\| \leqslant C$ for all $h > 0$.
- Q is maximal accretive, in particular it generates a continuous semigroup e^{-tQ} such that

$$\|e^{-tQ}\| \leqslant 1$$

- $\sigma(Q) \subset \{\mathrm{Re}(z) \geqslant \epsilon_0 h\}$ and

$$\forall\, \mathrm{Re}(z) \leqslant \epsilon h,\ \|(Q-z)^{-1}\| \leqslant Ch^{-1}$$

We apply quantitative Gearhardt-Prüss Theorem, it follows that

$$\forall t \geqslant 0,\ \|e^{-tQ}\| \leqslant Ce^{-\epsilon_0 ht}$$

Going back to P, we get

$$e^{-tP} = e^{-tP}\Pi_h + O(e^{-\epsilon_0 ht}).$$

Under the generic assumption the small eigenvalues $\lambda_{\mathbf{m}}$, $\mathbf{m} \in \mathcal{U}^{(0)}$ are distinct. One has $\Pi_h = \sum_{\mathbf{m}\in\mathcal{U}^{(0)}} \Pi_{\mathbf{m},h}$ with

$$\Pi_{\mathbf{m},h} = \frac{1}{2i\pi} \int_{\partial D(\lambda_{\mathbf{m}}, r_{\mathbf{m}})} (z-P)^{-1} dz$$

for some $r_{\mathbf{m}} > 0$ sufficiently small. Moreover, one can show that

- there exists $C > 0$ such that

$$\forall \mathbf{m} \in \mathcal{U}^{(0)}, \; \|\Pi_{\mathbf{m},h}\| \leqslant C$$

- the projector $\Pi_{\underline{\mathbf{m}}}$ on the smallest eigenvalue $\lambda_{\underline{\mathbf{m}}} = 0$ satisfies

$$\Pi_{\underline{\mathbf{m}}} u = \langle u, \varphi_{\underline{\mathbf{m}}} \rangle \varphi_{\underline{\mathbf{m}}}$$

  with $\varphi_{\underline{\mathbf{m}}} = Z_h e^{-(f-f(\underline{\mathbf{m}}))/h}$ normalized eigenstate associated to $\lambda_{\underline{\mathbf{m}}}$.
- This implies

$$e^{-tP} u_0 = \langle u_0, \varphi_{\underline{\mathbf{m}}} \rangle \varphi_{\underline{\mathbf{m}}} + \sum_{\mathbf{m}\in\mathcal{U}^{(0)}\setminus\underline{\mathbf{m}}} e^{-\lambda_{\mathbf{m}} t} \Pi_{\mathbf{m}} + O(e^{-\epsilon h t})$$

Bibliography

- T. Kato, Perturbation theory for linear operators, 1980
- F. Hérau and F. Nier, Isotropic hypoellipticity and trend to equilibrium for the Fokker-Planck equation with a high-degree potential, 2004
- F. Hérau, Hypocoercivity and exponential time decay for the linear inhomogeneous relaxation Boltzmann equation, 2006
- F. Hérau, M. Hitrik and J. Sjöstrand, Tunnel effect for Kramers-Fokker-Planck type operators, 2008
- J. Dolbeault, C. Mouhot, and C. Schmeiser, Hypocoercivity for kinetic equations with linear relaxation terms, 2009
- A. Guillin and B. Nectoux, Low-lying eigenvalues and convergence to the equilibrium of some piecewise deterministic Markov processes generators in the small temperature regime, 2020

Bibliography

- F. Bouchet and J. Reygner, Generalisation of the Eyring-Kramers transition rate formula to irreversible diffusion processes, 2016
- J.-F. Bony, D. Le Peutrec and L. Michel, Eyring-Kramers law for Fokker-Planck type differential operators, 2022
- B. Helffer, Spectral theory and its applications, 2013
- B. Helffer and J. Sjöstrand, Improving semigroup bounds with resolvent estimates, 2021