Most probable exit points for the overdamped Langevin dynamics

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   - Overdamped Langevin dynamics
   - Previous results
   - Quasi-stationary distribution (QSD)
2. Results
   - Hypotheses and notation
   - Results
   - Comments
3. About the proof when $X_0 \sim$QSD

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- Overdamped Langevin dynamics :

  $\hookrightarrow$ System $X = (X_t)_{t \geq 0}$ of d particles

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

  Where :

  - f potential function (assumed to be smooth here !)
  - $h = \kappa_B T$, $T \leftrightarrow$ temperature, $\kappa_B \leftrightarrow$ Boltzmann constant
  - $B = (B_1, \ldots, B_d) \leftrightarrow d$ independent Brownian motions

- When $0 < h \ll 1$, the process X is trapped during a long period of time near a local minimum of f before going to another region of $\mathbb{R}^d$

  $\hookrightarrow$ This regions are said metastable ($\leftrightsquigarrow$ tunneling effect)

  $\hookrightarrow$ Long period of inactivities between two "transitions"

- **General question :** For $\Omega \subset \mathbb{R}^d$ metastable and $h \ll 1$, what is the behaviour of the exit event from Ω ?

  Rk : Exit event from Ω $= \begin{cases} \text{time spent in } \Omega \\ + \text{ exit point distribution} \end{cases}$

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  what is the behaviour of the exit event from Ω ?

  Rk : Exit event from $\Omega \;=\; \begin{cases} \text{time spent in } \Omega \\ + \text{ exit point distribution} \end{cases}$

- We focus here on the most probable exit points :

  Let $\Omega \subset \mathbb{R}^d$ be a smooth open and connected set, and

  $$\tau_\Omega \;=\; \inf\{\, t \geq 0 \mid X_t \notin \Omega\} \quad \text{the first exit time from } \Omega.$$

Definition 1

X_{τ_Ω} concentrates on $\mathcal{Y} \subset \partial\Omega$ if :

– for any neigh. $\mathcal{V}_{\mathcal{Y}} \subset \partial\Omega$ of $\mathcal{Y}$, $\lim\limits_{h \to 0^+} \mathbb{P}(X_{\tau_\Omega} \in \mathcal{V}_{\mathcal{Y}}) = 1$

– for any $x \in \mathcal{Y}$ and $\mathcal{V}_x \subset \partial\Omega$ neigh. of x, $\lim\limits_{h \to 0^+} \mathbb{P}(X_{\tau_\Omega} \in \mathcal{V}_x) > 0$

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- When $\partial_n f > 0$ on $\partial\Omega$ and f admits one unique critical point x_0 in Ω (and hence $f(x_0) = \min_{\overline{\Omega}} f$) being non degenerate, it holds :

$$\forall x \in \Omega\,,\ \forall F \in \mathcal{C}^\infty(\partial\Omega,\mathbb{R}),\ \ \mathbb{E}^x[\,F(X_{\tau_\Omega})\,] \;=\; \frac{\int_{\partial\Omega} F\,\partial_n f\, e^{-\frac{2}{h}f}\,d\sigma}{\int_{\partial\Omega}\partial_n f\, e^{-\frac{2}{h}f}\,d\sigma} + o(1)$$

[Follows from M.I. Freidlin and A.D. Wentzell when $\mathrm{argmin}_{\partial\Omega} f = \{z_0\}$ (1970)
Result formally obtained in general by B.J. Matkowsky and Z. Schuss (1977)
Proved by S. Kamin (1978,1979), M.V. Day (1984, 1987), B. Perthame (1990)]

Rk 1 : $x \mapsto \mathbb{E}^x[\,F(X_{\tau_\Omega})\,]$ is the sol. to $\begin{cases} -\frac{h}{2}\Delta g + \nabla f\cdot\nabla g = 0 \\ g\big|_{\partial\Omega} = F \end{cases}$

Rk 2 : These results are also valid in the non-gradient case !

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Rk 2 : These results are also valid in the non-gradient case !

$\hookrightarrow$ When $X_0 = x \in \Omega$, X_{τ_Ω} concentrates on $\mathrm{argmin}_{\partial\Omega} f$
(with explicitly computable asymptotic relative probabilities)

- We want to obtain similar results for quite general domains Ω when X_0 is distributed according to the QSD of Ω and to extend them to deterministic initial conditions $X_0 = x$.
- More precisely, we look for geometric assumptions ensuring that :
  - when $X_0 \sim$ QSD, the distrib. of X_{τ_Ω} concentrates on $\mathcal{Y} \subset \mathrm{argmin}_{\partial\Omega} f$,
  - these results extend to $X_0 = x$ for some particular x to be specified

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- **Def :** A QSD ν on Ω is a measure supp. in Ω s.t. $\mathcal{L}^{\nu}(X_t \,|\, t < \tau_\Omega) = \nu$
- Infinitesimal generator of the dynamics :

$$L^{(0)} \;:=\; -\frac{h}{2}\Delta + \nabla f \cdot \nabla \;=\; -\frac{h}{2}\, e^{\frac{2}{h}f}\, \mathrm{div}\,(\, e^{-\frac{2}{h}f}\, \nabla \cdot\,)$$

- $\big(\, L^{(0)}\,,\, (H^2 \cap H^1_0)(\Omega, e^{-\frac{2}{h}f} dx)\,\big)$ s.a. ≥ 0 on $L^2_w = L^2(\Omega, e^{-\frac{2}{h}f} dx)$
- Discrete spectrum, the principal e.v. $\lambda_1(h) > 0$ is non degenerate
- The principal $\vec{\text{e.v.}}$ has a sign on Ω

Proposition 2

Let u_h be any $\vec{\text{e.v.}}$ associated with $\lambda_1(h) > 0$. Then

$$d\nu_h = \frac{u_h\; e^{-\frac{2}{h}f}\, dx}{\int_\Omega u_h(y)\; e^{-\frac{2}{h}f(y)} dy}$$

is a QSD for the process $(X_t \,|\, t < \tau_\Omega)$.

Properties of the QSD

Proposition 3 (Le Bris, Lelièvre, Luskin, Perez)

For every probability μ_0 on Ω and every t large enough,

$$\|\mathcal{L}^{\mu_0}(X_t | t < \tau_\Omega) - \nu_h\|_{TV} \leq C(\mu_0) e^{-(\lambda_2(h) - \lambda_1(h))\, t}$$

$\hookrightarrow$ The QSD is unique !

Proposition 4

When $X_0 \sim \nu_h$:

1. τ_Ω *are* X_{τ_Ω} *independent,*
2. $\tau_\Omega \sim \mathcal{E}(\lambda_1(h))$,
3. X_{τ_Ω} *has the following density on* $\partial\Omega$ *:*

$$z \in \partial\Omega \mapsto -\frac{h}{2\,\lambda_1(h)} \frac{\partial_n u_h(z)\; e^{-\frac{2}{h}f(z)}}{\int_\Omega u_h(y) e^{-\frac{2}{h}f(y)} dy}$$

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- "Morse" type hypotheses on f **(MH)** :
  - f is a smooth Morse function on $\overline{\Omega}$
  - ∇f does not vanish on $\partial\Omega$
  - $f\big|_{\partial\Omega}$ (or more generally $f\big|_{\{\sigma \text{ s.t. } \partial_n f(\sigma)>0\}}$) is a Morse function
  - $\mathcal{U}_0 := \{\text{local minima of } f \text{ in } \Omega\}$ is not empty

- Minimal energy needed to reach the boundary :
  - Let us define, for any $x \in \mathcal{U}_0$,

$$H_f(x) := \inf_{\substack{\gamma \in \mathcal{C}([0,1],\overline{\Omega}) \\ \gamma(0) = x \\ \gamma(1) \in \partial\Omega}} \max_{t\in[0,1]} f(\gamma(t))$$

  - and, for some arbitrary $x_1 \in \operatorname{argmax}\{H_f(x) - f(x),\ x \in \mathcal{U}_0\}$,

$$C_1 := \text{connected component of } \{f < H_f(x_1)\} \text{ containing } x_1$$

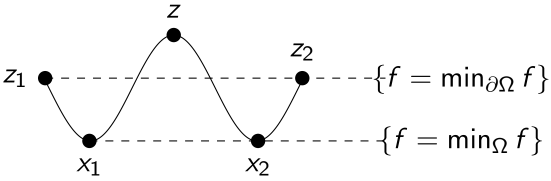
Geometric hypotheses **(GH)** :

- **(GH1)** $\mathrm{argmax}\{H_f(x) - f(x),\ x \in \mathcal{U}_0\} \subset C_1$

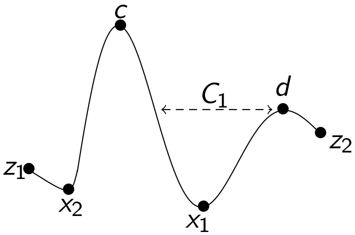
  ($\Rightarrow$ the definition of C_1 does not depend on the choice of x_1 !)

- **(GH2)** $\partial C_1 \cap \partial\Omega \neq \emptyset$

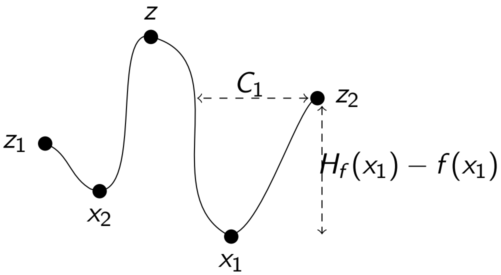
- **(GH3)** $\partial C_1 \cap \partial\Omega \subset \mathrm{argmin}_{\partial\Omega} f$



(GH1) not satisfied

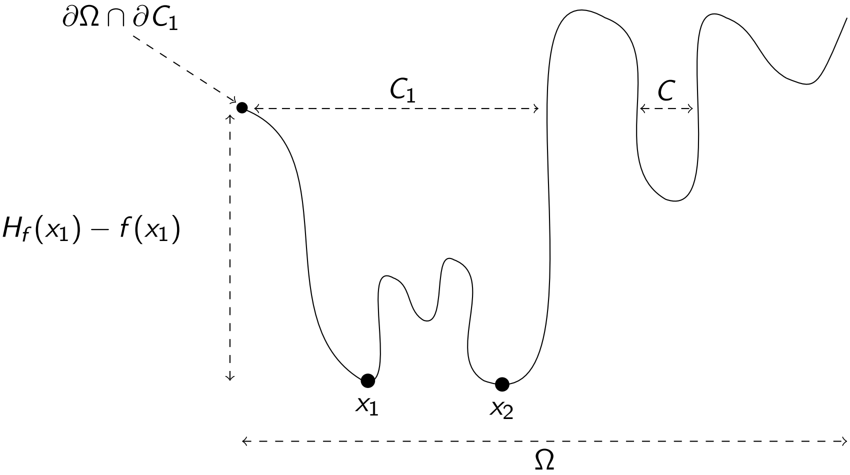


(GH1) but not (GH2)



(GH1), (GH2) but not (GH3)

An example where (GH) is satisfied



Generalized saddle points on $\partial\Omega$

- *Generalized* saddle points on $\partial\Omega$:

$$\begin{aligned}\mathcal{U}_1^{\partial\Omega} &= \{\text{local minima of } f\big|_{\partial\Omega} \text{ where } \partial_n f > 0\} \\ &= \{z_1, \dots, z_{m_1}\} \subset \partial\Omega\end{aligned}$$

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- $\mathcal{U}_1^{\partial\Omega} \cap \operatorname{argmin}_{\partial\Omega} f = \{z_1, \ldots, z_{k_1}\} \ (0 \leq k_1 \leq m_1)$

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- $\mathcal{U}_1^{\partial\Omega} \cap \mathrm{argmin}_{\partial\Omega} f = \{z_1, \dots, z_{k_1}\} \ (0 \leq k_1 \leq m_1)$

- $\partial C_1 \cap \partial\Omega = \partial C_1 \cap \mathcal{U}_1^{\partial\Omega} \cap \mathrm{argmin}_{\partial\Omega} f = \{z_1, \dots, z_{k_1^{\partial C_1}}\}$

Rk : From our hypotheses : $1 \leq k_1^{\partial C_1} \leq k_1 \leq m_1$

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Theorem 1 (with G. Di Gesù, T. Lelièvre et B. Nectoux)

We assume **(MH)** *and* **(GH)***.*

Let $F \in C^{\infty}(\partial\Omega, \mathbb{R})$ *and* $\{\Sigma_1, \dots, \Sigma_{k_1}\}$ *be a family of disjoint neigh. of* $\{z_1, \dots, z_{k_1}\} = \mathcal{U}_1^{\partial\Omega} \cap \operatorname{argmin}_{\partial\Omega} f$ *in* $\partial\Omega$*.*

We assume that $X_0 \sim \nu_h$ *or* $X_0 = x \in C_1$*. Then :*

1. *There exists* $c > 0$ *such that in the limit* $h \to 0^+$*,*

$$\mathbb{E}^{X_0}[\, F(X_{\tau_\Omega})\,] \;=\; \sum_{i=1}^{k_1} \mathbb{E}^{\nu_h}[\, \mathbf{1}_{\Sigma_i} F(X_{\tau_\Omega})\,] \;+\; O(e^{-\frac{c}{h}})$$

and

$$\sum_{i=k_1^{\partial C_1}+1}^{k_1} \mathbb{E}^{X_0}[\, \mathbf{1}_{\Sigma_i} F(X_{\tau_\Omega})\,] \;=\; O(h^{\frac{1}{4}})$$

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We assume that $X_0 \sim \nu_h$ *or* $X_0 = x \in C_1$. *Then :*

2. *For every* $i \in \{1, \ldots, k_1^{\partial C_1}\}$, *it holds when* $h \to 0^+$,

$$\mathbb{E}^{X_0}[\mathbf{1}_{\Sigma_i} F(X_{\tau_\Omega})] = F(z_i)\, a_i + O(h^{\frac{1}{4}})$$

where

$$a_i = \frac{\partial_n f(z_i)}{\sqrt{\det \operatorname{Hess} f\big|_{\partial\Omega}(z_i)}} \Big(\sum_{k=1}^{k_1^{\partial C_1}} \frac{\partial_n f(z_k)}{\sqrt{\det \operatorname{Hess} f\big|_{\partial\Omega}(z_k)}} \Big)^{-1}$$

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We assume that $X_0 \sim \nu_h$ *or* $X_0 = x \in C_1$. *Then :*

3. *Under some additional geometric assumption, it holds :*

$$\sum_{i=k_1^{\partial C_1}+1}^{k_1} \mathbb{E}^{X_0}[\mathbf{1}_{\Sigma_i} F(X_{\tau_\Omega})] = O(e^{-\frac{c}{h}}) + \cancel{O(h^{\frac{1}{4}})}$$

and for every $i \in \{1, \ldots, k_1^{\partial C_1}\}$,

$$\mathbb{E}^{X_0}[\mathbf{1}_{\Sigma_i} F(X_{\tau_\Omega})] = F(z_i)\, a_i + O(h) + \cancel{O(h^{\frac{1}{4}})}$$

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- When $X_0 \sim \nu_h$ or $X_0 = x$ as specified above, X_{τ_Ω} concentrates on

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$$\mathcal{Y} \;=\; \partial C_1 \cap \partial\Omega \;\subset\; \mathrm{argmin}_{\partial\Omega} f$$

- **But** X_{τ_Ω} does not concentrate on the sets

  $\{z_{k_1^{\partial C_1}+1}, \ldots, z_{k_1}\}$ and $\{$global minima of $f\big|_{\partial\Omega}$ where $\partial_n f \;<\; 0\}$

  which have energy $\min_{\partial\Omega} f$ (and can be non-empty)

- As a consequence, when

$$\partial_n f \; > \; 0 \;\; \text{on } \partial\Omega \quad \text{and} \quad (\nabla f)^{-1}(\{0\}) \; \subset \; \{f < \min_{\partial\Omega} f\},$$

it holds $k_1^{\partial C_1} = k_1$ (iff $\partial C_1 \cap \partial\Omega = \mathrm{argmin}_{\partial\Omega} f$) and for every $x \in \Omega$:

$$\mathbb{E}^x[\, F(X_{\tau_\Omega})\,] \; = \; \sum_{i=1}^{k_1} F(z_i)\, a_i \, + \, O(h^{\frac{1}{4}}) \; = \; \frac{\int_{\partial\Omega} F\, \partial_n f \; e^{-\frac{2}{h} f} \, d\sigma}{\int_{\partial\Omega} \partial_n f \; e^{-\frac{2}{h} f} \, d\sigma} + o(1)$$

$\hookrightarrow$ One recovers in particular the previous mentioned results

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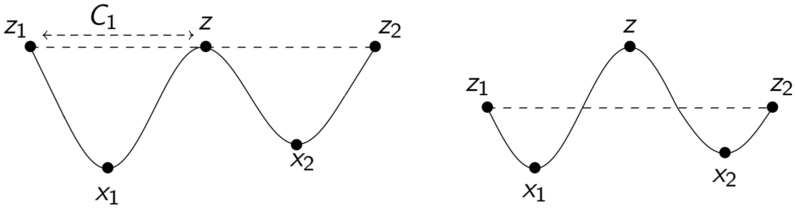
$$\mathbb{E}^x[\,F(X_{\tau_\Omega})\,] \; = \; \sum_{i=1}^{k_1} F(z_i)\,a_i \,+\, O(h^{\frac14}) \; = \; \frac{\int_{\partial\Omega} F\,\partial_n f\, e^{-\frac{2}{h}f}\, d\sigma}{\int_{\partial\Omega} \partial_n f\, e^{-\frac{2}{h}f}\, d\sigma} \,+\, o(1)$$

$\hookrightarrow$ One recovers in particular the previous mentioned results

- Two simple examples :



Here : $\mathbb{P}^{X_0}[X_{\tau_\Omega} = z_2] \simeq \sqrt{h}$ $\qquad$ $\mathbb{P}^{X_0}[X_{\tau_\Omega} = z_2] = \mathcal{O}(e^{-\frac{c}{h}})$

- Intermediate results about $\lambda_1(h)$:
  - Under **(MH)**, there exist $C_1, C_2 > 0$ such that when $h \to 0^+$,

$$\frac{C_1}{h^p} e^{-\frac{2}{h}(H_f(x_1)-f(x_1))} \le \lambda_1(h) \le \frac{C_2}{h^p} e^{-\frac{2}{h}(H_f(x_1)-f(x_1))}$$

    for some $p \in \{0, \frac{1}{2}\}$ and

$$\textbf{(GH1)} \text{ holds} \quad \text{iff} \quad \exists\, c > 0 \ \text{ s.t. } \ \lambda_1(h) = \lambda_2(h)\, O(e^{-\frac{c}{h}}).$$

  - Laslty, under **(MH)**, **(GH1)**, and **(GH2)**, it holds :

$$\lambda_1(h) = \frac{\sum_{j=1}^{k_1^{\partial C_1}} \partial_n f(z_j) \big(\det \mathrm{Hess} f\big|_{\partial\Omega}(z_j)\big)^{-\frac{1}{2}}}{\sqrt{\pi\, h}\, \sum_{x \in \mathrm{argmin}_{C_1} f} \big(\det \mathrm{Hess} f(x)\big)^{-\frac{1}{2}}} e^{-\frac{2}{h}(H_f(x_1)-f(x_1))}\big(1+O(\sqrt{h})\big)$$

- Some related results about the low spectrum of $L^{(0)}$ (in Ω or in $\mathbb{R}^d$) :
  - Probabilistic approach : Holley-Kusuoka-Stroock, Miclo, Mathieu, Bovier-Gayrard-Klein
  - Semi-classical approach : Helffer-Klein-Nier, Helffer-Nier, L.P., Michel
  - Langevin (in $\mathbb{R}^d$) : Hérau-Hitrik-Sjöstrand

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Let u_h be any $\overrightarrow{\text{e.v.}}$ associated with $\lambda_1(h)$ and $F \in C^\infty(\partial\Omega, \mathbb{R})$, then :

$$\mathbb{E}^{\nu_h}[\, F(X_{\tau_\Omega})\,] \;=\; -\frac{h}{2\,\lambda_1(h)}\frac{\int_{\partial\Omega} F(z)\,\partial_n u_h(z)\; e^{-\frac{2}{h}f(z)}\,dz}{\int_\Omega u_h(x)e^{-\frac{2}{h}f(x)}\,dx}$$

$\hookrightarrow$ we precisely estimate :

- $\lambda_1(h)$
- $\int_\Omega u_h(y)e^{-\frac{2}{h}f(y)}dy$
- $\partial_n u_h$ on $\partial\Omega$

Estimates on $\lambda_1(h)$ and on the low spectrum of $L^{(0)}$

- By standard techniques developed in semiclassical analysis, for $p \in \{0,1\}$ and $C > 0$ small enough :

$$\dim\left(\mathrm{Im}\ \mathbf{1}_{[0,C)}(L^{(p)})\right) = \dim\left(\mathrm{Im}\ \mathbf{1}_{[0,he^{-\frac{C}{h}})}(L^{(p)})\right) = \mathrm{Card}(\mathcal{U}_p)$$

where

$$\mathcal{U}_1 \ := \ \mathcal{U}_1^{\partial\Omega} \cup \{\text{saddle points of } f \text{ in } \Omega\}$$

- Use the supersymmetric extension "à la Witten"

$$L^{(1)} := L^{(0)} \otimes \mathrm{Id} + \mathrm{Hess}\, f\,,$$

$$\mathrm{Dom}(L^{(1)}) = \left\{v \in \Lambda^1 H^2(\Omega, e^{-\frac{2}{h}f}dx)\,;\, \mathbf{t}v = 0 \text{ et } \mathbf{t}(\mathrm{div}\,(e^{-\frac{2}{h}f}v)) = 0\right\}$$

$\hookrightarrow$ s.a. ≥ 0 on $\Lambda^1 L^2(\Omega, e^{-\frac{2}{h}f}dx)$ and

$$L^{(1)}\nabla \ = \ \nabla L^{(0)}$$

Estimates on $\lambda_1(h)$ and on the low spectrum of $L^{(0)}$

- Reduce the problem to a finite dimensional one :

$\hookrightarrow$ we study $\nabla : \mathrm{Im}\ \mathbf{1}_{[0,C)}(L^{(0)}) \to \mathrm{Im}\ \mathbf{1}_{[0,C)}(L^{(1)})$:

$$\begin{aligned} L^{(0)} &= -\frac{h}{2}\, e^{\frac{2}{h}f}\, \mathrm{div}\,(\, e^{-\frac{2}{h}f}\, \nabla \cdot\,) \\ &= \frac{h}{2}\nabla^* \nabla \quad (\text{ adjoint w.r.t. } e^{-\frac{2}{h}f}\, dx\ ) \end{aligned}$$

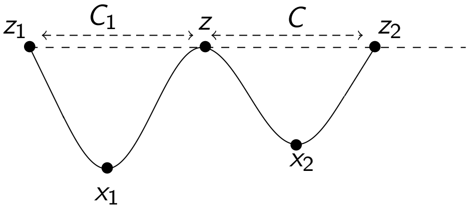
$\hookrightarrow \left\{ \text{E.v. of } L^{(0)}\big|_{\mathrm{Im}\ \mathbf{1}_{[0,C)}(L^{(0)})} \right\} = \left\{ \frac{h}{2}\Big(\text{Sing. V. of } \nabla\big|_{\mathrm{Im}\ \mathbf{1}_{[0,C)}(L^{(0)})}\Big)^2 \right\}$

$\hookrightarrow$ Construct $(u_j^{(p)})_{j\in\{1,\dots,\mathrm{Card}\,\mathcal{U}_p^{\overline{\Omega}}\}}$ an appropriate basis of

$$\mathrm{Im}\ \mathbf{1}_{[0,C)}(L^{(p)})\ , \quad p \in \{0,1\}$$

in which the matrix ∇ is estimable

On this simple example :



$\{f = \min_{\partial\Omega} f\} = \{f = H_f(x_1)\}$

$\hookrightarrow$ A "good" choice of "quasi-modes" first leads to the singular values of :

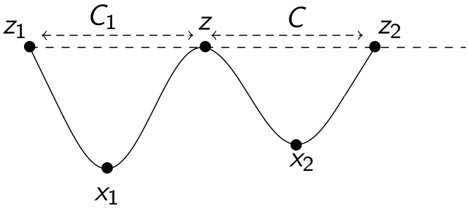
$$\begin{pmatrix} a_1 & O(e^{-\frac{c}{h}}) \\ b_1\, h^{\frac{1}{4}} & b_2\, h^{\frac{1}{4}} \\ O(e^{-\frac{c}{h}}) & a_2 \end{pmatrix} \times \begin{pmatrix} h^{-\frac{3}{4}} e^{-\frac{f(z_1)-f(x_1)}{h}} & 0 \\ 0 & h^{-\frac{3}{4}} e^{-\frac{f(z_2)-f(x_2)}{h}} \end{pmatrix}$$

where

$$a_i \sim -(\frac{2}{\sqrt{\pi}})^{\frac{1}{2}} |f'(z_i)|^{\frac{1}{2}} |f''(x_i)|^{\frac{1}{4}} \quad \text{et} \quad b_i \sim (-1)^i \frac{1}{\sqrt{\pi}} |f''(z)|^{\frac{1}{4}} |f''(x_i)|^{\frac{1}{4}}$$

Estimates on $\lambda_1(h)$ and on the low spectrum of $L^{(0)}$

On this simple example :



$\{f = \min_{\partial\Omega} f\} = \{f = H_f(x_1)\}$

$\hookrightarrow$ Which finally leads to :

$$\begin{aligned}\lambda_1(h) &= \frac{h}{2}\left(a_1^2 + O(\sqrt{h})\right) h^{-\frac{3}{2}} e^{-\frac{2}{h}(f(z_1)-f(x_1)} \\ &= \frac{1}{\sqrt{\pi h}}\,|f'(z_1)|\,|f''(x_1)|^{\frac{1}{2}}\, e^{-\frac{2}{h}(f(z_1)-f(x_1))}\left(1+O(\sqrt{h})\right)\end{aligned}$$

Estimates on $\int_\Omega u_h(y) e^{-\frac{2}{h}f(y)}dy$

Under (**HG1**) and $\min_{C_1} f = \min_{\overline{\Omega}} f$, one easily proves :

$$\int_\Omega u_h\, e^{-\frac{2}{h}f} = \int_{\mathcal{V}(\mathrm{argmin}_{C_1} f)} u_h\, e^{-\frac{2}{h}f}\,\left(1+O(e^{-\frac{c}{h}})\right)$$

$$= h^{\frac{d}{4}}\,\pi^{\frac{d}{4}}\,e^{-\frac{1}{h}\min_{\overline{\Omega}} f}\Big(\sum_{x\in\mathrm{argmin}_{C_1} f}\left(\det \mathrm{Hess} f(x)\right)^{-\frac{1}{2}}\Big)^{\frac{1}{2}}\left(1+O(h)\right)$$

$\hookrightarrow$ take a "good" quasi-mode $\tilde{u}_h = \frac{\chi}{\|\chi\|_{L^2_w}}$

$\hookrightarrow$ use (**HG1**) $\Leftrightarrow \exists\, c > 0$ t.q. $\lambda_1(h) = \lambda_2(h)\, O(e^{-\frac{c}{h}})$

$\hookrightarrow$ it then holds in L^2_w, for some fixed $\delta > 0$ small enough :

$$u_h + O(e^{-\frac{c}{h}}) = \mathbf{1}_{[0,\lambda_1(h)e^{\frac{\delta}{h}})}(L^{(0)})\,\tilde{u}_h = \tilde{u}_h + O(e^{-\frac{c}{h}})$$

$\hookrightarrow$ we conclude using Cauchy-Schwarz inequality and $\min_{C_1} f = \min_{\overline{\Omega}} f$!

Estimates on $\partial_n u_h$

- We have to conveniently estimate, on $\partial\Omega$,

$$\partial_n u = \vec{n} \cdot \nabla u_h$$

(where $u_h > 0$ unitary L^2_w)

$\hookrightarrow$ Supersymmetry :

$$\nabla u \ \in \ \mathrm{Im}\, \mathbf{1}_{[0,C)}(L^{(1)})$$

$\hookrightarrow$ In any o.n.b. $(\psi_j)_j$ of $\mathrm{Im}\, \mathbf{1}_{[0,C)}(L^{(1)})$, it holds :

$$\partial_n u \ = \ \sum_j \langle \nabla u, \psi_j \rangle \ \psi_j \cdot \vec{n}$$

- An accurate quasi-mode (but in L^2_w) for u_h is given by $\tilde{u}_h \ := \ \frac{\chi}{\|\chi\|_{L^2_w}}$

$\hookrightarrow$ We need to precisely compare their gradients !

- A "key" result (OK under **(HG1)** and **(HG2)**) :

$$\|\nabla(\mathbf{1}_{[0,C)}(L^{(0)})\,\tilde{u}_h)\|^2_{L^2_w} \;=\; \frac{2}{h}\lambda_1(h)\,(1+O(\sqrt{h}))$$

and for $\delta > 0$ small enough

$$\begin{aligned}
&\|\nabla\left(\mathbf{1}_{[0,C)}(L^{(0)}) - \mathbf{1}_{[0,\lambda_1(h)e^{\frac{\delta}{h}})}(L^{(0)})\right)\tilde{u}_h\|^2_{L^2_w} \\
&\quad= \|\nabla\,\mathbf{1}_{[0,C)}(L^{(0)})\,\tilde{u}_h\|^2_{L^2_w} - \|\nabla\,\mathbf{1}_{[0,\lambda_1(h)e^{\frac{\delta}{h}})}(L^{(0)})\,\tilde{u}_h\|^2_{L^2_w} \\
&\quad= \frac{2}{h}\lambda_1(h)\,O(\sqrt{h})
\end{aligned}$$

Thank you for your attention !