Low temperature asymptotics for Quasi Stationary Distributions in a bounded domain

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Joint work with T. Lelièvre

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Outline

- Quasi-Stationary Distributions
- Parallel Replica and Hyperdynamics
- Witten Laplacians
- Results

Definition of QSD

Consider the SDE in $\mathbb{R}^d$

$$dX_t = -\partial_x f(X_t)dt + \sqrt{2\beta^{-1}}dW_t \quad , \quad \beta = \frac{1}{kT}\,.$$

with $f \in \mathcal{C}^\infty(\mathbb{R}^d)$.

Ω domain of $\mathbb{R}^d$. A trajectory starting with $X_0 = x \in \Omega$ will be denoted $X_{x,t}$ and the exit time τ_x equals

$$\tau_x = \min\left\{t \in [0,+\infty),\ X_{x,t} \in \partial\Omega\right\}\,.$$

Definition:

A probability measure μ is a QSD in Ω if for

$$\forall \varphi \in \mathcal{C}^\infty(\overline{\Omega})\,, \forall t > 0\,, \mathbb{E}(\varphi(X_{x,t})|t < \tau_x) = \int_\Omega \varphi(x)\; d\mu(x)$$

when the law of $X_{x,0}$ is μ.

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Use of QSD

QSD can be defined with more general stochastic processes. They model the stochastic evolution of a population in a domain with possible individual escape or end. Applications (after P.K. Polett):Biology and ecology, Chemical kinetics, Epidemics, Genetics, Reliability, Telecommunication, Medicine, Neurosciences.

They provide the theoretical framework for analysing stochastic algorithms Parallel Replica and Fleming-Viot algorithms.

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Properties of QSD

In our case with a regular bounded domain Ω, there exists a unique QSD, $\mu = Z_{v1_\Omega}^{-1} v(x) 1_\Omega(x) e^{-\beta f(x)} dx$, where v is the non-negative eigenvector of the Dirichlet realization L^D of $L = -\partial_x f(x).\partial_x + \beta^{-1}\Delta_x$.

For any regular φ and any $x \in \Omega$, $\mathbb{E}(\varphi(X_{x,t}) | t < \tau_x)$ converges to $\int_{\Omega_+} \varphi(x)\ d\mu(x)$ as $t \to +\infty$.

When $X_{x,0}$ is distributed according the μ, the exit times τ and exit point X_τ are independent random variables with

- τ has the exponential law with coefficient λ_1, the first eigenvalue of L^D
- X_τ has the law given by

$$\mathbb{E}(\varphi(X_\tau)) = -\frac{\int_{\partial\Omega} \varphi \partial_n(ve^{\beta f})\ d\sigma}{\beta\lambda_1 \int_\Omega ve^{-\beta f}\ dx} = \frac{\int_{\partial\Omega} \varphi \partial_n(ve^{\beta f})\ d\sigma}{\int_{\partial\Omega} \partial_n(ve^{\beta f})\ d\sigma}.$$

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Aim

In a complex system (i.e. with a large number of degrees of freedom), one may identify a finite set of metastable states S . One wants to find the effective Markov process on S from suitable simulations of the whole system.
For a metastable domain $\Omega \in S$, the quasistationary distribution and the laws of τ and X_τ give respectively the exit process to the exterior of Ω and the reaction paths and proportions to other states of S .

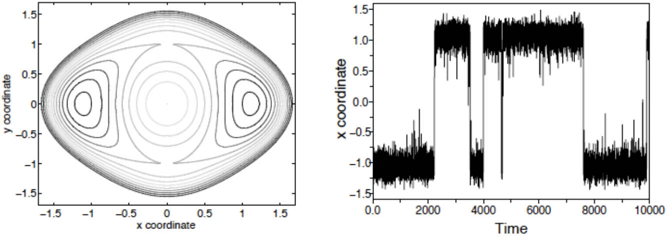

Figure: An example with $\sharp S = 2$.

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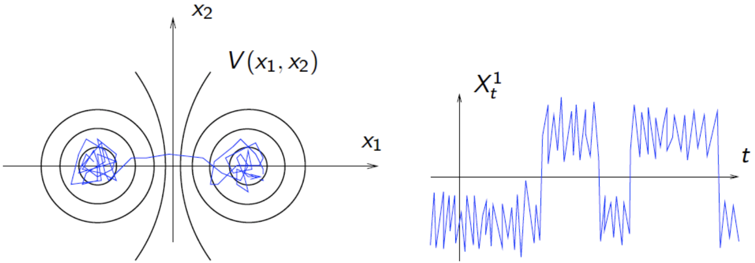

Figure: Here the metastable states are identified with $x_1 > 0$ and $x_1 < 0$

Parallel Replica

This method was introduced by A. Voter (1998).
One step consists in sampling as follows the exit time and exit position of a QSD in Ω: On parallel processors a large number K of independent particles $X_{x_k,t}$, $k = 1, \dots, K$ are simulated and the simulation is stopped as soon as one particle hits the boundary (time T). It can be proved that the distribution of $(X_{x_k,T})_{1\leq k\leq K}$ approximates the QSD.
REF Le Bris–Lelièvre–Luskin–Perez (2012).

Hyperdynamics

This is a way to accelerate the simulation with a little effect on the exit point law and some explicit transformation of the exit time law (proposed by A. Voter in 1997).

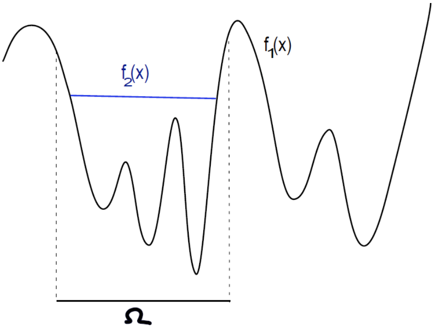

Figure: The potential is increased from f_1 to f_2 inside Ω.

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Guess :The exit time law coefficient is changed by multiplying with the "boost" factor

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The exit point law is not changed

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Fokker-Planck operators and Witten Laplacians

Remember

$$L = (\partial_x f(x) - \beta^{-1}\partial_x)).\partial_x \,.$$

Conjugating with $e^{-\frac{\beta f}{2}}$ (or $e^{\frac{\beta f}{2}}$) leads to

$$\frac{4}{\beta} e^{\frac{-\beta f}{2}} L e^{\frac{\beta f}{2}} = \Delta_{f,h}^{(0)}$$

$$\Delta_{f,h}^{(0)} = -h^2\Delta_x + |\partial_x f(x)|^2 - h\Delta f(x)\,, \quad h = \frac{2}{\beta}\,,$$

to be studied in $L^2(\Omega, dx)$. This is the semiclassical Witten Laplacian acting on functions.

More generally

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

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Witten Laplacians on compact manifolds

No boundary. f is a Morse function on Ω.

In his famous article of 81, E. Witten showed that the number of $\mathcal{O}(h^{3/2})$ eigenvalues of $\Delta^{(p)}_{f,h}$ is the number $m_p(\Omega)$ of critical points with index $p \to$ analytic approach to Morse inequalities. Continued in particular by Bismut and other collaborators for more general invariants (cf book by W. Zhang 01).

Result proved by Helffer–Sjöstrand in 85. The $\mathcal{O}(h^{3/2})$ eigenvalues are actually exponentially small.

After the works of Bovier–Eckhoff-Gayrard–Klein (04,04) using Freidlin-Wentzell and potential theory (capacities), accurate values of the exponentially small eigenvalues of $\Delta^{(0)}_{f,h}$ where given in Helffer–Klein–N. (04). Idea: Think of the eigenvalues of $\Delta^{(0)}_{f,h}\big|_{F_h} = d^*_{f,h}d_{f,h}\big|_{F^h}$ as the squared singular values of $d_{f,h}\big|_{F^h}$ (see also Bismut–Zhang 94) , then Gaussian elimination (Le Peutrec 09) summarizes former tricky inductions.

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Boundary Witten Laplacians

$\overline{\Omega}$ compact, f Morse, $f\big|_{\partial\Omega}$ Morse, $\|\nabla f\|$ does not vanish on $\partial\Omega$

In 95 Chang and Liu, proved that the number of $\mathcal{O}(h^{6/5})$-eigenvalues of Dirichlet or Neumann Witten Laplacians was equal to the number of generalized critical points.

$$D(\Delta_{f,h}^{N}) = \left\{\omega \in \bigwedge W^{2,2}(\Omega)\,, \quad \mathbf{n}\omega = 0\,,\, \mathbf{n}d_{f,h}\omega = 0\right\}\,.$$

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Idea: generalized saddle points Neumann (resp. Dirichlet) means $f = +\infty$(resp $f = -\infty$) outside $\overline{\Omega}$.

Helffer-N. (06) computes accurately the exp. small eigenvalues of $\Delta_{f,h}^{D,(0)}$. Le Peutrec (10) did it for $\Delta_{f,h}^{N,(0)}$.

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Morse function ?

In the QSD problem we want to study the tunnel effect between the global minimum of f and the boundary $\partial\Omega$. The expected results

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Idea: Formulate all the assumptions in terms of restricted Witten Laplacians.

Framework

$\Omega_- \subset\subset \Omega_+(=\Omega)$. $\nabla f \neq 0$ in $\overline{\Omega_+} \setminus \Omega_-$, $\partial_n f\big|_{\Omega_\pm} > 0$.

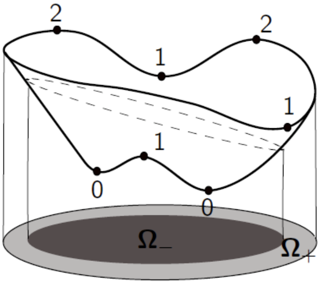

Figure: A typical $2D$ Morse example. The indices of the generalized critical points are labelled. .

Assumptions

There exist a constant $c_0 > 0$ and a function $\nu : (0, h_0) \to (0, +\infty)$ with

$$\forall \varepsilon > 0\,, \exists C_\varepsilon > 1, \quad \frac{1}{C_\varepsilon} e^{-\frac{\varepsilon}{h}} \leq \nu(h) \leq h,$$

and such that the following hypotheses are fulfilled.

Hyp 1 For $p = 0, 1$,

$$\# \left[\sigma(\Delta_{f,h}^{N,(p)}(\Omega_-)) \cap [0, \nu(h)]\right] = m_p^N(\Omega_-)$$
$$\left[\sigma(\Delta_{f,h}^{N,(p)}(\Omega_-)) \cap [0, \nu(h)]\right] \subset \left[0, e^{-\frac{c_0}{h}}\right]$$

with $m_p^N(\Omega_-)$ independent of h. In a neighborhood $\mathcal{V}_-$ of $\partial\Omega_-$ and for $\lambda(h) \in \sigma(\Delta_{f,h}^{N,(p)}(\Omega_-)) \cap (0, \nu(h)]$, the corresponding eigenvector satisfies

$$\|\psi(h)\|_{L^2(\mathcal{V}_-)} = \tilde{\mathcal{O}}(\sqrt{\lambda(h)})\,.$$

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$$\left[\sigma(\Delta_{f,h}^{N,(p)}(\Omega_-)) \cap [0, \nu(h)]\right] \subset \left[0, e^{-\frac{c_0}{h}}\right]$$

with $m_p^N(\Omega_-)$ independent of h. In a neighborhood $\mathcal{V}_-$ of $\partial\Omega_-$ and for $\lambda(h) \in \sigma(\Delta_{f,h}^{N,(p)}(\Omega_-)) \cap (0, \nu(h)]$, the corresponding eigenvector satisfies

$$\|\psi(h)\|_{L^2(\mathcal{V}_-)} = \tilde{\mathcal{O}}(\sqrt{\lambda(h)})\,.$$

Assumptions cont'

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Hyp 2

$$\sharp\left[\sigma(\Delta_{f,h}^{D,(1)}(\Omega_+\setminus\overline{\Omega_-}))\cap[0,\nu(h)]\right]=m_1^D(\Omega_+\setminus\overline{\Omega_-})\,,$$

$$\left[\sigma(\Delta_{f,h}^{D,(1)}(\Omega_+\setminus\overline{\Omega_-}))\cap[0,\nu(h)]\right]\subset\left[0,e^{-\frac{c_0}{h}}\right]\;,$$

with $m_1^D(\Omega_+\setminus\overline{\Omega_-})$ independent of $h\in(0,h_0)$.

Hyp 3

$$\{x\in\Omega_-\,,\partial f(x)=0\}\subset\left\{x\in\Omega_-,\ f(x)<\min_{\partial\Omega_+}f-c_0\right\}\,.$$

Notation

$$\kappa_f=\min_{\partial\Omega_+}f-\min_{\Omega_+}f\,.$$

Assumptions cont'

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Theorem 1

For $p=0,1$

$$m_0^D(\Omega_+) := \sharp\left[\sigma(\Delta_{f,h}^{D,(0)}(\Omega_+)) \cap [0,\nu(h)]\right] = m_0^N(\Omega_-)\,,$$

$$m_1^D(\Omega_+) := \sharp\left[\sigma(\Delta_{f,h}^{D,(1)}(\Omega_+)) \cap [0,\nu(h)]\right] = m_1^N(\Omega_-) + m_1^D(\Omega_+ \setminus \overline{\Omega_-})\,,$$

$$\sigma(\Delta_{f,h}^{D,(p)}(\Omega_+)) \cap [0,\nu(h)] \subset [0, e^{-\frac{c}{h}}]\,.$$

If $(u_k^{(1)})_{1\leq k\leq m_1^D(\Omega_+\setminus\overline{\Omega_+})}$ is an orthonormal system of the spectral subspace $\mathrm{Ran}1_{[0,\nu(h)]}(\Delta_{f,h}^{D,(1)}(\Omega_+ \setminus \overline{\Omega_-}))$, then

$$\lambda_1^{(0)}(\Omega_+) = \frac{h^2 \sum_{k=1}^{m_1^D(\Omega_+\setminus\overline{\Omega_-})} \left|\int_{\partial\Omega_+} e^{-\frac{f}{h}} \mathbf{i}_{n_\sigma} u_k^{(1)}\, d\sigma\right|^2}{\int_{\Omega_+} e^{-\frac{2f(x)}{h}}\, dx}(1+\mathcal{O}(e^{-\frac{c}{h}}))$$

$$= \tilde{O}(e^{-\frac{2\kappa_f}{h}})\,.$$

Theorem 1

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For $p = 0, 1$

$$m_0^D(\Omega_+) := \sharp\left[\sigma(\Delta_{f,h}^{D,(0)}(\Omega_+)) \cap [0,\nu(h)]\right] = m_0^N(\Omega_-)\,,$$

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If $(u_k^{(1)})_{1\leq k\leq m_1^D(\Omega_+\setminus\overline{\Omega_+})}$ is an orthonormal system of the spectral subspace $\mathrm{Ran}1_{[0,\nu(h)]}(\Delta_{f,h}^{D,(1)}(\Omega_+ \setminus \overline{\Omega_-}))$, then

$$\begin{aligned}\lambda_1^{(0)}(\Omega_+) &= \frac{h^2 \sum_{k=1}^{m_1^D(\Omega_+\setminus\overline{\Omega_-})} \left|\int_{\partial\Omega_+} e^{-\frac{f}{h}} \mathbf{i}_{n_\sigma} u_k^{(1)}\ d\sigma\right|^2}{\int_{\Omega_+} e^{-\frac{2f(x)}{h}}\ dx}(1+\mathcal{O}(e^{-\frac{c}{h}})) \\ &= \tilde{O}(e^{-\frac{2\kappa_f}{h}})\,.\end{aligned}$$

Theorem 1 cont'

The non negative normalized eigenfunction $u_1^{(0)}$ satisfies

$$\left\| u_1^{(0)} - \frac{e^{\frac{-f}{h}}}{\left(\int_{\Omega_+} e^{-\frac{2f(x)}{h}}\,dx\right)^{1/2}} \right\|_{W^{1.2}(\Omega_+)} = \mathcal{O}(e^{-\frac{c}{h}})\,,$$

$$\left\| d_{f,h}u_1^{(0)} + \sum_{k=1}^{m_1^D(\Omega_+\setminus\overline{\Omega_-})} \frac{h\int_{\partial\Omega_+} e^{-\frac{f(\sigma)}{h}}\,\mathbf{i}_{n_\sigma}\overline{u_k^{(1)}}\,d\sigma}{\left(\int_{\Omega_+} e^{-\frac{2f(x)}{h}}\,dx\right)^{1/2}} u_k^1 \right\|_{\bigwedge^1 W^{n,2}(\mathcal{V})} = \mathcal{O}(e^{-\frac{\kappa_f+c_{\mathcal{V}}}{h}})\,,$$

where $\mathcal{V}$ is any neighborhood of $\partial\Omega_+$ lying in $\Omega_+\setminus\overline{\Omega_-}$ and $c_{\mathcal{V}}>0$ does not depend on (n,h).

Changing f

Corollary

Let f_1 and f_2 satisfy Hyp 1,2,3 and $f_1 = f_2$ in $\Omega_+ \setminus \overline{\Omega_-}$, then

$$\frac{\lambda_1^{(0)}(f_2)}{\lambda_1^{(0)}(f_1)} = \frac{\int_{\Omega_+} e^{-2\frac{f_1(x)}{h}}\,dx}{\int_{\Omega_+} e^{-2\frac{f_2(x)}{h}}\,dx}(1+\mathcal{O}(e^{-\frac{c}{h}}))\,,$$

$$\frac{\partial_n\left[e^{-\frac{f_2}{h}}u_1^{(0)}(f_2)\right]\Big|_{\partial\Omega_+}}{\|\partial_n\left[e^{-\frac{f_2}{h}}u_1^{(0)}(f_2)\right]\|_{L^1(\partial\Omega_+)}} = \frac{\partial_n\left[e^{-\frac{f_1}{h}}u_1^{(0)}(f_1)\right]\Big|_{\partial\Omega_+}}{\|\partial_n\left[e^{-\frac{f_1}{h}}u_1^{(0)}(f_1)\right]\|_{L^1(\partial\Omega_+)}} + \mathcal{O}(e^{-\frac{c}{h}}) \quad \text{in } L^1(\partial\Omega_+)\,.$$

Theorem 2

Assume Hyp 1,2,3 and that $f\big|_{\partial\Omega_+}$ is a Morse function. Then

$$\lambda_1^{(0)}(\Omega_+) = \frac{\int_{\partial\Omega_+} 2\partial_n f(\sigma) e^{-2\frac{f(\sigma)}{h}}\, d\sigma}{\int_{\Omega_+} e^{-2\frac{f(x)}{h}}\, dx} \times (1 + \mathcal{O}(h))$$

$$-\frac{\partial_n \left[e^{-\frac{f}{h}} u_1^{(0)}\right]\Big|_{\partial\Omega_+}}{\left\|\partial_n \left[e^{-\frac{f}{h}} u_1^{(0)}\right]\right\|_{L^1(\partial\Omega_+)}} = \frac{(2\partial_n f) e^{-\frac{2f}{h}}\Big|_{\partial\Omega_+}}{\left\|(2\partial_n f) e^{-\frac{2f}{h}}\right\|_{L^1(\partial\Omega_+)}} + \mathcal{O}(h) \quad \text{in } L^1(\partial\Omega_+, d\sigma)\,.$$

A non-Morse potential

An example with one degenerate minimum and no saddle points.

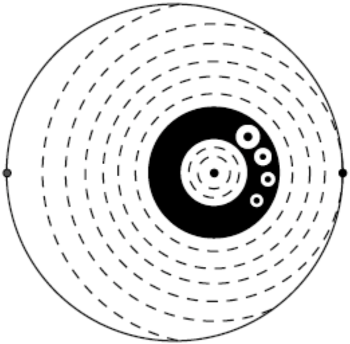

Figure: An example with $\sharp S = 2$.

In this example when Ω_- is a disk, concentric with Ω_+ ,
$m_0^N(\Omega_-) = 1$, $m_2^N(\Omega_-) = 5$ and .

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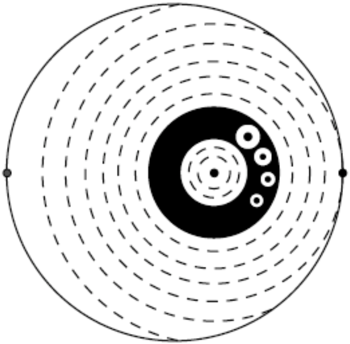

Figure: An example with $\sharp S = 2$.

In this example when Ω_- is a disk, concentric with Ω_+ , $m_0^N(\Omega_-) = 1$, $m_2^N(\Omega_-) = 5$ and $m_1^N(\Omega_-) = 5$.