A quasi-stationary approach to the narrow escape problem

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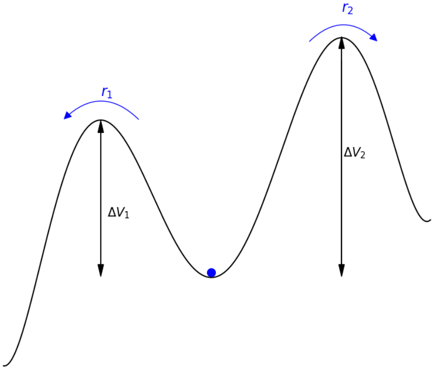
PhD under the supervision of Tony Lelièvre, Urbain Vaes & Gabriel Stoltz

Metastability of **energetic** origin



Thermal particle living in a potential well:

- Slow dynamics between the wells
- Long time to escape. This is a **rare event**

Toy model: Langevin particle in a double-well (φ^4) potential .

How much time does it take to **escape** the well?

Answer known since the 1930s:

Eyring-Kramers' formula*

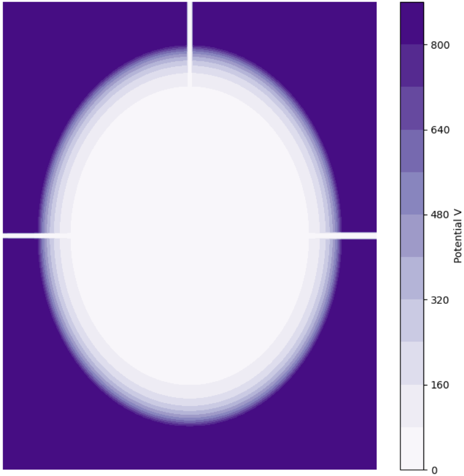
The escape time is exponentially distributed, with a rate r_i, with $i \in \{1, 2\}$:

$$r_i = C_i \exp\left(-\frac{\Delta V_i}{k_{\mathrm{B}} T}\right),$$

ΔV_i the height of the barrier, k_{B} the Boltzmann constant, T the temperature, C_i a constant.

* Also Arrhenius, Polanyi or Van't Hoff law.

What if energy is not the driving factor?



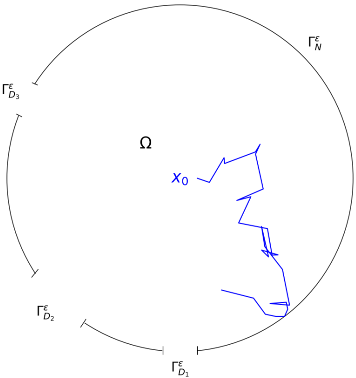
A potential made a confining well and a few **narrow canals**:

Still a long time to escape.
This is still a **rare event**

Is there an equivalent to the Eyring Kramers formula in this case?

The narrow escape problem [1]

Toy model of the metastability of entropic origin:



Setting:

- Domain Ω with holes $\Gamma_{D_i}^\varepsilon$ and reflecting boundary Γ_N^ε
- A Brownian motion starting at x_0 taking a long time to exit $\tau_\varepsilon = \inf\{t \geq 0 \,|\, X_t \notin \overline{\Omega}\}$

Goal: In the limit of small holes $\varepsilon \to 0$:

- Distribution of the escape time τ_ε
- The exit hole distribution X_{τ_ε}

[1] Introduced by Holcman and Schuss (2004), then large numbers of contributors: Ammari, Bénichou, Chen, Chevalier, Cheviakov, Friedman, Grebenkov, Singer, Straube, Voituriez, Ward...

Quasi-stationary distribution (QSD)

Definition

$$\text{If } X_0 \sim \nu_\varepsilon, \ \text{ then } \forall t > 0, \mathbb{P}(X_t \mid t < \tau_\varepsilon) = \nu_\varepsilon$$

The quasi-stationary distribution is the distribution of X_t that is stationary by the dynamics conditionned on the fact that the Brownian motion has not escaped yet.

Why is it natural?

- Counterpart of the stationary distribution for metastable systems

Why is it useful here?

- If $X_0 \sim \nu_\varepsilon$,

$$\tau_\varepsilon \sim \mathrm{Exp}(\lambda_\varepsilon) \text{ independent of } X_{\tau_\varepsilon}$$

$$X_{\tau_\varepsilon} \sim \int \partial_n \nu_\varepsilon$$

- Markov jump process [2]

[2] Di Gesù, Lelièvre, Le Peutrec and Nectoux, *Faraday Discussion*, (2016)

Yaglom's limit

$$\text{If } X_0 \in \Omega, \quad \text{then} \quad \lim_{t \to +\infty} \mathbb{P}(X_t \,|\, t < \tau_\varepsilon) = \nu_\varepsilon$$

The quasi-stationary distribution is attained after a large time of simulation.

Consider the adjoint generator (Fokker-Planck) $\mathcal{L}_\varepsilon^*$ of the process:
Then the stationary distribution s is given by $\mathcal{L}^* s = 0 = 0\, s$.
The QSD ν_ε is given by the eigenvector with the smallest eigenvalue: $-\mathcal{L}_\varepsilon^* \nu_\varepsilon = \lambda_\varepsilon \, \nu_\varepsilon$.
Qualitative idea: Consider the eigen-decomposition of $\mathcal{L}_\varepsilon^*$ (it exists as $\mathcal{L}_\varepsilon$ is self-adjoint and has a compact resolvant), then

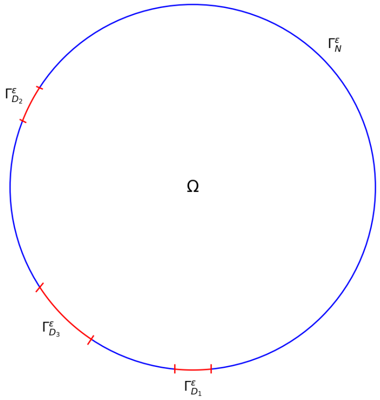
$$\rho(t) = \sum_k \langle \rho(0),\, u_\varepsilon^k \rangle \mathrm{e}^{-\lambda_\varepsilon^k t} u_\varepsilon^k ,$$

At large time, the dominant term is the one with the smallest eigenvalue, which is identified to the QSD by Yaglom's limit.

The QSD as an eigenvalue problem

We want to find the QSD ν_ε

$$\begin{cases} -\Delta \nu_\varepsilon = \lambda_\varepsilon \nu_\varepsilon & \text{in } \Omega_\varepsilon \\ \partial_n \nu_\varepsilon = 0 & \text{on } \Gamma_N^\varepsilon \\ \nu_\varepsilon = 0 & \text{on } \Gamma_{D_i}^\varepsilon \end{cases}$$



But thanks to [3]:

Flat angle between Γ_N^ε and $\Gamma_{D_i}^\varepsilon$: $\partial_n \nu_\varepsilon \notin L^2(\partial\Omega)$

90° angle between Γ_N^ε and $\widetilde{\Gamma}_{D_i}^\varepsilon$: $\partial_n \nu_\varepsilon \in L^2(\partial\Omega)$

We need to be able to integrate to get the exit hole distribution X_τ .

[3] Jakab, Mitrea and Mitrea, *Indiana University Mathematics Journal*, (2009)

Why modifying the domain?

We want to find the QSD ν_ε

$$\begin{cases} -\Delta \nu_\varepsilon = \lambda_\varepsilon \nu_\varepsilon & \text{in } \Omega_\varepsilon \\ \partial_n \nu_\varepsilon = 0 & \text{on } \Gamma_N^\varepsilon \\ \nu_\varepsilon = 0 & \text{on } \Gamma_{D_i}^\varepsilon \end{cases}$$

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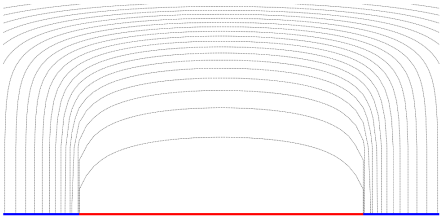
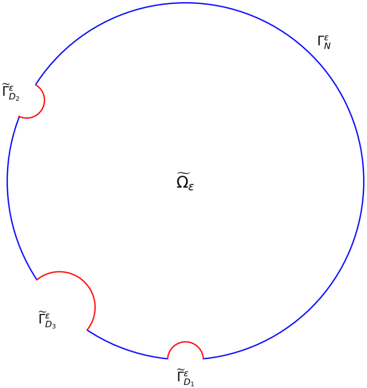


Figure: Level curves of the solution ν_ε near a flat hole.

[3] Jakab, Mitrea and Mitrea, *Indiana University Mathematics Journal*, (2009)

A more regular narrow escape problem



Similar eigenvalue problem:

$$\begin{cases} -\Delta \nu_\varepsilon = \lambda_\varepsilon \nu_\varepsilon & \text{in } \widetilde{\Omega}_\varepsilon \\ \partial_n \nu_\varepsilon = 0 & \text{on } \Gamma_N^\varepsilon \\ \nu_\varepsilon = 0 & \text{on } \widetilde{\Gamma}_{D_i}^\varepsilon \end{cases}$$

Previous work: Asymptotic expansion for the disk and the ball [4]

My PhD work: Asymptotic expansion for general domains in $N \geq 2$ dimensions

[4] Lelièvre, Rachid and Stoltz, *preprint* (2024)

What does the quasi-stationary distribution look like?

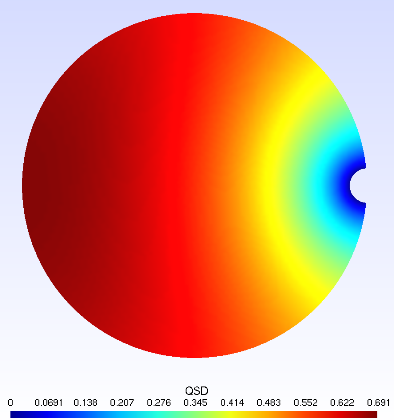


Figure: Dimension 2: Circle

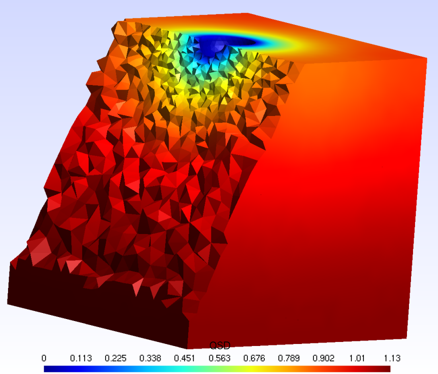
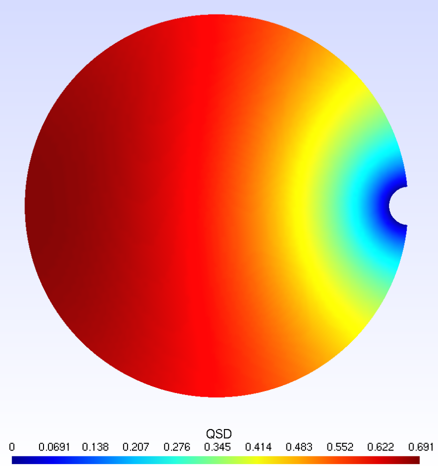


Figure: Dimension 3: Cube

How to build the quasimode?

From the experiments, ν_ε is almost constant far from the holes:



We can approximate the solution ν_ε by a quasimode (semi-classic technique):

$$\varphi_\varepsilon = 1 + K_\varepsilon f$$

with K_ε the approximation of the eigenvalue and f the solution when the hole is a point:

$$\begin{cases} -\Delta f = 1 & \text{in } \Omega \\ \partial_n f = 0 & \text{on } \partial\Omega \setminus \{x^{(h)}\} \end{cases}$$

with $x^{(h)}$ the center of the hole.

Point charge at the boundary

From the compatibility condition:

$$\int_\Omega \Delta f = \oint_{\partial\Omega} \partial_n f$$

The distribution f satisfies:

$$\begin{cases} -\Delta f = 1 & \text{in } \Omega \\ \partial_n f = -|\Omega|\delta_{x^{(h)}} & \text{on } \partial\Omega \end{cases} \tag{1}$$

$\Rightarrow$ Neumann's Green function with the singularity pushed to the boundary .
The Narrow escape problem has been related to f before in the literature. [1, 5]

[5] Silbergleit, Mandel and Nemenman (link with electrostatic)

Key idea:

- We know the solution to (1) on the half plane $\mathbb{R}^+ \times \mathbb{R}^{n-1}$:

$$f_{\text{halfplane}}(x) = \frac{1}{\left|x - x^{(h)}\right|^{n-2}} + S(x),$$

with S a smooth function such that $-\Delta S = 1$.

- Consider the change of variable $\Psi \colon \Omega \cap B(x^{(h)}, \delta) \to \mathbb{R}^+ \times \mathbb{R}^{n-1}$ that flattens locally the domain. Then by Taylor expansion of Ψ :

$$f(x) \sim f_{\text{halfplane}} \circ \Psi(x) \propto \frac{1}{\left|x - x^{(h)}\right|^{n-2}} \left(1 + O\left(\left|x - x^{(h)}\right|\right)\right)$$

The quasimode is a good approximation of the QSD

This reasoning can be extended to N holes of radius ε_i, taking:

$$\varphi_\varepsilon = 1 + \sum_{i=1}^{N} K_\varepsilon^i f_i, \qquad \text{and } \overline{K_\varepsilon} = \sum_{i=1}^{N} K_\varepsilon^i$$

Theorem (here for $n > 3$ for simplicity)

The quasimode φ_ε verifies:

$$\begin{cases} -\Delta\varphi_\varepsilon = \overline{K_\varepsilon} = \overline{K_\varepsilon}\varphi_\varepsilon + O\left(\overline{K_\varepsilon}^2 \|f_i\|_{\infty,i,\widetilde{\Omega}_\varepsilon}\right) & \text{in } \widetilde{\Omega}_\varepsilon \\ \partial_n \varphi_\varepsilon = 0 & \text{on } \Gamma_N^\varepsilon \\ \varphi_\varepsilon = O\left(\left(K_\varepsilon^i\right)^{\frac{1}{n-2}}\right) & \text{on } \widetilde{\Gamma}_{D_i}^\varepsilon \end{cases}$$

'

Theorem

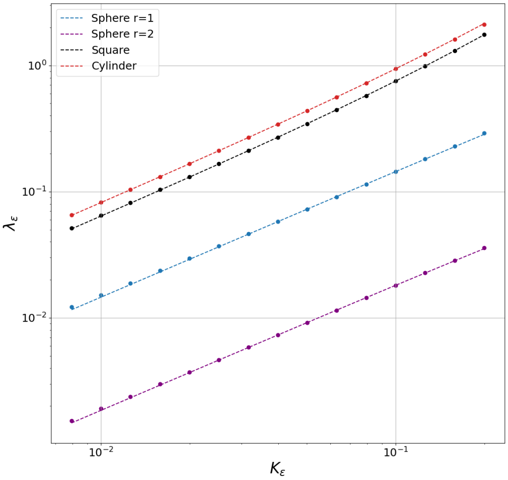
Let

$$K_\varepsilon^i = \begin{cases} \varepsilon_i^{n-2}, & \text{for } n \geq 3 \\ -(\log \varepsilon_i)^{-1}, & \text{for } n = 2 \end{cases}$$

Then there exists a $C_n > 0$ such that the eigenvalue λ_ε scales as:

$$\lambda_\varepsilon = \left(\mathbb{E}[\tau_\varepsilon]\right)^{-1} = C_n \overline{K_\varepsilon} + \begin{cases} O(\overline{K_\varepsilon}^{\frac{n-1}{n-2}}) & \text{for } n > 3 \\ O(\overline{K_\varepsilon}^2 \log(\overline{K_\varepsilon})), & \text{for } n = 3 \\ O(\overline{K_\varepsilon}^2), & \text{for } n = 2 \end{cases}$$

The error for $n > 3$ does not worsen with n , $K_\varepsilon^{\frac{n-1}{n-2}} = \varepsilon^{n-1}$

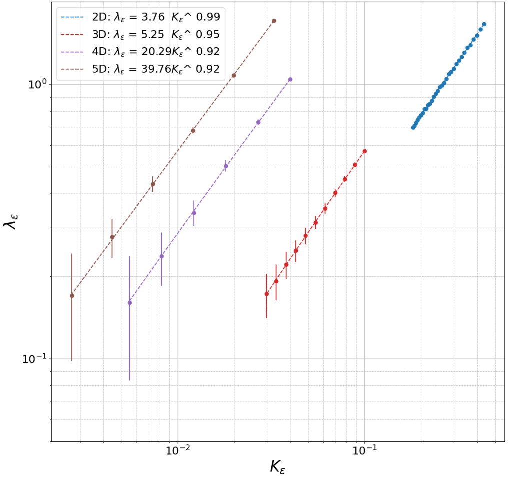


The constant C_n is given by the singularity expansion of f:

$$C_n = \frac{\max\{n-2, 1\}}{2} \frac{|\mathscr{C}(0,1)|}{|\Omega|}$$

In **dimension** 3 we find for the simple shapes through FEM:

Shape	C_3	C_3 (simu)
Sphere radius 1	1.500	1.46 ± 0.02
Sphere radius 2	0.187	0.18 ± 0.01
Cube	6.282	6.28 ± 0.02
Cylinder	8.000	8.06 ± 0.01



- Monte Carlo simulation of the exit time τ_ε for a unit ball in dimension $\{2, 3, 4, 5\}$
- It's a rare event so very long simulations...
- Correct scaling in K_ε, but:

Dimension	C_n^{ball}	C_n^{ball} (simu)
2	2	3 ± 1
3	4.5	5 ± 3
4	16	20 ± 2
5	32.5	39 ± 3

Importance of the initial condition

The previous simulations where done with the inital condition as $X_0 \sim \delta_0 \neq \nu_\varepsilon$.
Fleming–Viot algorithm $\rightarrow$ estimate the QSD on the flight using the Yaglom limit

Test: the unit sphere in dimension 3:

Initialisation	ν_ε	δ_0	$\nu_\varepsilon^{\mathrm{FV}}$
C_n	4	5 ± 3	3.7 ± 0.6
$K_\varepsilon^?$	1	0.95 ± 0.08	1.0 ± 0.1

Results on the exit hole distribution

With the same method, we can also compute the exit hole distribution:

Theorem

The exit hole distribution scales as:

$$P(X_\tau \in \Gamma_{D_i}) = \frac{K_\varepsilon^i}{K_\varepsilon} + \begin{cases} O(\varepsilon_i) & \text{for } n > 3 \\ O(K_\varepsilon^i \log(K_\varepsilon^i)), & \text{for } n = 3 \\ O(K_\varepsilon^i), & \text{for } n = 2 \end{cases}$$

Numerical results on the exit hole distribution

Obtained through Monte-Carlo simulations, average over 10^4 simulations and several values of ε:

Unit sphere in dimension 3

- 2 holes of radius $\varepsilon_1 = \varepsilon_2/2$.
- By the theorem $\mathbb{P}(X_\tau \in \Gamma_{D_2}) = \frac{2}{3} + O(\varepsilon)$

$\Rightarrow \mathbb{P}(X_\tau \in \Gamma_{D_2})|_{\mathrm{simu}} = 0.665 \pm 0.001$

Unit sphere in dimension 4

- 4 holes of radius ε, $0.7\,\varepsilon$, $0.8\,\varepsilon$, $0.9\,\varepsilon$.
- By the theorem $\mathbb{P}(X_\tau \in \Gamma_{D_2}) = \frac{2}{3} + O(\varepsilon^2)$

Hole	Theorem	Monte-Carlo
1	0.284	0.33 ± 0.02
2	0.205	0.17 ± 0.02
3	0.235	0.22 ± 0.02
4	0.264	0.27 ± 0.02

Conclusion

- The QSD is a useful tool to study the narrow escape problem
- With this approach we can solve it for any (locally smooth) smooth domain in any dimension
- We get the scaling of the escape time and the exit hole distribution

Future work: How does the shape of the hole influence the escape time? $\rightarrow$ the slit

The slit