Entropic metastability in the narrow escape problem

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

In collaboration with:

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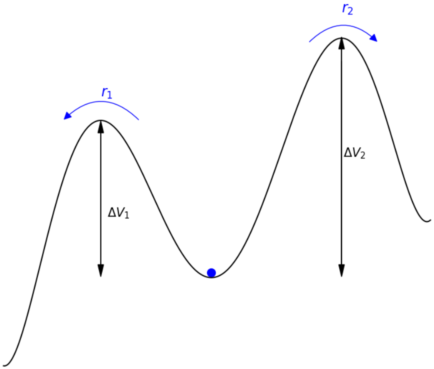
Metastability of **energetic** origin



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 potential

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

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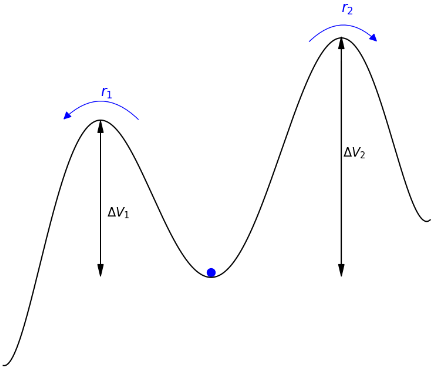

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Eyring-Kramers' formula

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

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

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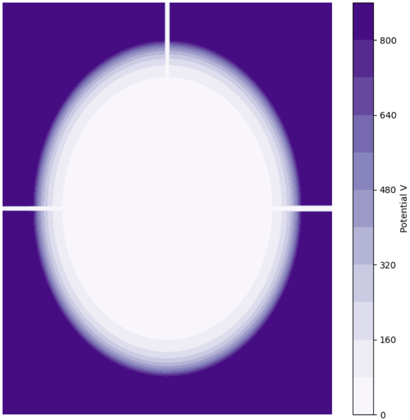
What if energy is not the driving factor?



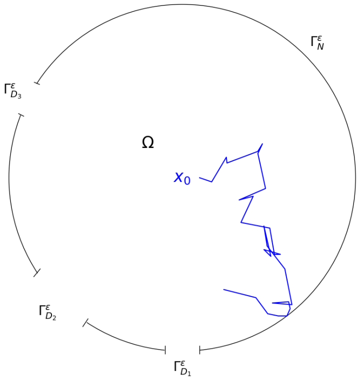
A potential made of a confining well and a few **narrow canals**:

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

Toy model of the metastability of entropic origin:



Setting:

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

$$\mathrm{d}X_t = \sqrt{2}\,\mathrm{d}B_t - \mathbb{1}_{\Gamma_{\mathrm{D}}^\varepsilon}(X_t)n(X_t)\mathrm{d}L_t.$$

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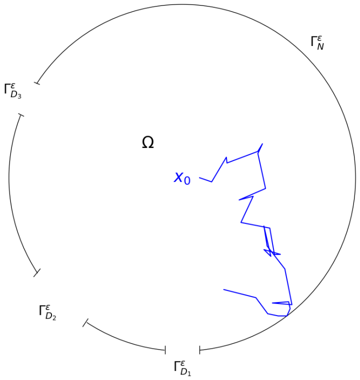

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Goal: In the limit of small holes $\varepsilon \to 0$:

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

A spectral approach to solve the narrow escape problem

Let $\rho(x, t)$be the density of probability to be at y at time $t < \tau_\varepsilon$ starting from ρ_0 then it verifies the Fokker-Plank equation:

$$\begin{cases} \partial_t \rho = \Delta \rho & \text{in } \Omega \\ \partial_n \rho = 0 & \text{on } \Gamma_N^\varepsilon \\ \rho = 0 & \text{on } \Gamma_D^\varepsilon \\ \rho(\cdot, 0) = \rho_0 & \text{in } \Omega \end{cases} \quad (1)$$

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The operator $\mathcal{L}_\varepsilon$ associated to (1) is self-adjoint with compact resolvent

→ there exists an orthonormal basis in $H^1(\Omega)$ of eigenfunctions $(u_\varepsilon^k)_{k\geq 0}$ and eigenvalues $(\lambda_\varepsilon^k)_{k\geq 0}$ ranked in increasing order $\lambda_\varepsilon^0 < \lambda_\varepsilon^1 < \dots$

$$\rho(x,t) = \sum_{k\geq 0} \langle \rho_0,\, u_\varepsilon^k \rangle \mathrm{e}^{-\lambda_\varepsilon^k t} u_\varepsilon^k(x)$$

Large time behaviour

If the eigengap $\lambda_\varepsilon^1 - \lambda_\varepsilon^0$ is large, then the large time behaviour of $\rho(x, t)$ is dominated by the first eigenmode

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From the probability, we deduce the behaviour of quantities of interest:

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- The law of the exit hole will be dictated by u_ε^0
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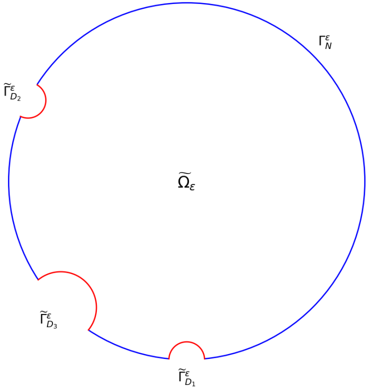
$\Rightarrow$ Rigorous approach: the quasi-stationary distribution [1]

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

The narrow escape problem as an eigen problem



We want to find the eigencouple $(\lambda_\varepsilon^0, u_\varepsilon^0)$ solution of:

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

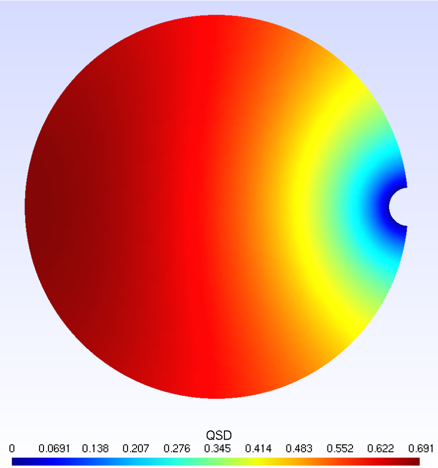
Previous work: Asymptotic scaling for the disk and the ball [1]

My PhD work: Asymptotic scaling for general domains in $d \geq 2$ dimensions

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

How to build the quasimode (1 hole)?

From the simulations, u_ε^0 is almost constant far from the hole:



We can approximate the solution u_ε^0 by a quasimode (semi-classical technique):

$$u_0^\varepsilon \simeq \varphi_\varepsilon = 1 + K_\varepsilon f$$

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

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

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

Theorem [Asymptotic of the exit time]

Consider N identical holes of radius r_ε. Then there exists a $C_{d,\Omega} > 0$ such that the eigenvalue λ_ε^0 scales as:

$$\lambda_\varepsilon^0 = \left(\mathbb{E}[\tau_\varepsilon]\right)^{-1} = \begin{cases} C_{d,\Omega}\, N\, r_\varepsilon^{d-2} & + \mathrm{O}(r_\varepsilon^{d-1}), & \text{for } d > 3 \\ C_{3,\Omega}\, N\, r_\varepsilon & + \mathrm{O}({r_\varepsilon}^2 \log(r_\varepsilon)), & \text{for } d = 3 \\ C_{2,\Omega}\, N\, (\log(r_\varepsilon))^{-1} & + \mathrm{O}\left([\log(r_\varepsilon)]^{-2}\right), & \text{for } d = 2 \end{cases}$$

Where does the scaling comes from?

The fundamental solution of the laplacian Λ in dimension d:

$$\lambda_\varepsilon^0 \sim C_{d,\Omega}\Lambda(r_\varepsilon)^{-1} \qquad \text{and} \qquad C_{d,\Omega} = \frac{\max\{d-2,\, 1\}}{2} \frac{|\mathscr{C}(0,1)|}{|\Omega|}$$

Exit time for N exit holes and $d \geq 2$

Theorem [Exit hole distribution]

The probability to exit through hole $i \in \{1, \dots, N\}$is given by:

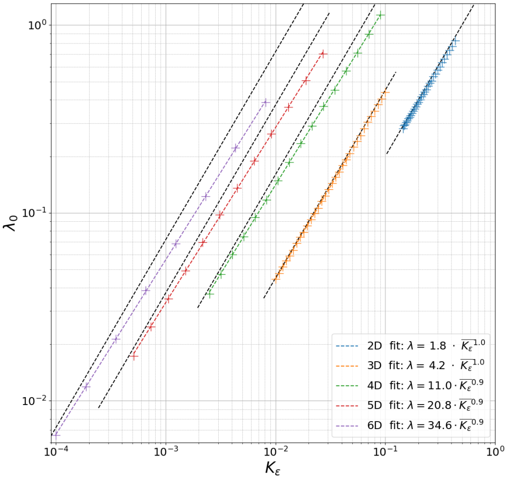
$$\mathbb{P}_\varepsilon(X_\tau \in \Gamma^\varepsilon_{D_i}) = \frac{\lambda^\varepsilon_{(0,i)}}{\lambda^\varepsilon_0}$$

where $\lambda^\varepsilon_{(0,i)}$is the eigenvalue of the problem where there is only the hole i.

In dimension 2, the eigenvalues scales as a logarithmic function of the radius. with 2 holes

- Even if one hole is **twice bigger** than the other:

$$r^{(1)}_\varepsilon = 2r^{(2)}_\varepsilon \Rightarrow \qquad \mathbb{P}_\varepsilon(X_\tau \in \Gamma^\varepsilon_{D_1}) \approx \frac{1}{2}$$



- Monte Carlo simulation of the exit time τ_ε for a unit ball in dimension $\{2, 3, 4, 5, 6\}$
- Correct scaling in K_ε, the asymptotic regime has not yet been reached in higher dimension:

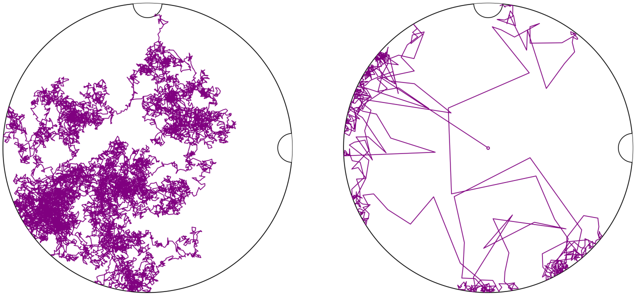
Dimension	C_d^{ball}	C_d^{ball} (simu)
2	2	1.8
3	4.5	4.2
4	16	11
5	32.5	20.8
6	72	34.6

Monte Carlo simulation of the narrow escape problem

Naive Monte-Carlo is computationally expensive

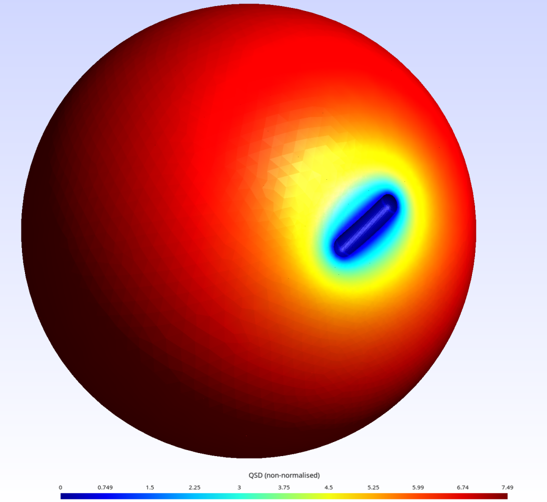
- Time step should be small compared to $(r_i^\varepsilon)^2$ for $i \in \{1, \dots, N\}$
- Mean exit time increases as $\varepsilon \to 0$

Example: in dimension 3 with $r_i^\varepsilon \propto \varepsilon$, the mean exit time scales as $\frac{1}{\varepsilon}$
$\rightsquigarrow$ Simulation cost of M exit events scales as $M\varepsilon^{-3}$



Conclusion

- The narrow escape is a toy model of metastability of entropic origin
- With our approach we can solve it for any (locally) smooth domain in any dimension
- We get the scaling of the escape time and the law of exit hole



Future work:

- Study the influence of the hole geometry on the escape event $\rightarrow$ the slit