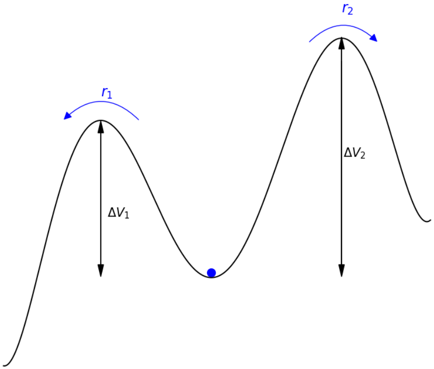
Entropic metastability in the narrow escape problem

Louis Carillo

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



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

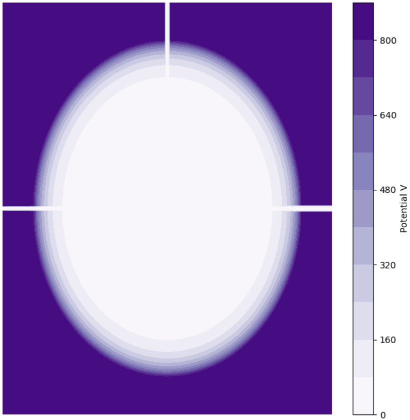
How much time does it take to **escape** the well?

Eyring-Kramers' formula

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

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

What if energy is not the driving factor?



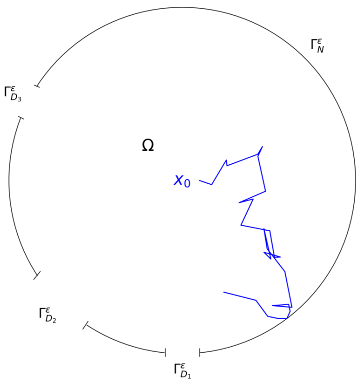
A potential made a confining well and a few **narrow canals**:

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 law of exit hole 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...

An approach to solve the narrow escape problem

Let $\rho(t,x) = \mathbb{P}_x(t < \tau_\varepsilon)$, the survival probability at time t starting from x then

$$\partial_t \rho = \Delta \rho \quad \text{in } \Omega \quad + \text{ boundary conditions}$$

With the eigen decomposition $(\lambda_k, u_k)_{k\geq 0}$ of the Laplacian Δ

$$\rho(t,x) = \sum_{k\geq 0} \langle 1,\ u_\varepsilon^k \rangle \mathrm{e}^{-\lambda_\varepsilon^k t} u_\varepsilon^k(x)$$

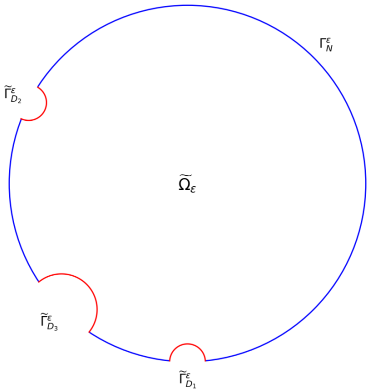
At large time, the dominant term is the one with the smallest eigenvalue λ_ε^0.

$$\mathbb{P}_x(t < \tau_\varepsilon) \approx \langle 1,\ u_\varepsilon^0 \rangle \mathrm{e}^{-\lambda_\varepsilon^0 t} u_\varepsilon^0(x)$$

Rigorous approach: the quasi-stationary distribution (QSD) [2]

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

The narrow escape problem as an eigenvalue problem



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

Eigenvalue problem with modified holes:

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

$\lambda_0^\varepsilon \Rightarrow$ exit time distribution
$u_0^\varepsilon \Rightarrow$ law of exit point

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

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

How does u_ε^0 look like?

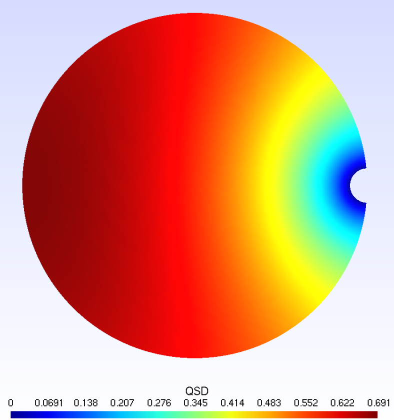


Figure: Dimension 2: Circle

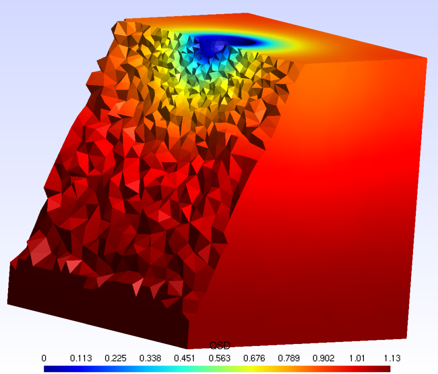
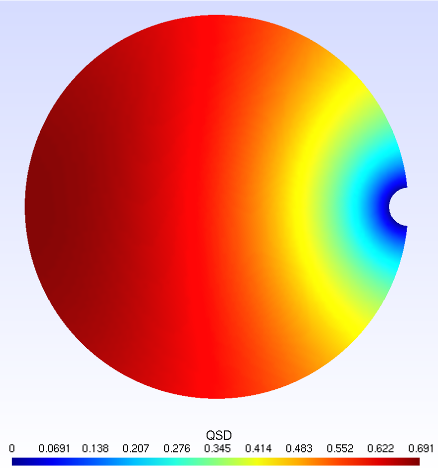


Figure: Dimension 3: Cube

From the experiments, u_ε^0 is almost constant far from the holes:



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

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

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

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

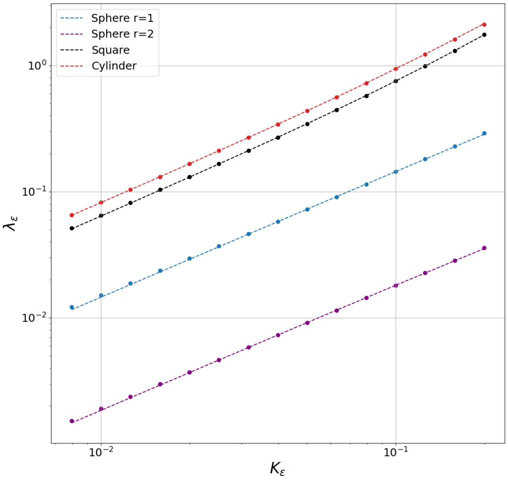
with $x^{(h)}$ the center of the hole.

Theorem [Asymptotic of the exit time]

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

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

Similar expansions are possible with multiple holes,
for instance with $r_\varepsilon = \sum_{i=1}^{N} (r_\varepsilon^{(i)})^{d-2}$ for $d \geq 3$ and N holes



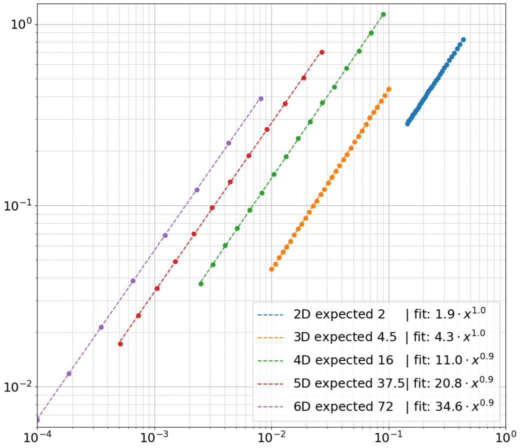
The constant $C_{d,\Omega}$ is given by:

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

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

Shape	$C_{3,\Omega}$	$C_{3,\Omega}$ (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

Measure of the exit time in higher dimension



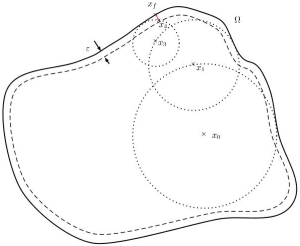
- Monte Carlo simulation of the exit time τ_ε for a unit ball in dimension $\{2, 3, 4, 5\}$
- It is a rare event so very long simulations...
- Correct scaling in K_ε, but:

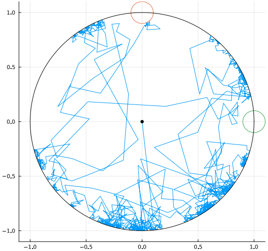
Dimension	C_d^{ball}	C_d^{ball} (simu)
2	2	1.9
3	4.5	4.3
4	16	11
5	32.5	20.8
6	72	34.6

Several reasons:

- Asymptotics requires very small $\varepsilon \approx 10^{-3}$
- Trade-off $\sqrt{\Delta t} \ll \varepsilon$ and $N_{\text{step}} \simeq \Delta t\, \varepsilon^{2-d}$

Solution: Adaptive timestep algorithm: walk-on-sphere





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 → the slit