A quasi-stationary approach to the narrow escape problem

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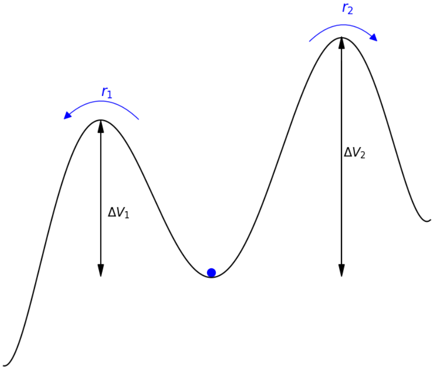
PhD under the supervision of Tony Lelièvre, Urbain Vaes & Gabriel Stoltz

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*

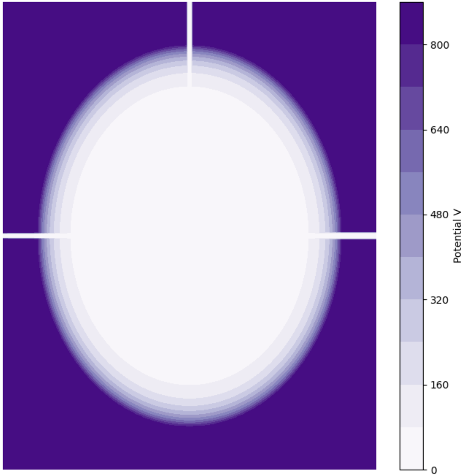
The escape time is exponentially distributed, with a rate r_i, with $i \in \{1, 2\}$:

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

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?

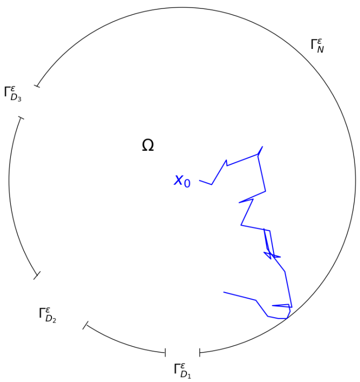


A potential made a confining well and a few **narrow canals**:

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

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

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

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

The QSD ν_ε is the distribution of X_t that is stationary by the dynamics conditionned on the fact that the Brownian motion has not escaped yet

Property: Yaglom's limit

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

The QSD is attained after a large time of simulation, in our context

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Fundamental properties of the QSD

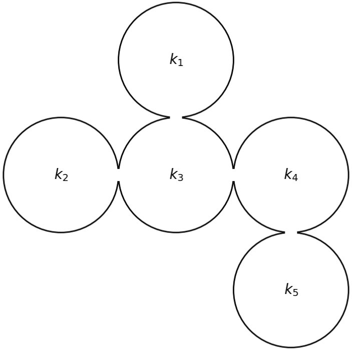
Assume that $X_0 \sim \nu_\varepsilon$. Then

- The exit time τ is *exponentially distributed* $\sim \mathrm{Exp}(\lambda_\varepsilon)$

$$\begin{aligned}\mathbb{P}_{\nu_\varepsilon}[\tau \geq s+t] &= \mathbb{P}_{\nu_\varepsilon}[\tau \geq s+t \,|\, \tau \geq s]\,\mathbb{P}_{\nu_\varepsilon}[\tau \geq s] \\ &= \mathbb{P}_{\nu_\varepsilon}[\tau \geq t]\,\mathbb{P}_{\nu_\varepsilon}[\tau \geq s].\end{aligned}$$

- The exit point X_τ is *independent* of the exit time τ

$$\begin{aligned}\mathbb{P}_{\nu_\varepsilon}[X_\tau \in A, \tau \geq t] &= \mathbb{P}_{\nu_\varepsilon}[X_\tau \in A \,|\, \tau \geq t]\,\mathbb{P}_{\nu_\varepsilon}[\tau \geq t] \\ &= \mathbb{P}_{\nu_\varepsilon}[X_\tau \in A]\,\mathbb{P}_{\nu_\varepsilon}[\tau \geq t]\end{aligned}$$



In the setting with a stationary distribution:

One can build a Markov-chain model [2],
$\rightsquigarrow$ labyrinth of simple shapes

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

Quasi-stationary distribution and Eigenvalue problems

In the setting with a stationary distribution:
Consider the adjoint generator (Fokker-Planck) $\mathcal{L}_\varepsilon^*$ of the process:
Then the stationary distribution s is given by $\mathcal{L}^* s = 0 = 0\, s$

In the metastable setting:
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

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

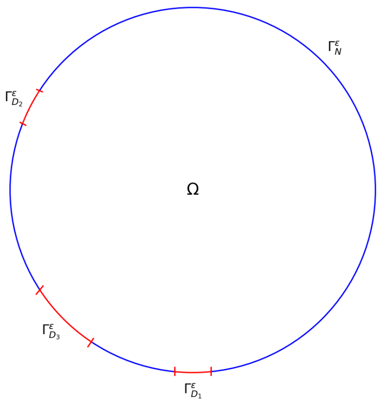
At large time, the dominant term is the one with the smallest eigenvalue, which is identified to the QSD by Yaglom's limit.

We want to find the QSD ν_ε

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

Then the narrow escape problem is solved:

- $\mathbb{E}[\tau_\varepsilon] = \lambda_\varepsilon^{-1}$, the mean exit time
- $\mathbb{P}_{\nu_\varepsilon}[X_\tau \in \Gamma_{D_i}^\varepsilon] \propto \int_{\Gamma_{D_i}^\varepsilon} \partial_n \nu_\varepsilon$, the exit hole distribution



The QSD as an eigenvalue problem

We want to find the QSD ν_ε

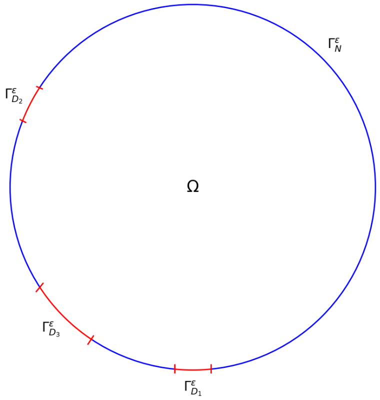
$$\begin{cases} -\Delta\nu_\varepsilon = \lambda_\varepsilon\nu_\varepsilon & \text{in } \Omega_\varepsilon \\ \partial_n\nu_\varepsilon = 0 & \text{on } \Gamma_N^\varepsilon \\ \nu_\varepsilon = 0 & \text{on } \Gamma_{D_i}^\varepsilon \end{cases}$$

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 do integration by parts 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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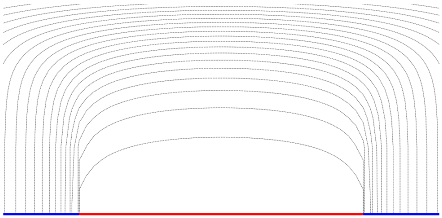
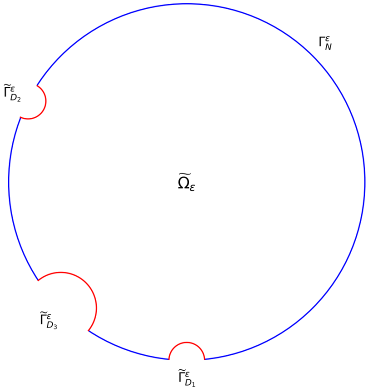


Figure: Level curves of the solution ν_ε near a flat hole.

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

A more regular narrow escape problem



Similar eigenvalue problem:

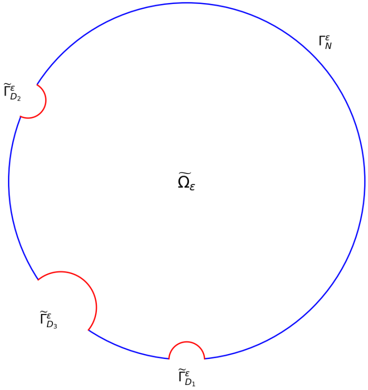
$$\begin{cases} -\Delta \nu_\varepsilon = \lambda_\varepsilon \nu_\varepsilon & \text{in } \widetilde{\Omega}_\varepsilon \\ \partial_n \nu_\varepsilon = 0 & \text{on } \Gamma_N^\varepsilon \\ \nu_\varepsilon = 0 & \text{on } \widetilde{\Gamma}_{D_i}^\varepsilon \end{cases} \tag{1}$$

N holes of radius $r_\varepsilon^{(i)}$ centered at $x^{(i)} \in \partial\Omega$

Domain $\widetilde{\Omega}_\varepsilon = \Omega \backslash \overline{\cup_{i=1}^N B(x^{(i)}, r_\varepsilon^{(i)})}$

New holes: $\widetilde{\Gamma}_{D_i}^\varepsilon = \partial B(x^{(i)}, r_\varepsilon^{(i)}) \cap \overline{\Omega}$

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 scaling for the disk and the ball [4]

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

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

What does the quasi-stationary distribution look like?

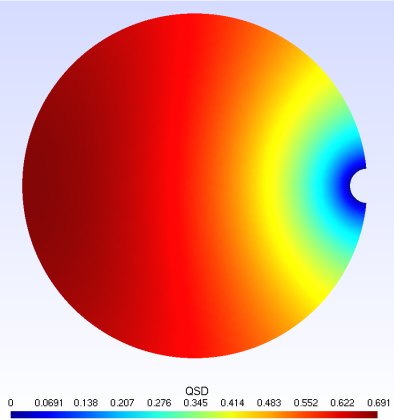


Figure: Dimension 2: Circle

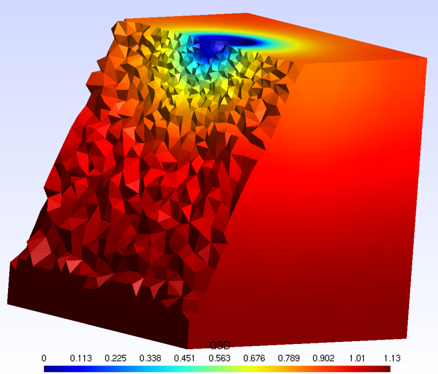


Figure: Dimension 3: Cube

Explicit solution to (1) with 1 exit hole

In (1), when $\varepsilon \to 0$, it holds $|\Gamma_{\mathrm{D}}^{\varepsilon}| \to 0$ so we expect $\lambda_\varepsilon \to 0$ and $\nu_\varepsilon \to \mathrm{cst}$. This motivates looking for a solution of the form $\nu_\varepsilon = 1 + v_\varepsilon$, with

$$\begin{cases} -\Delta v_\varepsilon = \lambda_\varepsilon + \lambda_\varepsilon v_\varepsilon & \text{on } \Omega_\varepsilon \\ \partial_n v_\varepsilon = 0 & \text{on } \Gamma_{\mathrm{N}}^{\varepsilon} \\ v_\varepsilon = -1 & \text{on } \Gamma_{\mathrm{D}}^{\varepsilon} \end{cases}$$

Taking formally the limit $\varepsilon \to 0$, we find that $v_\varepsilon/\lambda_\varepsilon$ should converge to a function f satisfying

$$\begin{cases} -\Delta f = 1 & \text{on } \Omega \\ \partial_n f = 0 & \text{on } \partial\Omega \setminus \{x_1\} \end{cases}$$

We will now try to build such f.

Observations on f

From the compatibility condition:

$$\int_{\partial\Omega} \partial_n f = \int_\Omega \Delta f = -|\Omega|$$

The distribution f formally satisfies:

$$\begin{cases} -\Delta f = 1 & \text{in } \Omega \\ \partial_n f = -|\Omega|\delta_{x^{(1)}} & \text{on } \partial\Omega \end{cases} \tag{2}$$

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

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

Construction of f for 1 exit hole

Let $\Lambda\colon \mathbb{R}^d \to \mathbb{R}$ denote the fundamental solution of the Laplacian

$$\Lambda(x) \propto \begin{cases} \log(x) & \text{if } d = 2 \\ -\frac{1}{|x|^{d-2}} & \text{if } d \geq 3 \end{cases}$$

Lemma: Construction of a quasimode

If $\partial\Omega$ is locally smooth around $\{x_1\}$, there exists $(f,\ C_{d,\Omega})$ solution to (2), such that $f : \Omega \mapsto \mathbb{R}$ is smooth on Ω and of the form $f(x) = C_{d,\Omega}^{-1}\Lambda(x - x_1) + R(x)$

The remainder term $R\colon \Omega \to \mathbb{R}$ satisfies

$$R(x) = \begin{cases} \mathrm{O}(1) & \text{if } d = 2 \\ \mathrm{O}\big(-\log|x - x_1|\big) & \text{if } d = 3 \\ \mathrm{O}\big(|x - x_1|^{-(d-3)}\big) & \text{if } d \geq 4 \end{cases}$$

Sketch of proof. Consider the change of variables

$$\Psi : \Omega \cap B(x_1, \delta) \to \mathbb{R}^+ \times \mathbb{R}^{d-1}$$

that locally flattens the boundary $\partial\Omega$ while preserving the normals and satisfies $\Psi(x_1) = 0$

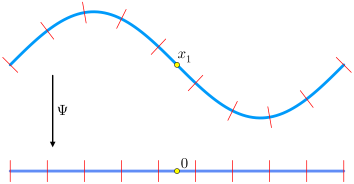


Figure: Local change of coordinates Ψ

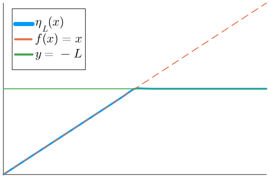


Figure: Smooth cutoff function η_L

We will take the ansatz $f = C_{d,\Omega}^{-1} \eta_L \circ \Lambda \circ \Psi + S$.

Proof of the lemma on f: step 2/3

Ansatz : $f = C_{d,\Omega}^{-1} \eta_L \circ \Lambda \circ \Psi + S$

- In the first term $\eta_L \circ \Lambda \circ \Psi(x)$ equals $\Lambda(x - x_1)$ to leading order, in a neighborhood of x_1, as $\Psi(x) = x - x_1 + O(|x - x_1|^2)$
- By substitution we look for S satisfying

$$\begin{cases} -\Delta S = 1 - C_{d,\Omega}^{-1} \Delta(\eta_L \circ \Lambda \circ \Psi) & \text{on } \Omega \\ \partial_n S = 0 & \text{on } \partial\Omega \end{cases}$$

This problem admits a unique mean-zero weak solution if RHS is mean-zero,
$\rightsquigarrow$ defines $C_{d,\Omega}$ as

$$|\Omega| C_{d,\Omega} = \int_\Omega \Delta(\eta_L \circ \Lambda \circ \Psi)$$

Determine $C_{d,\Omega}$:

1. $\Delta(\eta_L \circ \Lambda \circ \Psi) \in L^p(\Omega)$ with $1 < p \leq \frac{d}{d-1}$
2. Computation using Green's theorem:

$$\int_\Omega \Delta(\eta_L \circ \Lambda \circ \Psi) = \int_{\partial\Omega} \partial_n(\eta_L \circ \Lambda \circ \Psi)$$

Proof that S is subsingular:

Using the integral representation of S (layer potential techniques [6]), we have that, in the limit $x \to x^{(1)}$

$$S(x) = \mathrm{O}\left(\int_\Omega \Lambda(x-y)\Delta S(y)\,\mathrm{d}y\right) = \mathrm{o}\Big(\Lambda(x-y)\Big)$$

[6] Ammari, Kang and Lee, *American Mathematical Society*, (2009)

The Dirichlet condition (still with 1 exit hole)

Remember that

- f "=" $\lim_{\varepsilon\to 0} \lambda_\varepsilon^{-1} v_\varepsilon$ with $v_\varepsilon = \nu_\varepsilon - 1 = -1$ on $\tilde{\Gamma}_D^\varepsilon$
- Close to x_1, we have $f \sim C_{d,\Omega}^{-1}\Lambda$.

$\leadsto$ A good approximation of $(\lambda_\varepsilon, \nu_\varepsilon)$ is the pair $(\widehat{\lambda}_\varepsilon, \widehat{\nu}_\varepsilon)$, with $\widehat{\lambda}_\varepsilon := C_{d,|\Omega|}\left(\Lambda(r_1^\varepsilon)\right)^{-1}$ and $\widehat{\nu}_\varepsilon := 1 + \widehat{\lambda}_\varepsilon f$, satisfies the initial problem with small residuals

$$\begin{cases} -\Delta \widehat{\nu}_\varepsilon = \widehat{\lambda}_\varepsilon \widehat{\nu}_\varepsilon - \widehat{\lambda}_\varepsilon^2 f & \text{on } \Omega_\varepsilon \\ \partial_n u_\varepsilon = 0 & \text{on } \Gamma_{\mathrm{N}}^\varepsilon \\ \nu_\varepsilon = \widehat{\lambda}_\varepsilon R & \text{on } \Gamma_{\mathrm{D}}^\varepsilon \end{cases}$$

These resilduals have been quantified in the previous lemma

Estimate of the error on the eigenvalue

Reminder: ν_ε is the QSD, $\widehat{\nu}_\varepsilon$ is the quasimode
Similarily to [4], we have $\langle \widehat{\nu}_\varepsilon, \nu_\varepsilon \rangle = 1 + \mathrm{O}(\lambda_\varepsilon) + \mathrm{O}(\widehat{\lambda}_\varepsilon)$
By *Green's identity*, we have

$$\begin{aligned}
\lambda_\varepsilon \langle \widehat{\nu}_\varepsilon, \nu_\varepsilon \rangle &= -\langle \widehat{\nu}_\varepsilon, \Delta \nu_\varepsilon \rangle \\
&= -\langle \Delta \widehat{\nu}_\varepsilon, \nu_\varepsilon \rangle + \langle \partial_n \widehat{\nu}_\varepsilon, \nu_\varepsilon \rangle_{\Gamma^\varepsilon} - \langle \widehat{\nu}_\varepsilon, \partial_n \nu_\varepsilon \rangle_{\Gamma^\varepsilon} \\
&= \widehat{\lambda}_\varepsilon \langle \widehat{\nu}_\varepsilon, \nu_\varepsilon \rangle - \widehat{\lambda}_\varepsilon^2 \langle f, \nu_\varepsilon \rangle + 0 - \widehat{\lambda}_\varepsilon \langle R, \partial_n \nu_\varepsilon \rangle_{\Gamma^\varepsilon_{\mathrm{D}}}
\end{aligned}$$

Therefore we deduce that

$$\left| \lambda_\varepsilon - \widehat{\lambda}_\varepsilon \right| \langle \widehat{\nu}_\varepsilon, \nu_\varepsilon \rangle \leq \mathcal{O}(\widehat{\lambda}_\varepsilon^2) + \widehat{\lambda}_\varepsilon \|R\|_{L^\infty(\Gamma^\varepsilon_{\mathrm{D}})} \|\partial_n \nu_\varepsilon\|_{L^1(\Gamma^\varepsilon_{\mathrm{D}})}$$

To conclude: the bound on R comes from the lemma,
and it can be shown that $\|\partial_n \nu_\varepsilon\|_{L^1(\Gamma^\varepsilon_{\mathrm{D}})} = \mathrm{O}(\lambda_\varepsilon)$ [4].

Results for N exit holes and $d \geq 2$

We define

$$K_\varepsilon^i = -\Lambda(r_i^\varepsilon) = \begin{cases} -\dfrac{1}{\log(r_i^\varepsilon)} & \text{if } d = 2 \\ (r_i^\varepsilon)^{d-2} & \text{if } d \geq 3 \end{cases} \qquad \overline{K}_\varepsilon = K_1 + \cdots + K_N$$

Theorem (Eigenvalue)

The mean exit time when $X_0 \sim \nu_\varepsilon$ is given by $\mathbb{E}_{\nu_\varepsilon}[\tau] = \frac{1}{\lambda_\varepsilon}$, where

$$\lambda_\varepsilon = C_{d,\Omega}\overline{K}_\varepsilon + \begin{cases} \mathrm{O}\left(\overline{K}_\varepsilon^2\right) & \text{for } d = 2 \\ \mathrm{O}\left(\overline{K}_\varepsilon^2 \log\left(\overline{K}_\varepsilon\right)\right) & \text{for } d = 3 \\ \mathrm{O}\left(\overline{K}_\varepsilon^{\frac{d-1}{d-2}}\right) & \text{for } d \geq 4 \end{cases}$$

Results for N exit holes and $d \geq 2$

Theorem (Exit hole distribution)

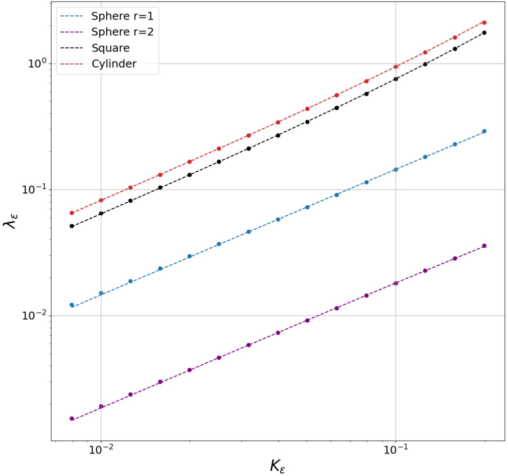
$$\mathbb{P}_\varepsilon(X_\tau \in \Gamma^\varepsilon_{D_i}) = \frac{K^i_\varepsilon}{\overline{K_\varepsilon}} + \begin{cases} \mathrm{O}(\overline{K_\varepsilon}), & \text{for } d = 2 \\ \mathrm{O}(\overline{K_\varepsilon}\log(\overline{K_\varepsilon})), & \text{for } d = 3 \\ \mathrm{O}(\overline{K_\varepsilon}^{\frac{1}{d-2}}) & \text{for } d \geq 4 \end{cases}$$

Does the bound worsen with the dimension?

No! For $d \geq 4$, for the eigenvalue

$$\lambda_\varepsilon = C_{d,\Omega}\,(r_i^\varepsilon)^{d-2}\left(1 + \mathrm{O}\left(\sum_{i=1}^{N} r_i^\varepsilon\right)\right)$$

The same can be done with the exit hole distribution



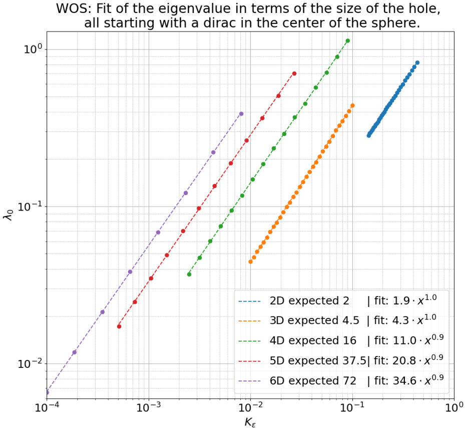
The constant $C_{d,\Omega}$ is given by:

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

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



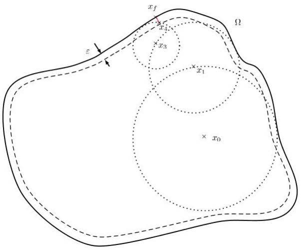
- Monte Carlo simulation of the exit time τ_ε for a unit ball in dimension $\{2, 3, 4, 5\}$
- It's a rare event so very long simulations...
- Correct scaling in K_ε, but:

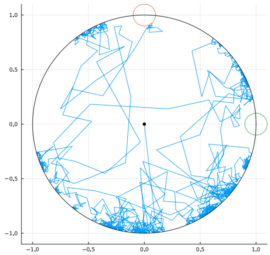
Dimension	C_d^{ball}	C_d^{ball} (simu)
2	2	1.9
3	4.5	4.3
4	16	11
5	32.5	20.8
6	72	34.6

Several reasons:

- The previous simulations where done with the inital condition $X_0 \sim \delta_0 \neq \nu_\varepsilon$.
- Trade-off $\sqrt{\Delta t} \ll \varepsilon$ and $N_{\text{step}} \simeq \Delta t \overline{K}_\varepsilon$

Solution: Adaptative timestep algorithm: walk on sphere





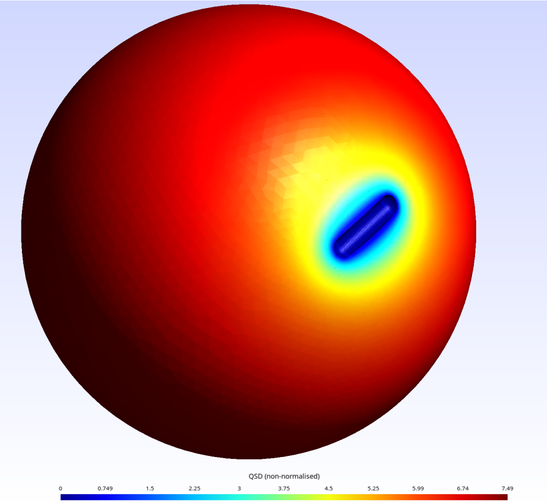
Conclusion

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

Future work:

Precise assymptotics starting for deterministic initial conditions

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


QSD (non-normalised)
0
0.749
1.5
2.25
3
3.75
4.5
5.25
5.99
6.74
7.49