A quasi-stationary approach to the narrow escape problem

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

The QSD as an eigenvalue problem

We want to find the QSD ν_ε

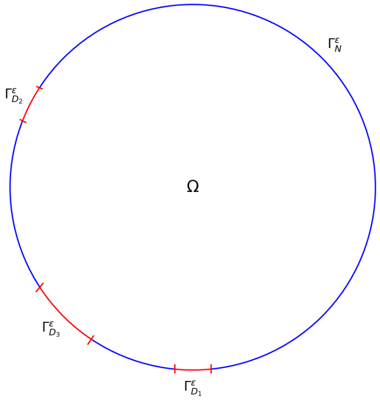
$$\begin{cases} -\Delta\nu_\varepsilon = \lambda_\varepsilon \nu_\varepsilon & \text{in } \Omega_\varepsilon \\ \partial_n \nu_\varepsilon = 0 & \text{on } \Gamma_N^\varepsilon \\ \nu_\varepsilon = 0 & \text{on } \Gamma_{D_i}^\varepsilon \end{cases}$$

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

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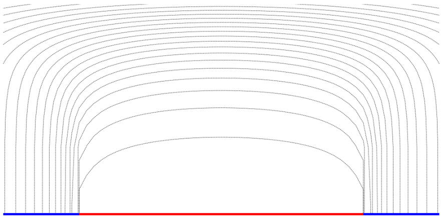
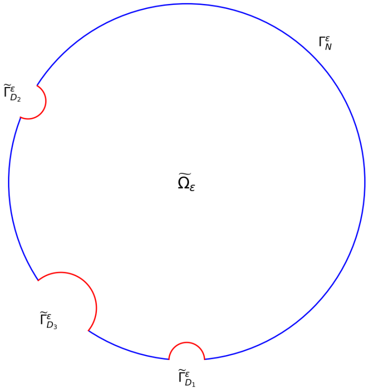


Figure: Level curves of the solution ν_ε near a flat hole.

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



Similar eigenvalue problem:

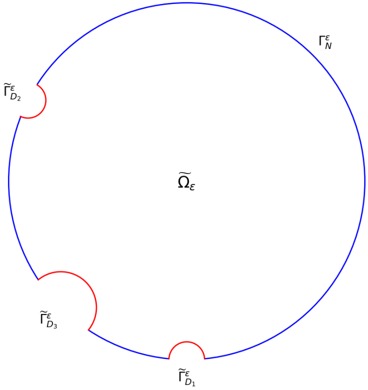
$$\begin{cases} -\Delta \nu_\varepsilon = \lambda_\varepsilon \nu_\varepsilon & \text{in } \widetilde{\Omega}_\varepsilon \\ \partial_n \nu_\varepsilon = 0 & \text{on } \Gamma_N^\varepsilon \\ \nu_\varepsilon = 0 & \text{on } \widetilde{\Gamma}_{D_i}^\varepsilon \end{cases} \tag{1}$$

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:

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

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?

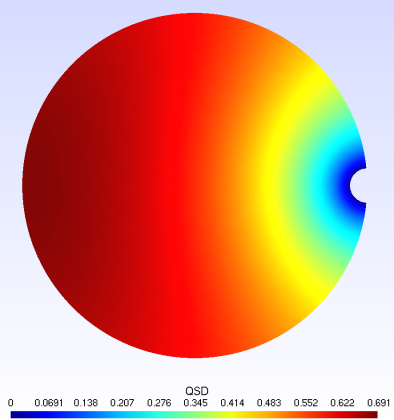


Figure: Dimension 2: Circle

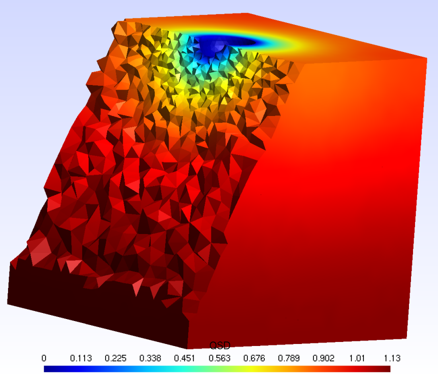
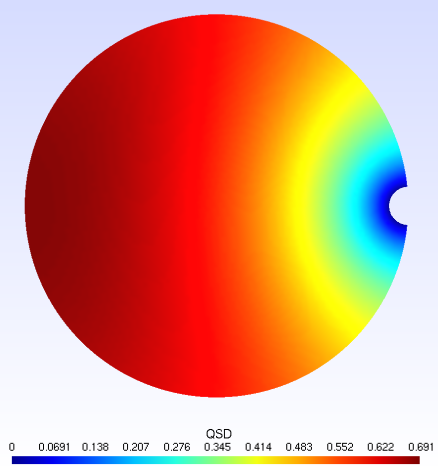


Figure: Dimension 3: Cube

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



We can approximate the solution ν_ε by a quasimode, for 1 hole i:

$$\varphi_\varepsilon = 1 + K_\varepsilon^i f_i$$

with f_i such that:

$$\begin{cases} -\Delta f_i = C_d & \text{in } \Omega \\ \partial_n f_i = 0 & \text{on } \partial\Omega \backslash \{x^{(i)}\} \end{cases} \tag{2}$$

with $x^{(i)}$ the center of the hole and $C_d > 0$

Then,

$$-\Delta \varphi_\varepsilon = C_d K_\varepsilon^i = C_d K_\varepsilon^i \varphi_\varepsilon + O(\dots)$$

Lemma

There exists (f_i, C_d) such that:

- f_i is solution of (2) in Ω
- $\operatorname{sing\,supp} f_i = \{x^{(i)}\}$
- $f_i \in C^\infty\left(\widetilde{\Omega}_\varepsilon\right)$
- $f_i(x) = -\left(r_\varepsilon^{(i)}\right)^{2-d}\left(1 + O\left(r_\varepsilon^{(i)}\right)\right)$ uniformly in $x \in \widetilde{\Gamma}_D^\varepsilon$

in the limit $\varepsilon \to 0$

The proof will be carried out in $d > 3$, in 3 steps

Proof of the lemma on f: step 1/3

From the compatibility condition:

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

The distribution f formally satisfies:

$$\begin{cases} -\Delta f_i = C_d & \text{in } \Omega \\ \partial_n f_i = -C_d |\Omega| \delta_{x^{(i)}} & \text{on } \partial\Omega \end{cases} \tag{3}$$

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

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

Proof of the lemma on f: step 2/3

Fundamental solution of the laplacian , $\Gamma\colon x \mapsto -|x|^{2-d}$ satisfies:

$$\begin{cases} -\Delta\Gamma = 0 & \text{in } \mathbb{R}^+ \times \mathbb{R}^{d-1}, \\ \partial_n \Gamma = 0 & \text{on } \partial\left(\mathbb{R}^+ \times \mathbb{R}^{d-1}\right) \setminus \{0\}, \end{cases}$$

Consider the change of variables $\Psi_i\colon \Omega \cap B(x^{(i)}, \delta) \to \mathbb{R}^+ \times \mathbb{R}^{d-1}$ that flattens locally the domain, with $\Psi_i(x^{(i)}) = 0$, such that

$$\partial_n \left(\Gamma \circ \Psi_i\right) = \partial_n \Gamma = 0, \quad \text{for } x \in \partial\Omega \cap B(x^{(i)}, \delta) \setminus \{x^{(i)}\}$$

As $\Psi_i(x) = x - x^{(i)} + o\left(x - x^{(i)}\right)$, by Taylor expansion:

$$-\Delta\left(\Gamma \circ \Psi_i\right) = O\left(\left|x - x^{(i)}\right|^{1-d}\right) \in L^p(\Omega), \quad \text{for } p < \frac{d}{d-1}$$

Proof of the lemma on f: step 3/3

The solution f_i is built as:

$$f_i = \Gamma \circ \Psi_i + S_i,$$

with $S_i \in W^{1,p}$ chosen such that f_i verifies the original PDE (2):

$$\begin{cases} -\Delta S_i = \Delta\left(\Gamma \circ \Psi_i\right) + C_d & \text{in } \Omega \\ \partial_n S_i = -N & \text{on } \partial\Omega \end{cases} \tag{4}$$

where $N = \partial_n\left(\Gamma \circ \Psi_i\right)$ and $N(x^{(i)}) = 0$

- The value of C_d determined by compatibility on (4)
- Using the integral representation of S_i (layer potential techniques [6]), we have that $S_i(x) = O(|x - x^{(i)}|\Gamma(x - x^{(i)}))$, in the limit $x \to x^{(i)}$

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

Behaviour of the quasimode near the hole

This construction can be extended to N holes of radius $r_\varepsilon^{(i)}$, taking:

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

Then for $x \in \widetilde{\Gamma}_{D_i}^{\varepsilon}$:

$$\varphi_\varepsilon(x) = 1 - K_\varepsilon^i \left(r_\varepsilon^{(i)}\right)^{2-d} + O\left(K_\varepsilon^i \left(r_\varepsilon^{(i)}\right)^{3-d}\right) + \sum_{j\neq i} K_\varepsilon^j f_j(x)$$

Scaling of K_ε^i

For φ_ε to be close to 0 on $\widetilde{\Gamma}_{D_i}^{\varepsilon}$, we take

$$K_\varepsilon^i = \left(r_\varepsilon^{(i)}\right)^{d-2}$$

Results

Theorem (Operator) 1.2 from [4]

The operator $\mathcal{L}_\varepsilon$ associated to (1) is non-negative, self-ajoint, has a compact resolvent

$$\exists c > 0, \exists \varepsilon_0 > 0, \forall \varepsilon \in (0, \varepsilon_0), \ \dim \mathrm{Ran} \pi_{[0, c\overline{K}_\varepsilon]}(\mathcal{L}_\varepsilon) = 1$$

Theorem (Eigenvalue)

$$\lambda_\varepsilon = \left(\mathbb{E}[\tau_\varepsilon]\right)^{-1} = C_d \sum_{i=1}^{N} \left(r_\varepsilon^{(i)}\right)^{d-2} \left(1 + O\left(\sum_{i=1}^{N} r_\varepsilon^{(i)}\right)\right)$$

Theorem (Exit hole distribution)

$$P(X_\tau \in \Gamma_{D_i}^{\varepsilon}) = \frac{\left(r_\varepsilon^{(i)}\right)^{d-2}}{\sum_{i=1}^{N} \left(r_\varepsilon^{(i)}\right)^{d-2}} + O\left(\sum_{i=1}^{N} r_\varepsilon^{(i)}\right)$$

Results in any dimension $d \geq 2$

$$K_\varepsilon^i = \left(r_\varepsilon^{(i)}\right)^{d-2} \quad \text{for } d > 2, \qquad K_\varepsilon^i = -\log\left(r_\varepsilon^{(i)}\right)^{-1} \quad \text{for } d = 2$$

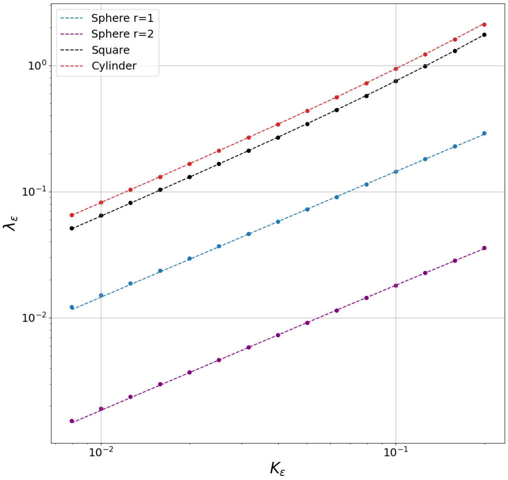
Theorem (Eigenvalue)

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

Theorem (Exit hole distribution)

$$P(X_\tau \in \Gamma_{D_i}^\varepsilon) = \frac{K_\varepsilon^i}{\overline{K_\varepsilon}} + \begin{cases} O(\overline{K_\varepsilon}^{\frac{d-1}{d-2}}) & \text{for } d > 3 \\ O(\overline{K_\varepsilon} \log(\overline{K_\varepsilon})), & \text{for } d = 3 \\ O(\overline{K_\varepsilon}), & \text{for } d = 2 \end{cases}$$

Measure of the exit time through Finite Element Method (FEM)

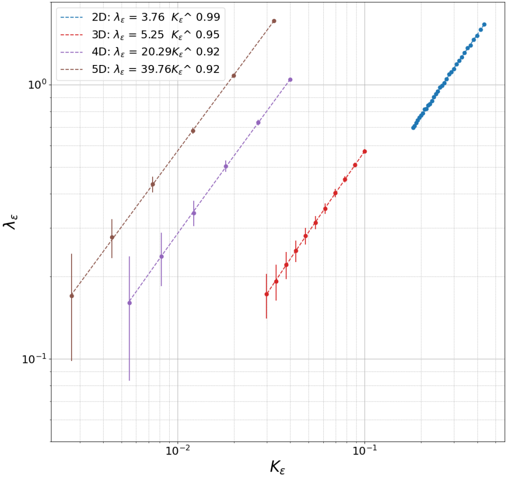


The constant C_d is given by:

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

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

Shape	C_3	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_d^{ball}	C_d^{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 $X_0 \sim \delta_0 \neq \nu_\varepsilon$.
Fleming–Viot algorithm $\rightarrow$ estimate the QSD on the fly using the Yaglom limit

Test: the unit sphere in dimension 3, fit of $\lambda_\varepsilon = C_3 \overline{K_\varepsilon}^\alpha$:

Initialisation	ν_ε	δ_0	$\nu_\varepsilon^{\mathrm{FV}}$
C_3	4	5 ± 3	3.7 ± 0.6
α	1	0.95 ± 0.08	1.0 ± 0.1

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 $\varepsilon = 0.5\varepsilon$.
- Estimate of $\mathbb{P}(X_\tau \in \Gamma^\varepsilon_{D_2})$

By the theorem: $\frac{2}{3} + O(\varepsilon)$
By the simulation: 0.665 ± 0.001

Unit sphere in dimension 4

- 4 holes of radius ε, $0.7\,\varepsilon$, $0.8\,\varepsilon$, $0.9\,\varepsilon$.
- Estimate of $\mathbb{P}(X_\tau \in \Gamma^\varepsilon_{D_i})$

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

Proof of the results on the Eigenvalue

By the Green identity, we can write:

$$
\begin{aligned}
\lambda_0^\varepsilon = \frac{\lambda_0^\varepsilon \langle \varphi^\varepsilon, u_0^\varepsilon \rangle}{\langle \varphi^\varepsilon, u_0^\varepsilon \rangle} = \frac{\langle \varphi^\varepsilon, -\Delta u_0^\varepsilon \rangle}{\langle \varphi^\varepsilon, u_0^\varepsilon \rangle} &= \frac{\langle -\Delta \varphi^\varepsilon, u_0^\varepsilon \rangle - \langle \varphi^\varepsilon, \partial_n u_0^\varepsilon \rangle_{\Gamma^\varepsilon} + \langle \partial_n \varphi^\varepsilon, u_0^\varepsilon \rangle_{\Gamma^\varepsilon}}{\langle \varphi^\varepsilon, u_0^\varepsilon \rangle} \\
&= \frac{\langle -\Delta \varphi^\varepsilon, u_0^\varepsilon \rangle - \langle \varphi^\varepsilon, \partial_n u_0^\varepsilon \rangle_{\Gamma_D^\varepsilon}}{\langle \varphi^\varepsilon, u_0^\varepsilon \rangle} \\
&= \frac{\langle C_d \overline{K_\varepsilon}, u_0^\varepsilon \rangle - \langle O(\overline{K_\varepsilon}^{\frac{1}{n-2}}), \partial_n u_0^\varepsilon \rangle_{\Gamma_D^\varepsilon}}{\langle 1 + O(\overline{K_\varepsilon}), u_0^\varepsilon \rangle}
\end{aligned}
$$

By injecting all we know about the quasimode.
This sums up to being able to estimate the L^1 norm of the quasimode u_0 and its normal derivative

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

The slit