

Drexel University — Mathematics Department Colloquium

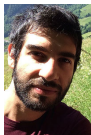
Metastability of stochastic partial differential equations and Fredholm determinants

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Based on joint works with Giacomo Di Gesù,
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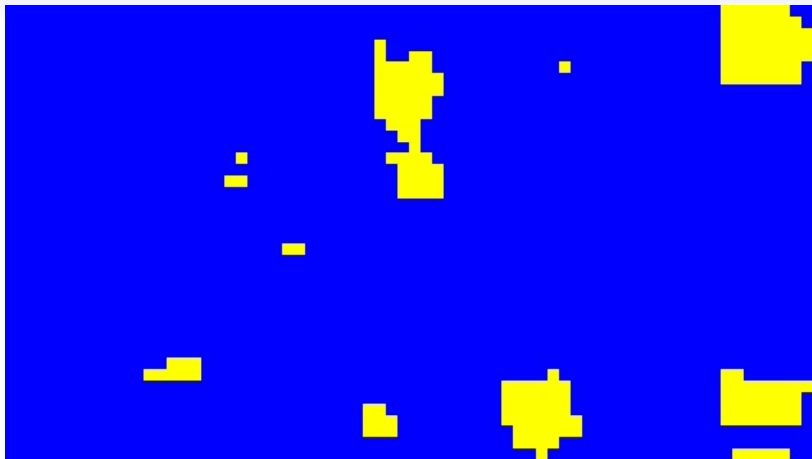
What is metastability?



Supercooled water

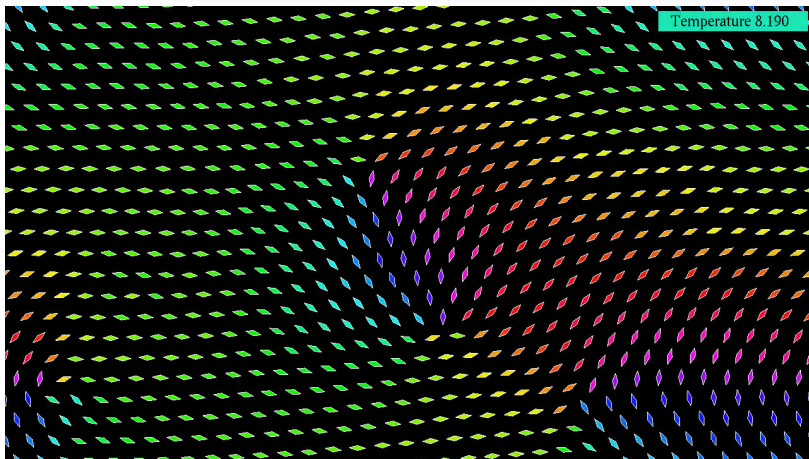
(Source: https://youtu.be/fSPzMva9_CE)

What is metastability?



Ising model with Glauber dynamics at low temperature
(Online: https://youtu.be/_vrtfDcjfxU)

What is metastability?



Particles interacting with a Lennard–Jones potential,
coupled to a thermostat (stochastic differential equation, or SDE)
(Online: <https://youtu.be/tIII17AG10C0>)

Reversible diffusion in a double-well

$$dx_t = -\nabla V(x_t) dt + \sqrt{2\varepsilon} dW_t$$

$V: \mathbb{R}^d \rightarrow \mathbb{R}$ confining potential

$$\tau_y^x = \inf\{t > 0: x_t \in \mathcal{B}_\varepsilon(y)\}$$

first-hitting time of small ball $\mathcal{B}_\varepsilon(y)$,
when starting in x

Arrhenius' law (1889): $\mathbb{E}[\tau_y^x] \simeq e^{[V(z)-V(x)]/\varepsilon}$

Eyring–Kramers law (1935, 1940):

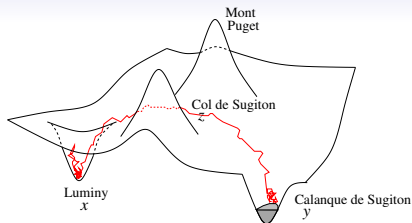
Eigenvalues of Hessian of V at minimum x : $0 < \nu_1 \leq \nu_2 \leq \dots \leq \nu_d$

Eigenvalues of Hessian of V at saddle z : $\lambda_1 < 0 < \lambda_2 \leq \dots \leq \lambda_d$

$$\mathbb{E}[\tau_y^x] = 2\pi \sqrt{\frac{\lambda_2 \dots \lambda_d}{|\lambda_1| \nu_1 \dots \nu_d}} e^{[V(z)-V(x)]/\varepsilon} [1 + o_\varepsilon(1)]$$

Arrhenius' law: proved by [Freidlin, Wentzell, 1979] using large deviations

Eyring–Kramers law: [Bovier, Eckhoff, Gayard, Klein, 2004] using potential theory,
[Helffer, Klein, Nier, 2004] using Witten Laplacian, ...



Potential-theoretic proof

$$dx_t = -\nabla V(x_t) dt + \sqrt{2\varepsilon} dW_t$$

- ▷ **Generator:** $\mathcal{L} = \varepsilon \Delta - \nabla V \cdot \nabla = \varepsilon e^{V/\varepsilon} \nabla \cdot e^{-V/\varepsilon} \nabla$
- ▷ **Invariant probability:** $\pi(dx) = \frac{1}{Z} e^{-V(x)/\varepsilon} dx \Rightarrow \mathcal{L}^\dagger \pi = 0$
- ▷ **Reversible:** $\langle f, \mathcal{L}g \rangle = \langle \mathcal{L}f, g \rangle$ for $\langle f, g \rangle = \int_{\mathbb{R}^d} e^{-V(x)/\varepsilon} f(x)g(x) dx$
- ▷ **Dirichlet form:** $\mathcal{E}(f) = \langle f, -\mathcal{L}f \rangle = \varepsilon \int_{\mathbb{R}^d} e^{-V(x)/\varepsilon} |\nabla f(x)|^2 dx$
 $\mathcal{E}(f, g) = \langle f, -\mathcal{L}g \rangle$

Expected hitting time

- ▷ Expected hitting time:

$$w_A(x) = \mathbb{E}^x[\tau_A] \quad \text{satisfies} \quad \begin{cases} (\mathcal{L}w_A)(x) = -1 & x \in A^c \\ w_A(x) = 0 & x \in A \end{cases}$$

- ▷ Green function:

$$\begin{cases} (\mathcal{L}G_A)(x) = \delta(x - y) & x \in A^c \\ G_A(x, y) = 0 & x \in A \end{cases}$$

$$\Rightarrow \quad w_A(x) = - \int_{A^c} G_A(x, y)(dy)$$

Committor

▷ Committor:

$$h_{AB}(x) = \mathbb{P}^x\{\tau_A < \tau_B\} \quad \text{satisfies} \quad \begin{cases} (\mathcal{L}h_{AB})(x) = 0 & x \in (A \cup B)^c \\ h_{AB}(x) = 1 & x \in A \\ h_{AB}(x) = 0 & x \in B \end{cases}$$

▷ Equilibrium measure: $e_{AB}(dx) = (-\mathcal{L}h_{AB})(dx)$ measure on $x \in \partial A$

$$\Rightarrow \quad h_{AB}(x) = - \int_A G_B(x, y) e_{AB}(dy)$$

Capacity

Capacity: $\text{cap}(A, B) = \int_{\partial A} e^{-V(x)/\varepsilon} e_{AB}(dx)$

$\Rightarrow \nu_{AB}(dx) = \frac{1}{\text{cap}(A, B)} e^{-V(x)/\varepsilon} e_{AB}(dx)$ is a probability measure on ∂A

Theorem (“Magic” formula):

$$\mathbb{E}^{\nu_{AB}}[\tau_B] := \int_{\partial A} \mathbb{E}^x[\tau_B] \nu_{AB}(dx) = \frac{1}{\text{cap}(A, B)} \int_{B^c} e^{-V(x)/\varepsilon} h_{AB}(x) dx$$

Dirichlet principle

Theorem: Dirichlet principle

Let $\mathcal{H}_{AB} = \{h : \mathbb{R}^d \rightarrow [0, 1] : h|_A = 1, h|_B = 0\}$. Then

$$\text{cap}(A, B) = \inf_{h \in \mathcal{H}_{AB}} \mathcal{E}(h) = \mathcal{E}(h_{AB})$$

Thomson principle

Theorem: Thomson principle [Landim, Mariani, Seo 2018]

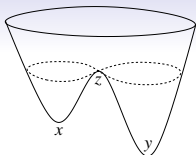
Let $\mathcal{U}_{AB} = \{f: \nabla \cdot f|_{(A \cup B)^c} = 0, \int_{\partial A} f(x) \cdot n_A(x) \sigma(dx) = 1\}$. Then

$$\text{cap}(A, B) = \sup_{f \in \mathcal{U}_{AB}} \frac{1}{\mathcal{D}(f)} = \frac{1}{\mathcal{D}(f_{AB})} \quad \mathcal{D}(f) = \frac{1}{\varepsilon} \int e^{V(x)/\varepsilon} |f(x)|^2 dx$$

Proof of Eyring–Kramers law

$$dx_t = -\nabla V(x_t) dt + \sqrt{2\varepsilon} dW_t$$

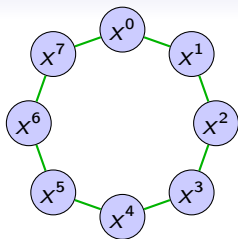
▷ A, B small balls around x, y



A particle system

[B, Fernandez, Gentz, Nonlinearity 2007]

- ▷ N particles on a circle $\mathbb{Z}/N\mathbb{Z}$
- ▷ Bistable local dynamics
- ▷ Ferromagnetic nearest neighbour coupling
- ▷ Independent noise on each site



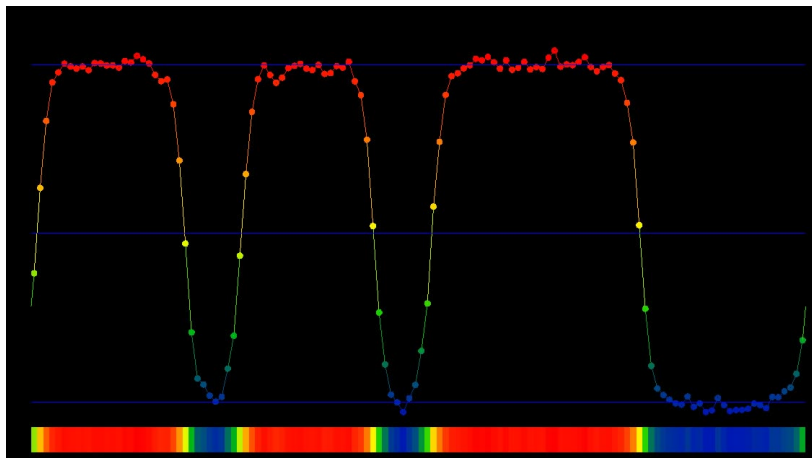
$$dx_t^i = [x_t^i - (x_t^i)^3] dt + \frac{\gamma}{2} [x_t^{i+1} - 2x_t^i + x_t^{i-1}] dt + \sqrt{2\varepsilon} dW_t^i$$

Gradient system $dx_t = -\nabla V(x_t) dt + \sqrt{2\varepsilon} dW_t$

potential $V(x) = \sum_i U(x^i) + \frac{\gamma}{4} \sum_i (x^{i+1} - x^i)^2$ $U(\xi) = \frac{1}{4}\xi^4 - \frac{1}{2}\xi^2$

Coarsening dynamics with noise

([Link to simulation](#))



Deterministic Allen–Cahn PDE

[Chafee & Infante 74, Allen & Cahn 75]

$$\partial_t u(t, x) = \Delta u(t, x) + f(u(t, x))$$

- ▷ $x \in [0, L]$, L : bifurcation parameter
- ▷ $u(t, x) \in \mathbb{R}$
- ▷ Either periodic or zero-flux Neumann boundary conditions
- ▷ In this talk: $f(u) = u - u^3$ (results more general)

Energy function:

$$V[u] = \int_0^L \left[\frac{1}{2} u'(x)^2 - \frac{1}{2} u(x)^2 + \frac{1}{4} u(x)^4 \right] dx \quad \rightarrow \min$$

Scaling limit of particle system with $\gamma = 2 \frac{N^2}{L^2}$

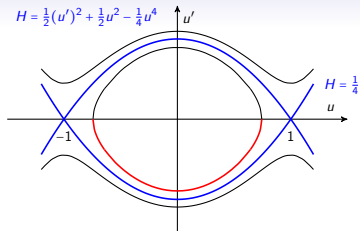
Stationary solutions: $u_0''(x) = -u_0(x) + u_0(x)^3$ critical points of V

Stability: Sturm–Liouville problem $\partial_t v_t(x) = v_t''(x) + [1 - 3u_0(x)^2]v_t(x)$

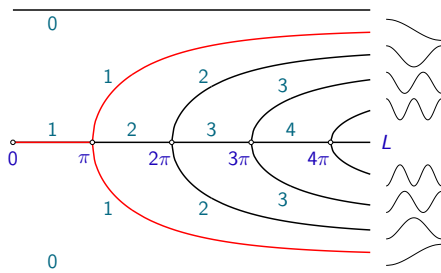
Stationary solutions

$$u_0''(x) = -f(u_0(x)) = -u_0(x) + u_0(x)^3$$

- ▷ $u_{\pm}(x) \equiv \pm 1$
- ▷ $u_0(x) \equiv 0$
- ▷ Nonconstant solutions satisfying b.c.
(expressible in terms of Jacobi elliptic fcts)
- ▷ Neumann b.c: $2k$ nonconstant solutions when $L > k\pi$



Number of positive eigenvalues
(= unstable directions)
Transition state



- ▷ Periodic b.c: k families when $L > 2k\pi$

Eyring–Kramers law for 1D SPDEs: heuristics

$$\partial_t u(t, x) = \Delta u(t, x) + f(u(t, x)) + \sqrt{2\varepsilon} \xi(t, x) \quad (f(u) = u - u^3)$$

Initial condition: u_{in} near $u_- \equiv -1$ with eigenvalues $\nu_k = \left(\frac{\beta k \pi}{L}\right)^2 + 2$

Target: $u_+ \equiv 1$, $\tau_+ = \inf\{t > 0: \|u_t - u_+\|_{L^\infty} < \rho\}$

Transition state: ($\beta = 1$ for Neumann b.c., $\beta = 2$ for periodic b.c.)

$$u_{\text{ts}}(x) = \begin{cases} u_0(x) \equiv 0 & \text{if } L \leq \beta\pi \quad \text{with ev } \lambda_k = \left(\frac{\beta k \pi}{L}\right)^2 - 1 \\ u_1(x) \text{ } \beta\text{-kink stationary sol.} & \text{if } L > \beta\pi \quad \text{with ev } \lambda'_k \end{cases}$$

[Faris & Jona-Lasinio 82]: large-deviation principle

\Rightarrow Arrhenius law: $\mathbb{E}^{u_{\text{in}}}[\tau_+] \simeq e^{(V[u_{\text{ts}}] - V[u_-])/\varepsilon}$

[Maier & Stein 01]: formal computation; for Neumann b.c.

$\Rightarrow \mathbb{E}^{u_{\text{in}}}[\tau_+] \simeq 2\pi \sqrt{\frac{1}{|\lambda_0| \nu_0}} \prod_{k=1}^{\infty} \frac{\lambda_k}{\nu_k} e^{(V[u_{\text{ts}}] - V[u_-])/\varepsilon}$

Eyring–Kramers law for 1D SPDEs: main result

Theorem: Neumann b.c. [B & Gentz, 2013]

- ▷ If $L < \pi - c$ with $c > 0$, then

$$\mathbb{E}^{u_{\text{in}}}[\tau_+] = 2\pi \sqrt{\frac{1}{|\lambda_0|\nu_0} \prod_{k=1}^{\infty} \frac{\lambda_k}{\nu_k}} e^{(V[u_{\text{ts}}] - V[u_-])/\varepsilon} \underbrace{\left[1 + \mathcal{O}(\varepsilon^{1/2} |\log \varepsilon|^{3/2})\right]}_{\text{error not optimal}}$$

- ▷ If $L > \pi + c$, then same formula with extra factor $\frac{1}{2}$ (since 2 saddles) and λ'_k instead of λ_k

- ▷ Results also for L near π and periodic b.c.

- ▷ Prefactor involves a **Fredholm determinant**:

Δ_{\perp} Laplacian acting on mean zero functions

$$\prod_{k=1}^{\infty} \frac{\lambda_k}{\nu_k} = \det[(-\Delta_{\perp} - 1)(-\Delta_{\perp} + 2)^{-1}] = \det[\mathbb{1} - 3(-\Delta_{\perp} + 2)^{-1}]$$

converges because $\log \det = \text{Tr} \log$ and $(-\Delta_{\perp} + 2)^{-1}$ is **trace class**

(limit = $\frac{\sqrt{2} \sin(L)}{\sinh(\sqrt{2}L)}$)

Ideas of the proof ($L < \pi$)

- ▷ Spectral Galerkin approximation: $u(t, x) = \sum_{|k| \leq N} z_k(t) e_k(x)$ (Fourier)
- ▷ Use Dirichlet and Thomson principles to bound capacity
View integrals as expectations under Gaussian measures
- ▷ Conclusion: $\text{cap}(A, B) = \varepsilon \sqrt{\frac{|\lambda_0|}{2\pi\varepsilon}} \sqrt{\frac{(2\pi\varepsilon)^N}{\det[-\Delta_L - 1]}} [1 + \mathcal{O}(\varepsilon)]$

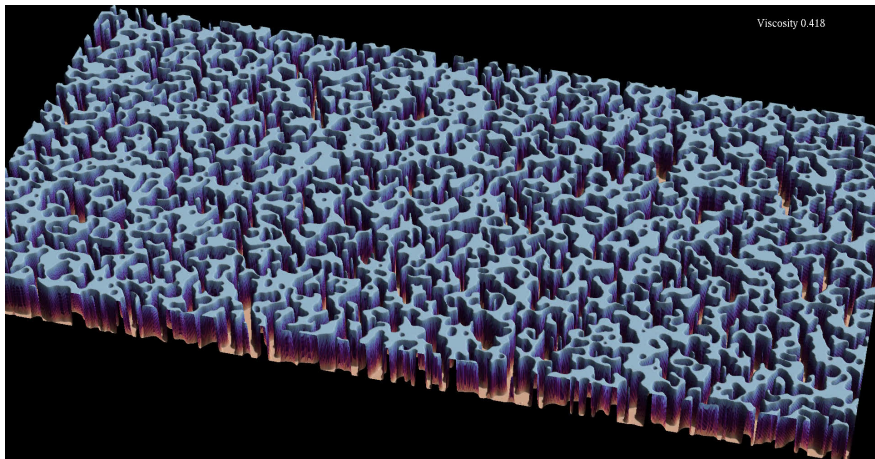
Other elements of the proof:

- ▷ A priori bounds on h_{AB} : large deviations (or symmetry argument)
- ▷ Convergence of hitting times as $N \rightarrow \infty$: a priori estimate for $\mathbb{E}[\tau_B^2]$
- ▷ Coupling argument for start in u_{in} [Martinelli, Olivieri & Scoppola]
- ▷ Bifurcation at $L = \beta\pi$

The two-dimensional case

$$\partial_t u = \Delta u + u - u^3 + \sqrt{2\varepsilon}\xi$$

([Link to simulation](#))



The two-dimensional case

- ▷ Large-deviation principle: [Hairer & Weber, 2015]
- ▷ Naive computation of prefactor fails:

$$\begin{aligned}\log \prod_{k \in (\mathbb{N}^2)^*} \frac{1 - \left(\frac{L}{|k|\pi}\right)^2}{1 + 2\left(\frac{L}{|k|\pi}\right)^2} &\simeq \sum_{k \in (\mathbb{N}^2)^*} \log \left(1 - \frac{3L^2}{|k|^2\pi^2}\right) \\ &\simeq - \sum_{k \in (\mathbb{N}^2)^*} \frac{3L^2}{|k|^2\pi^2} \simeq -\frac{3L^2}{\pi^2} \int_1^\infty \frac{r \, dr}{r^2} = -\infty\end{aligned}$$

- ▷ In fact, the equation needs to be **renormalised**

Theorem: [Da Prato & Debussche 2003]

Let ξ^δ be a mollification on scale δ of white noise. Then

$$\partial_t u = \Delta u + [1 + 3\varepsilon C(\delta)]u - u^3 + \sqrt{2\varepsilon}\xi^\delta$$

with $C(\delta) \simeq \log(\delta^{-1})$ admits local solution converging as $\delta \rightarrow 0$

(Global version: [Mourrat & Weber 2015])

[Mourrat & Weber 2014]: **Renormalised** eq = scaling limit of **Ising–Kac model**

Main result in dimension 2

Theorem: [B, Di Gesù, Weber, 2017]

For $L < 2\pi$, appropriate $A \ni u_-$, $B \ni u_+$, $\exists \mu_N$ probability measures on ∂A :

$$\limsup_{N \rightarrow \infty} \mathbb{E}^{\mu_N} [\tau_B] \leq \frac{2\pi}{|\lambda_0|} \sqrt{\prod_{k \in \mathbb{Z}^2} \frac{|\lambda_k|}{\nu_k} e^{\frac{\nu_k - \lambda_k}{|\lambda_k|}} e^{(V[u_{ts}] - V[u_-])/\varepsilon} [1 + c_+ \sqrt{\varepsilon}]}$$

$$\liminf_{N \rightarrow \infty} \mathbb{E}^{\mu_N} [\tau_B] \geq \frac{2\pi}{|\lambda_0|} \sqrt{\prod_{k \in \mathbb{Z}^2} \frac{|\lambda_k|}{\nu_k} e^{\frac{\nu_k - \lambda_k}{|\lambda_k|}} e^{(V[u_{ts}] - V[u_-])/\varepsilon} [1 - c_- \varepsilon]}$$

- ▷ Inverse of prefactor involves **Carleman–Fredholm determinant**:

$$\det_2(\mathbb{1} + T) = \det(\mathbb{1} + T) e^{-\text{Tr } T}$$

with $T = 3(-\Delta_{\perp} - 1)^{-1}$

\det_2 defined whenever T is only **Hilbert–Schmidt** (true for $d \leq 3$)

- ▷ [Tatsoulis & Weber 2018]: Same result for $\mathbb{E}^{u_0} [\tau_B]$

Renormalisation

Problem: Stoch. convolution $w_t(x) = \int_0^t e^{\Delta(t-s)} \xi(s, x) ds$ is **distribution**

▷ δ -mollification should be equivalent to Galerkin approx. $|k| \leq N = \delta^{-1}$

▷ $\lim_{t \rightarrow \infty} \int_0^t e^{(\Delta-1)(t-s)} \xi_N(s, x) ds = \phi_N$ is a **Gaussian free field**, s.t.

$$L^2 C_N := L^2 \mathbb{E} \phi_N^2 = \mathbb{E} \|\phi_N\|_{L^2}^2 = \sum_{|k| \leq N} \frac{1}{2(\mu_k+1)} = \frac{\text{Tr}(P_N[-\Delta+1]^{-1})}{2} \simeq \log(N)$$

▷ Galerkin-truncated renormalised potential

$$V_N = \frac{1}{2} \int_{\mathbb{T}^2} [\|\nabla u_N(x)\|^2 - u_N(x)^2] dx + \frac{1}{4} \int_{\mathbb{T}^2} :u_N(x)^4: dx$$

▷ Using **Nelson estimate**: $\text{cap}(A, B) \simeq \sqrt{\frac{|\lambda_0| \varepsilon}{2\pi}} \prod_{0 < |k| \leq N} \sqrt{\frac{2\pi \varepsilon}{\lambda_k}}$

▷ $\int h_{A,B} e^{-V_N/\varepsilon} dz \simeq \prod_{|k| \leq N} \sqrt{\frac{2\pi \varepsilon}{\nu_k}} e^{-V_N(L,0)/\varepsilon}$, $-V_N(L,0) = \frac{1}{4} L^2 + \frac{3}{2} L^2 C_N \varepsilon$

▷ Prefactor proportional to (since $\nu_k = \lambda_k + 3$)

$$\prod_{0 < |k| \leq N} \frac{\lambda_k}{\lambda_k+3} e^{3/\lambda_k} \quad \text{converges since} \quad \log \left[\frac{\lambda_k}{\lambda_k+3} e^{3/\lambda_k} \right] = \mathcal{O} \left(\frac{1}{|k|^4} \right)$$

References

- ▷ N. B., Bastien Fernandez & Barbara Gentz, *Metastability in interacting nonlinear stochastic differential equations I: From weak coupling to synchronisation & II: Large- N behaviour*, Nonlinearity **20**, 2551–2581; 2583–2614 (2007)
- ▷ N. B. & Barbara Gentz, *Sharp estimates for metastable lifetimes in parabolic SPDEs: Kramers' law and beyond*, Electronic J. Probability **18**, (24):1–58 (2013)
- ▷ N. B., Giacomo Di Gesù & Hendrik Weber, *An Eyring–Kramers law for the stoch. Allen–Cahn equation in dimension two*, Electronic J. Probability **22**, 1–27 (2017)
- ▷ A. Bovier and F. den Hollander, *Metastability. A potential-theoretic approach*, Springer, Cham, 2015
- ▷ C. Landim, M. Mariani, and I. Seo, *Dirichlet's and Thomson's principles for non-selfadjoint elliptic operators with application to non-reversible metastable diffusion processes*, Arch. Ration. Mech. Anal., 231(2):887–938, 2019
- ▷ N. B., *Kramers' law: Validity, derivations and generalisations*, Markov Processes Relat. Fields **19**, 459–490 (2013)
- ▷ N. B., *An Introduction to Singular Stochastic PDEs: Allen-Cahn Equations, Metastability and Regularity Structures*, EMS Press (2022), DOI 10.4171/elm/34
- ▷ N. B., *Metastability of Stochastic Partial Differential Equations and Fredholm Determinants*, EMS Newsletter 117, 6–14 (2020)

Thanks for your attention!