

IRTG Bielefeld–Seoul Winter School - Stochastic Dynamics

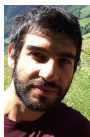
Metastable dynamics of Markov processes

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Based on joint works with Manon Baudel, Giacomo Di Gesù,
Bastien Fernandez, Barbara Gentz, Damien Landon and Hendrik Weber



What is metastability?

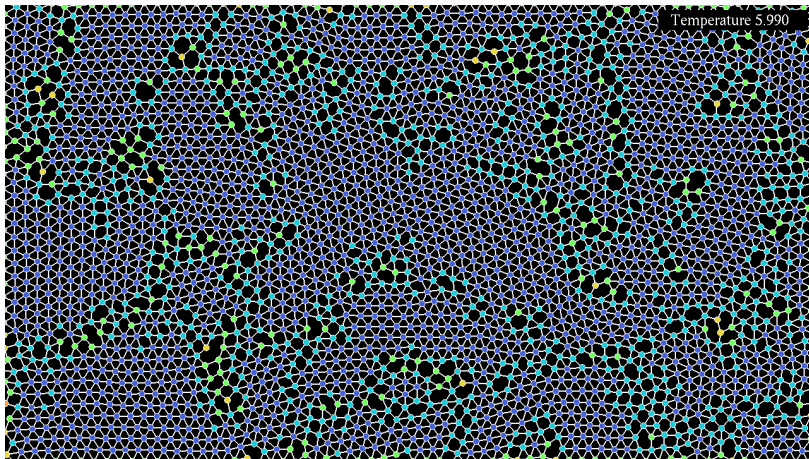
Supercooled water

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

What is metastability?

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

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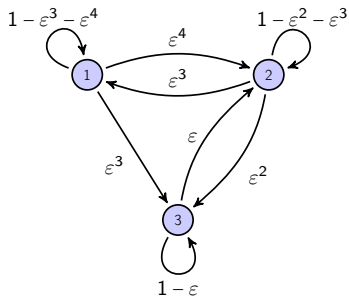


Particles interacting with a Lennard–Jones potential, coupled to a thermostat (stochastic differential equation, or SDE)

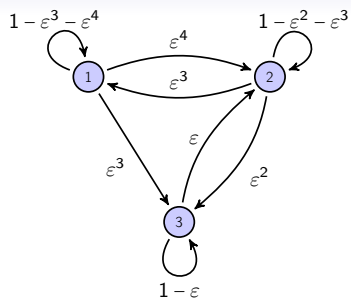
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2. Continuous-space Markov chains and SDEs
3. Example: the FitzHugh–Nagumo equation
4. The case of reversible SDEs: The potential-theoretic approach
5. The stochastic Allen–Cahn PDE

1. Metastable Markov chains on a finite set



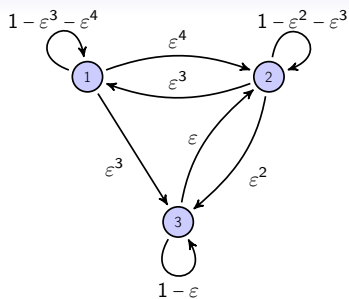
A simple example



$$P = \begin{pmatrix} 1 - \epsilon^3 - \epsilon^4 & \epsilon^4 & \epsilon^3 \\ \epsilon^3 & 1 - \epsilon^2 - \epsilon^3 & \epsilon^2 \\ 0 & \epsilon & 1 - \epsilon \end{pmatrix}$$

$$0 \leq \epsilon \leq \epsilon_{\max}$$

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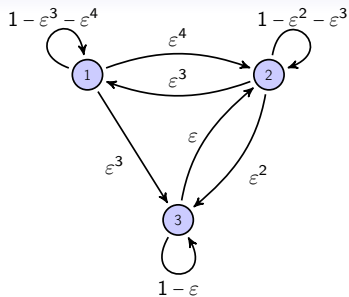


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- ▷ $\epsilon = 0$: $P = \text{Id}$
- ▷ $0 < \epsilon \leq \epsilon_{\max}$: irreducible, aperiodic, **not** reversible

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Stationary distribution:

Speed of convergence to π_0 ?

Eigenvalues of P :

Main question

How to easily determine leading term of **spectral gap** $1 - \lambda_1$?

- ▷ Linear algebra/analytic methods (singular perturbation theory), e.g. [Schweitzer 68, Hassin & Haviv 92, Avrachenkov & Lasserre 99]
- ▷ Probabilistic methods, e.g. [Wentzell 72, Freidlin & Wentzell 70s, Miclo 95, Beltràn & Landim 2010, Cameron & Vanden-Eijnden 2014, Betz & Le Roux 2016, Cameron & Gan 2016]

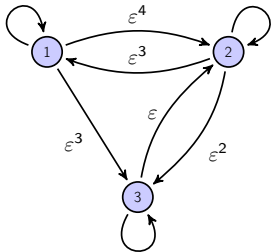
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Some probabilistic tools:

- ▷ W -graphs
- ▷ **Lumping** of states
- ▷ Speeding up time



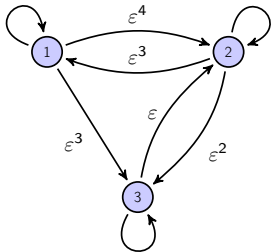
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- ▶ Speeding up time
- ▶ Here: **trace process**



Killed process

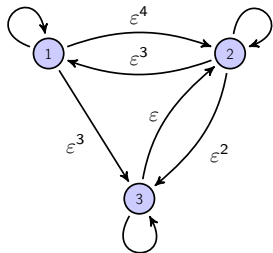
\mathcal{X} finite, $\{X_n\}_{n \in \mathbb{N}_0}$ irreducible aperiodic M.C., transition matrix P , $A \subset \mathcal{X}$

▷ Process **killed** upon leaving A : $P_A(x, y) = P(x, y) \mathbb{1}_{\{x, y \in A\}}$

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$$A = \{1, 2\}$$

Trace process [Landim, Beltran]

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▷ **Trace process** on A : process monitored only when in A

$${}_A P(x, y) = \mathbb{P}^x \{X_{\tau_A^+} = y\}, \quad \tau_A^+ = \inf\{n \geq 1: X_n \in A\}$$

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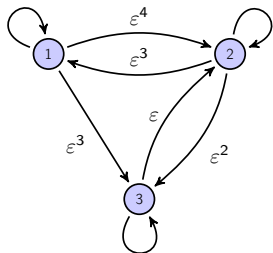
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Matrix representation (**Schur complement**)

$$P = \begin{pmatrix} P_A & P_{AA^c} \\ P_{A^c A} & P_{A^c} \end{pmatrix} \Rightarrow {}_A P = P_A + P_{AA^c} [\mathbb{1} - P_{A^c}]^{-1} P_{A^c A}$$

Application to the example

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A nice application of the trace process

Recall: the chain is **not** assumed to be reversible:

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Proposition: $\forall x, y \in A$

$$\pi_0(x)\mathbb{P}^x\{\tau_y^+ < \tau_x^+\} = \pi_0(y)\mathbb{P}^y\{\tau_x^+ < \tau_y^+\}$$

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- ▷ First proof in non-reversible case: [Betz & Le Roux 2016]

Using $\pi_0(x) = 1/\mathbb{E}^x[\tau_x^+]$

- ▷ Alternative proof using trace process: [Baudel & B 2017]

Remark: $\pi_0|_A$ is invariant by AP

Good domains

Definition: For $A \subset \mathcal{X}$, let

$$p_{\text{in}}(A) = \inf_{x \in A^c} \mathbb{P}^x \{X_1 \in A\}$$

$$p_{\text{out}}(A) = \sup_{x \in A} \mathbb{P}^x \{X_1 \in A^c\}$$

A is a **good domain** if $\lim_{\varepsilon \rightarrow 0} \frac{p_{\text{out}}(A)}{p_{\text{in}}(A)} = 0$

Good domains

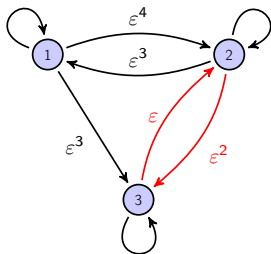
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Example:



Main idea

For a good domain A ,

$P = \begin{pmatrix} P_A & P_{AA^c} \\ P_{A^cA} & P_{A^c} \end{pmatrix}$ is well-approximated by $\widehat{P} = \begin{pmatrix} P_A & 0 \\ P_{A^cA} & P_{A^c} \end{pmatrix}$

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Norm: $\|Q\| = \sup_{\|\varphi\|_\infty=1} \|Q\varphi\|_\infty = \sup_{\|\mu\|_1=1} \|\mu Q\|_1 = \sup_{x \in \mathcal{X}} \sum_{y \in \mathcal{X}} |Q(x, y)|$

Lemma: $\|P - \widehat{P}\| = 2p_{\text{out}}(A)$

Main idea

Fact from spectral theory (using complex analysis, Riesz projector):
 $\hat{\lambda}$ simple eigenvalue of \hat{P} at distance $> \|P - \hat{P}\|$ from remaining spectrum
 $\Rightarrow P$ has unique eigenvalue at distance $\mathcal{O}(\|P - \hat{P}\|)$ from $\hat{\lambda}$

Consequence: If $A^c = \{x\}$ then $p_{\text{in}}(A) = 1 - P(x, x) = 1 - \hat{\lambda}$
 $\Rightarrow 1 - \lambda = 1 - \hat{\lambda} + \mathcal{O}(p_{\text{out}}(A)) = (1 - \hat{\lambda}) \left[1 + \mathcal{O}\left(\frac{p_{\text{out}}(A)}{p_{\text{in}}(A)}\right) \right]$

Example: $\hat{\lambda}_2 = 1 - \varepsilon$ perturbs to $\lambda_2 = 1 - \varepsilon + \mathcal{O}(\varepsilon^2)$

The argument does not suffice to compare spectra of P_A and ${}_A P$

$$\hat{P} = \begin{pmatrix} 1 - \varepsilon^3 - \varepsilon^4 & \varepsilon^3 + \varepsilon^4 & 0 \\ \varepsilon^3 & 1 - \varepsilon^3 & 0 \\ 0 & \varepsilon & 1 - \varepsilon \end{pmatrix}$$

Laplace transforms

$u \in \mathbb{C} \Rightarrow \mathbb{E}^x[e^{u\tau_A^+}]$ exists for

$$|e^{-u}| > 1 - p_{\text{in}}(A) \quad (*)$$

Follows from $\mathbb{P}^y\{\tau_A^+ > n\} \leq (1 - p_{\text{in}}(A))^n \quad \forall y \in A^c$

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Proposition [Feynman–Kac type relation]

Under (*),

$$\begin{cases} (P\phi)(x) = e^{-u} \phi(x) & x \in A^c \\ \phi(x) = \bar{\phi}(x) & x \in A \end{cases}$$

admits unique solution $\phi(x) = \mathbb{E}^x[e^{u\tau_A} \bar{\phi}(X_{\tau_A})]$, $\tau_A = \inf\{n \geq 0: X_n \in A\}$

Proof:

Laplace transforms

Corollary [Reduction to eigenvalue problem on A]

Under (\star) , $P\phi = e^{-u}\phi$ in \mathcal{X} \Leftrightarrow ${}_A P^u \phi = e^{-u}\phi$ in A
where ${}_A P^u(x, y) = \mathbb{E}^x[e^{u(\tau_A^+ - 1)} \mathbb{1}_{\{X_{\tau_A^+} = y\}}]$ is such that ${}_A P^0 = {}_A P$

Proof of \Rightarrow :

Laplace transforms

Proposition

$$\|_A P^u - {}_A P^0\| \leq \frac{|1 - e^{-u}| \sup_{x \in A} \mathbb{E}^x[\tau_A^+ - 1]}{1 - |1 - e^{-u}| \sup_{x \in A^c} \mathbb{E}^x[\tau_A^+]} \leq \frac{|1 - e^{-u}| p_{\text{out}}(A)}{p_{\text{in}}(A) - |1 - e^{-u}|}$$

Main result – nondegenerate case

Algorithm in **nondegenerate** case:

- ▷ **Assume** $\exists x \in \mathcal{X}$ such that $1 - P(x, x) \gg 1 - P(y, y) \forall y \neq x$
- ▷ Take $A = \mathcal{X} \setminus \{x\}$ (A is a good set)
- ▷ Then $\mathbb{1} - P$ has ev $1 - \lambda = P(x, x)[1 + \mathcal{O}(p_{\text{in}}(A)/p_{\text{out}}(A))]$ $\in \mathbb{R}$
- ▷ Compute ${}_A P$ and start again with P replaced by ${}_A P$

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Theorem [Baudel & B, 2017]

- ▷ Non-degenerate case: $\exists A_1 \subset A_2 \subset \dots \subset A_n = \mathcal{X}$ s.t.
 $\#(A_{k+1} \setminus A_k) = 1$, each A_k good set for ${}_A P$
Renumber states s.t. $A_k = \{1, \dots, k\}$. Then
- ▷ $\lambda_0 = 1, \lambda_k = 1 - \mathbb{P}^{k+1} \{ \tau_{A_k}^+ < \tau_{k+1}^+ \} \left[1 + \mathcal{O} \left(\frac{p_{\text{out}}(A_k | A_{k+1})}{p_{\text{in}}(A_k | A_{k+1})} \right) \right] \in \mathbb{R}$

Main result – nondegenerate case

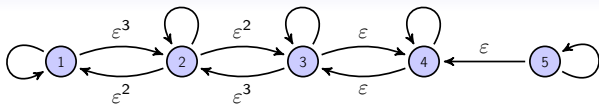
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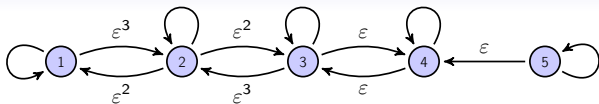
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- ▶ k th right eigenvector ϕ_k close to $\mathbb{P}^x\{\tau_{k+1} < \tau_{A_k}\}$
- ▶ k th left eigenvector π_k close to **quasistationary distribution (QSD)** of P_{A_k} (left eigenvect of P_{A_k} for Perron–Frobenius principal eigenval)

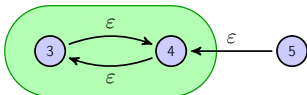
Algorithm in degenerate case



Algorithm in degenerate case



Degenerate part, leading order:



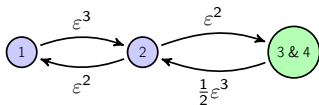
Eigenvalues:

1

$1 - \epsilon$

$1 - 2\epsilon$

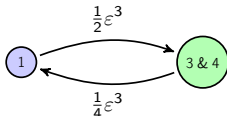
Effective trace process:



Eigenvalues:

$1 - 2\epsilon^2$

Trace on $\{1, 3\&4\}$:



$1 - \frac{3}{4}\epsilon^3$

1

2. Continuous-space Markov chains and SDEs

$$\mathbb{P}\{X_{n+1} \in A | X_n = x\} = \int_A k_\sigma(x, y) dy$$

Deterministic Poincaré maps

$$\text{ODE} \quad \dot{z} = f(z) \quad z \in \mathbb{R}^n$$

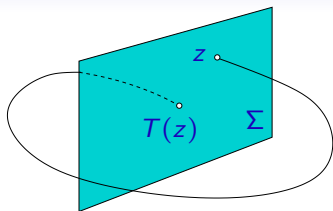
$$\text{Flow: } z_t = \varphi_t(z_0)$$

$\Sigma \subset \mathbb{R}^n$: $(n-1)$ -dimensional manifold

Poincaré map (or first-return map):

$$T: \Sigma \rightarrow \Sigma$$

$$T(z) = \varphi_\tau(z) \text{ where } \tau = \inf\{t > 0: \varphi_t(z) \in \Sigma\}$$



Deterministic Poincaré maps

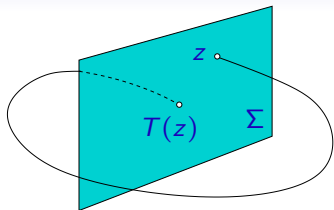
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Benefits:

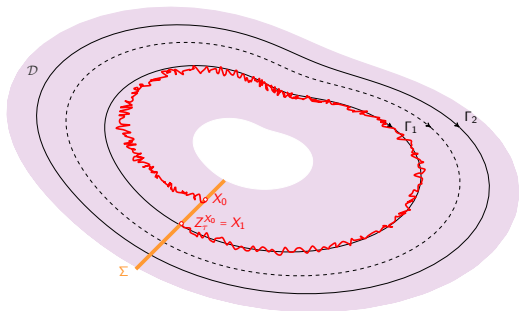
1. **Dimension reduction**: T is an $(n-1)$ -dimensional map
2. **Stability** of periodic orbits: no neutral direction
3. **Bifurcations** of periodic orbits easier to study (period doubling, Hopf, ...)

Question: how about SDEs

$$dz_t = f(z_t) dt + \sigma g(z_t) dW_t ?$$

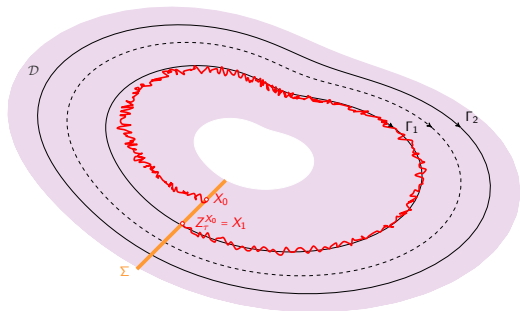
Random Poincaré maps

$dz_t = f(z_t) dt + \sigma g(z_t) dW_t \Rightarrow$ Sample path $(Z_t^{z_0}(\omega))_{t \geq 0}$



Random Poincaré maps

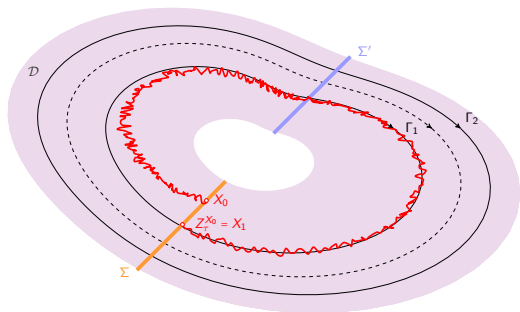
$$dz_t = f(z_t) dt + \sigma g(z_t) dW_t \quad \Rightarrow \quad \text{Sample path } (Z_t^{z_0}(\omega))_{t \geq 0}$$



 $z_0 = X_0 \in \Sigma \quad \Rightarrow \quad \inf\{t > 0: Z_t^{X_0} \in \Sigma\} = 0$

Random Poincaré maps

$$dz_t = f(z_t) dt + \sigma g(z_t) dW_t \quad \Rightarrow \quad \text{Sample path } (Z_t^{z_0}(\omega))_{t \geq 0}$$



$$\triangle! \quad z_0 = X_0 \in \Sigma \quad \Rightarrow \quad \inf\{t > 0: Z_t^{X_0} \in \Sigma\} = 0$$

$$\text{Solution: } \tau_0 = 0, \quad \tau'_{n+1} = \inf\{t > \tau_n: Z_t^{X_0} \in \Sigma'\} \\ \tau_{n+1} = \inf\{t > \tau'_{n+1}: Z_t^{X_0} \in \Sigma\}$$

$$X_n = Z_{\tau_n}^{X_0} \in \Sigma \quad \Rightarrow \quad (X_n)_{n \geq 0} \text{ is a Markov chain} \quad K(x, A) := \mathbb{P}^x\{X_1 \in A\}$$

$(X_n, \omega) \mapsto X_{n+1}$: random Poincaré map

[J. Weiss, E. Knobloch, 1990], [P. Hitczenko, G. Medvedev, 2009]

Continuous-space Markov chains

$(X_n)_{n \in \mathbb{N}_0}$ Markov chain in $\mathcal{X} \subset \mathbb{R}^d$ with kernel K_σ :

$$\mathbb{P}\{X_{n+1} \in A | X_n = x\} = K_\sigma(x, A) = \int_A K_\sigma(x, dy)$$

- ▷ $K_0(x, A) = \mathbb{1}_{\{\Pi(x) \in A\}}$ defined by deterministic map $\Pi : \mathcal{X} \rightarrow \mathcal{X}$
- ▷ For $\sigma > 0$, K_σ admits continuous density k_σ

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Example 1: Randomly perturbed map

$$X_{n+1} = \Pi(X_n) + \sigma \xi_{n+1}$$

$(\xi_n)_{n \geq 1}$ i.i.d. r.v. with density (e.g. $\sigma \xi_n$ Gaussian of variance σ^2)

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- ▷ For $\sigma > 0$, K_σ admits continuous density k_σ

Example 1: Randomly perturbed map

$$X_{n+1} = \Pi(X_n) + \sigma \xi_{n+1}$$

$(\xi_n)_{n \geq 1}$ i.i.d. r.v. with density (e.g. $\sigma \xi_n$ Gaussian of variance σ^2)

Example 2: Random Poincaré map

SDE

$$dz_t = f(z_t) dt + \sigma g(z_t) dW_t$$

X_n suitably defined location of n th return to surface of section $\Sigma \subset \mathcal{X}$

Assumptions

Assumption 1: Deterministic dynamics

$\Pi : \mathcal{X} \rightarrow \mathcal{X}$ admits positively invariant compact set $\mathcal{X}_0 \subset \mathcal{X}$, finitely many limit sets in \mathcal{X}_0 , all hyperbolic fixed points, N of which are stable

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K_σ satisfies LDP with good rate function I ($K_\sigma(x, A) \sim e^{-\inf_A I(x, \cdot)/\sigma^2}$)
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Assumption 4: Uniform positivity (Doebelin-type condition)

$\forall x_i^*$ stable fixed point, $\exists B_i$ nbh of x_i^* s.t. $k_i =_{B_1 \cup \dots \cup B_i} k_{B_i}$ satisfies

$$\sup_{x \in B_i} k_i^n(x, y) \leq L \inf_{x \in B_i} k_i^n(x, y) \quad \forall y \in B_i \quad \text{for some } L \in (1, 2), n(\sigma) \in \mathbb{N}$$

Metastable hierarchy (SDE case)

Freidlin–Wentzell theory:

Rate function: $I_{[0,T]}(\gamma) = \frac{1}{2} \int_0^T (\dot{\gamma}_s - f(\gamma_s))^T [gg^T(\gamma_s)]^{-1} (\dot{\gamma}_s - f(\gamma_s)) ds$

Large-deviation principle: $\mathbb{P}\{(z_t)_{0 \leq t \leq T} \in \Lambda\} \simeq e^{-\inf_{\gamma \in \Lambda} I_{[0,T]}(\gamma)/\sigma^2}$

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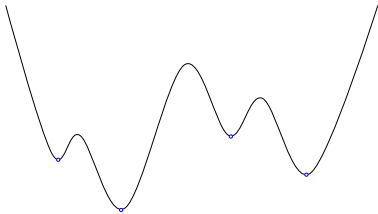
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$\exists \theta > 0$ s.t. $\forall 2 \leq k \leq N$

$$\min_{\ell < k} H(k, \ell) \leq \min_{\substack{i < k \\ j \neq i}} H(i, j) - \theta$$



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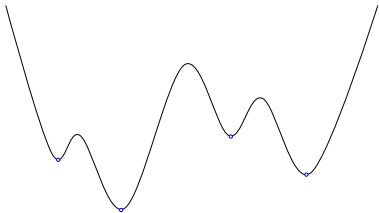
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Remark: Using Doob's h -transform, one may replace Assumption 3 by

Assumption 3': Confinement

$\exists \theta' > 0$ such that $\min_i H(i, \partial D) \geq \max_{i \neq j} H(i, j) + \theta'$

Main result

Theorem [Baudel & B, 2017]

▷ Non-degenerate case (x_1^*, \dots, x_N^* in metastable order)

◊ Eigenvalues of K_σ :

$$\lambda_0 = 1$$

$$\lambda_k = 1 - \mathbb{P}^{\hat{\pi}_0^{k+1}} \{ \tau_{B_1 \cup \dots \cup B_k}^+ < \tau_{B_{k+1}}^+ \} [1 + \mathcal{O}(e^{-\theta/\sigma^2})] \in \mathbb{R} \quad 1 \leq k < N$$

$$|\lambda_k| < \varrho = 1 - \frac{c}{\log(\sigma^{-1})} \quad k \geq N$$

where $\hat{\pi}_0^{k+1}$ is a certain QSD on B_{k+1} and $c, \theta > 0$

- ◊ k th right eigenfunction ϕ_k close to $\mathbb{P}^x \{ \tau_{B_{k+1}} < \tau_{B_1 \cup \dots \cup B_k} \}$
- ◊ k th left eigenfunction π_k close to QSD of $K_{(B_1 \cup \dots \cup B_k)^c}$

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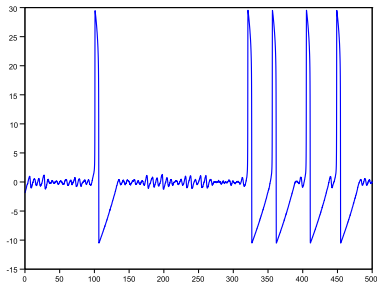
$$\lambda_k = 1 - \mathbb{P}^{\hat{\pi}_0^{k+1}} \{ \tau_{B_1 \cup \dots \cup B_k}^+ < \tau_{B_{k+1}}^+ \} [1 + \mathcal{O}(e^{-\theta/\sigma^2})] \in \mathbb{R} \quad 1 \leq k < N$$

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- ▷ Expected hitting times:
$$\mathbb{E}^x [\tau_{B_1 \cup \dots \cup B_k}] = [1 - \lambda_k]^{-1} [1 + \mathcal{O}(e^{-\kappa/\sigma^2})] \quad \forall x \in B_{k+1}, 1 \leq k \leq N-1$$
 - ▷ Degenerate case: similar to finite chain...

3. FitzHugh–Nagumo equations



Stochastic FitzHugh–Nagumo equation

$$dx_t = \frac{1}{\varepsilon} [x_t - x_t^3 + y_t] dt$$

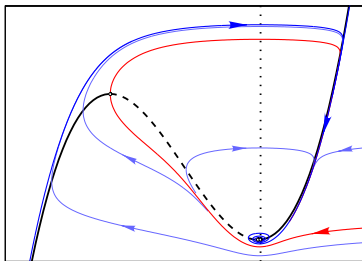
neuron membrane potential

$$dy_t = [a - x_t - by_t] dt$$

open ion channels

- ▷ $b = 0$ for simplicity in this talk, bifurcation parameter $\delta := \frac{3a^2-1}{2}$

$$\varepsilon = 0.1$$
$$\delta = 0.02$$



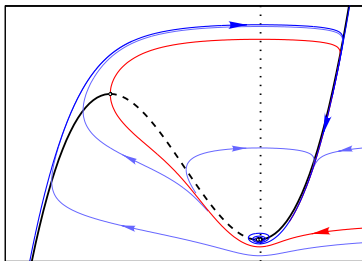
Stochastic FitzHugh–Nagumo equation

$$dx_t = \frac{1}{\varepsilon} [x_t - x_t^3 + y_t] dt + \frac{\sigma_1}{\sqrt{\varepsilon}} dW_t^{(1)} \quad \text{neuron membrane potential}$$

$$dy_t = [a - x_t - by_t] dt + \sigma_2 dW_t^{(2)} \quad \text{open ion channels}$$

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- ▷ $W_t^{(1)}, W_t^{(2)}$: independent Wiener processes
- ▷ $0 < \sigma_1, \sigma_2 \ll 1$, $\sigma = \sqrt{\sigma_1^2 + \sigma_2^2}$

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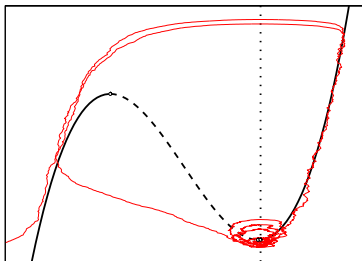
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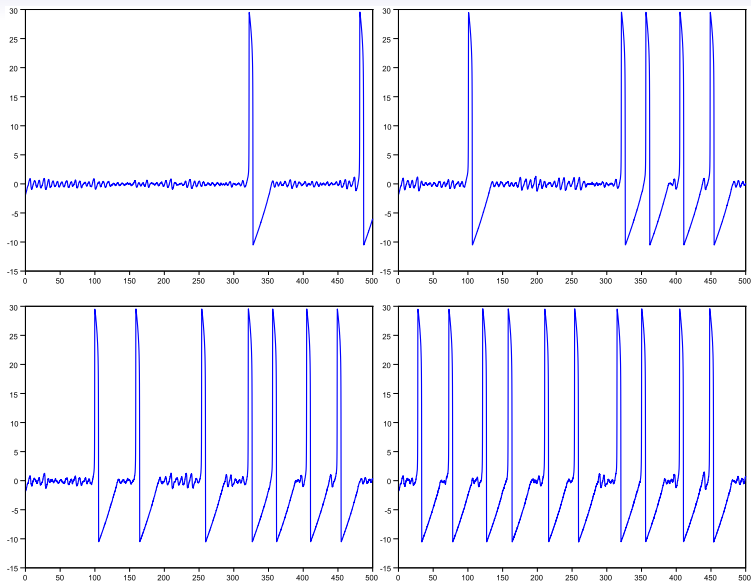
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$$\begin{aligned}\varepsilon &= 0.1 \\ \delta &= 0.02 \\ \sigma_1 &= \sigma_2 = 0.03\end{aligned}$$

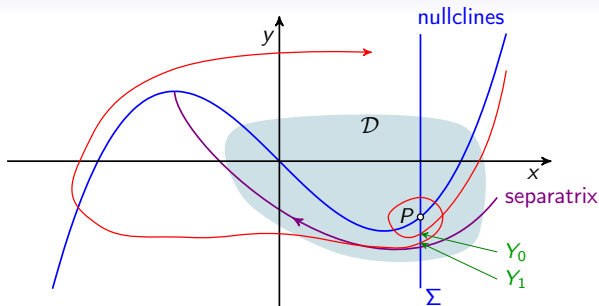


Mixed-mode oscillations (MMOs)



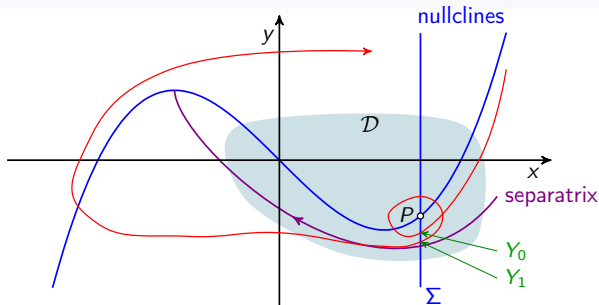
Time series $t \mapsto -x_t$ for $\varepsilon = 0.01$, $\delta = 3 \cdot 10^{-3}$, $\sigma = 1.46 \cdot 10^{-4}, \dots, 3.65 \cdot 10^{-4}$

Random Poincaré map



Y_0, Y_1, \dots substochastic Markov chain describing process killed on ∂D
Number of small oscillations: $N = \inf\{n \geq 1: Y_n \notin \Sigma\}$

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Theorem 1 [B & Landon, 2012]

N is asymptotically geometric: $\lim_{n \rightarrow \infty} \mathbb{P}\{N = n + 1 | N > n\} = 1 - \lambda_0$

where $\lambda_0 \in \mathbb{R}_+$: principal eigenvalue of the kernel K , $\lambda_0 < 1$ if $\sigma > 0$

Random Poincaré map

Theorem 1 [B & Landon, 2012]

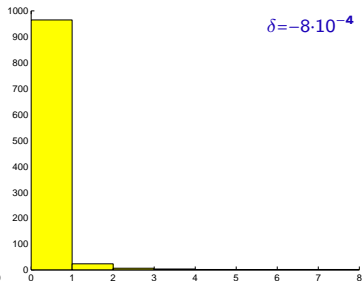
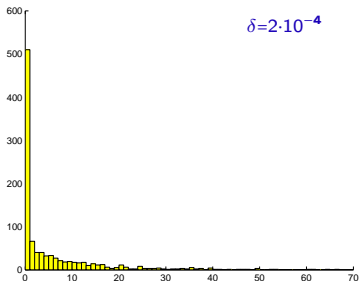
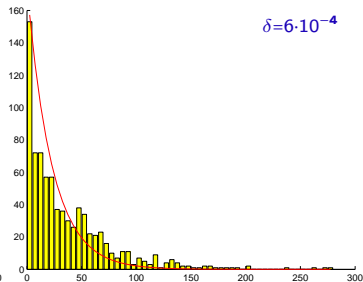
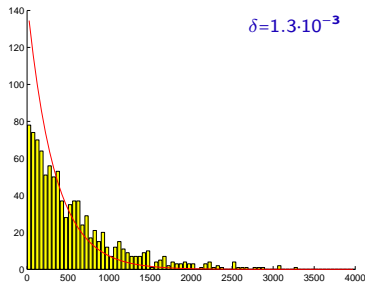
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Proof:

Histograms of distribution of N (1000 spikes)

$$\sigma = \varepsilon = 10^{-4}$$



Weak-noise regime

Theorem 2 [B & Landon, 2012]

Assume ε and $\delta/\sqrt{\varepsilon}$ sufficiently small

There exists $\kappa > 0$ s.t. for $\sigma^2 \leq (\varepsilon^{1/4}\delta)^2 / \log(\sqrt{\varepsilon}/\delta)$

▷ Principal eigenvalue:

$$1 - \lambda_0 \leq \exp\left\{-\kappa \frac{(\varepsilon^{1/4}\delta)^2}{\sigma^2}\right\}$$

▷ Expected number of small oscillations:

$$\mathbb{E}^{\mu_0}[N] \geq C(\mu_0) \exp\left\{\kappa \frac{(\varepsilon^{1/4}\delta)^2}{\sigma^2}\right\}$$

where $C(\mu_0)$ = probability of starting on Σ above separatrix

Proof:

Dynamics near the separatrix

Change of variables:

- ▷ Translate to Hopf bif. point
- ▷ Scale space and time
- ▷ Straighten nullcline $\dot{x} = 0$

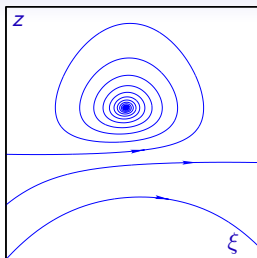
⇒ variables (ξ, z) where nullcline: $\{z = \frac{1}{2}\}$

$$d\xi_t = \left(\frac{1}{2} - z_t - \frac{\sqrt{\varepsilon}}{3} \xi_t^3 \right) dt$$

$$dz_t = \left(\mu + 2\xi_t z_t + \frac{2\sqrt{\varepsilon}}{3} \xi_t^4 \right) dt$$

where

$$\mu = \frac{\delta}{\sqrt{\varepsilon}}$$



Dynamics near the separatrix

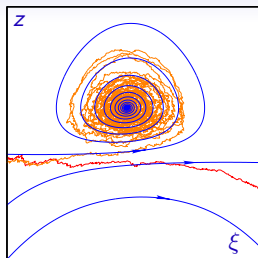
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$$dz_t = \left(\tilde{\mu} + 2\xi_t z_t + \frac{2\sqrt{\varepsilon}}{3} \xi_t^4 \right) dt - 2\tilde{\sigma}_1 \xi_t dW_t^{(1)} + \tilde{\sigma}_2 dW_t^{(2)}$$



where

$$\tilde{\mu} = \frac{\delta}{\sqrt{\varepsilon}} - \tilde{\sigma}_1^2 \quad \tilde{\sigma}_1 = -\sqrt{3} \frac{\sigma_1}{\varepsilon^{3/4}} \quad \tilde{\sigma}_2 = \sqrt{3} \frac{\sigma_2}{\varepsilon^{3/4}}$$

Upward drift dominates if $\tilde{\mu}^2 \gg \tilde{\sigma}_1^2 + \tilde{\sigma}_2^2 \Rightarrow (\varepsilon^{1/4} \delta)^2 \gg \sigma_1^2 + \sigma_2^2$

Rotation around P : use that $2z e^{-2z-2\xi^2+1}$ is constant for $\tilde{\mu} = \varepsilon = 0$

Take $A = \{z > \tilde{\mu}^{1-\gamma}\}$ with $0 < \gamma < \frac{1}{4}$



From below to above threshold

Linear approximation:

$$dz_t^0 = (\tilde{\mu} + tz_t^0) dt - \tilde{\sigma}_1 t dW_t^{(1)} + \tilde{\sigma}_2 dW_t^{(2)}$$

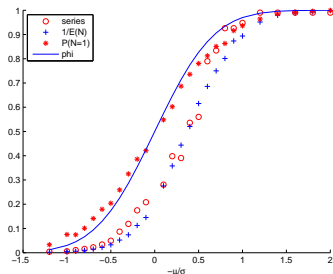
$$\Rightarrow \mathbb{P}\{\text{no small osc}\} \simeq \Phi\left(-\pi^{1/4} \frac{\tilde{\mu}}{\sqrt{\tilde{\sigma}_1^2 + \tilde{\sigma}_2^2}}\right) \quad \Phi(x) = \int_{-\infty}^x \frac{e^{-y^2/2}}{\sqrt{2\pi}} dy$$

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*: $\mathbb{P}\{\text{no small osc}\}$

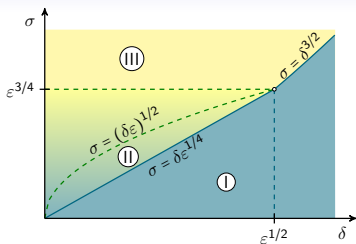
+: $1/\mathbb{E}[N]$

o: $1 - \lambda_0$

curve: $x \mapsto \Phi(\pi^{1/4} x)$

$$x = -\frac{\tilde{\mu}}{\sqrt{\tilde{\sigma}_1^2 + \tilde{\sigma}_2^2}} = -\frac{\epsilon^{1/4}(\delta - \sigma_1^2/\epsilon)}{\sqrt{\sigma_1^2 + \sigma_2^2}}$$

Summary: Parameter regimes



$$\sigma_1 = \sigma_2:$$

$$\mathbb{P}\{N = 1\} \simeq \Phi\left(-\frac{(\pi\epsilon)^{1/4}(\delta - \sigma^2/\epsilon)}{\sigma}\right)$$

$$\Phi(x) = \frac{1}{\sqrt{2\pi}} \int_{-\infty}^x e^{-y^2/2} dy$$

see also

[Muratov & Vanden Eijnden '08]

Regime I: rare isolated spikes

Theorem 2 applies ($\delta \ll \epsilon^{1/2}$)

Interspike interval \simeq exponential

Regime II: clusters of spikes

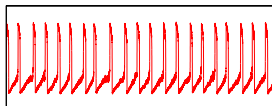
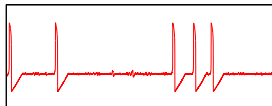
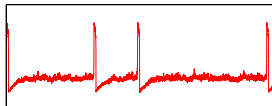
interspike osc asympt geometric

$\sigma = (\delta\epsilon)^{1/2}$: geom(1/2)

Regime III: repeated spikes

$\mathbb{P}\{N = 1\} \simeq 1$

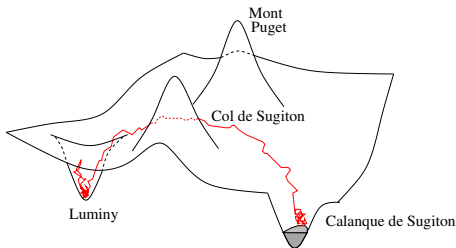
Interspike interval \simeq constant



References, parts 1–3

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- ▷ Manon Baudel & N. B., *Spectral theory for random Poincaré maps*, *SIAM J. Math. Analysis* **49**, 4319–4375 (2017)
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- ▷ Garrett Birkhoff, *Extensions of Jentzsch's theorem*, *Trans. Amer. Math. Soc.*, 85:219–227, 1957.

4. The case of reversible SDEs: The potential-theoretic approach



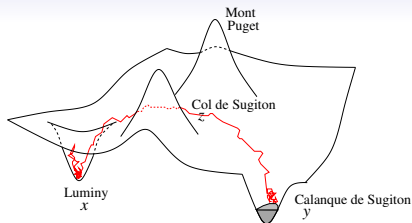
Reversible diffusion in a double-well

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

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



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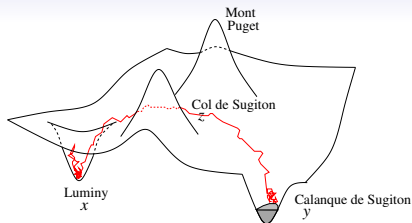
Arrhenius' law (1889): $\mathbb{E}[\tau_y^x] \simeq e^{[V(z)-V(x)]/\varepsilon}$

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 : $\lambda_1 < 0 < \lambda_2 \leq \dots \leq \lambda_d$

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



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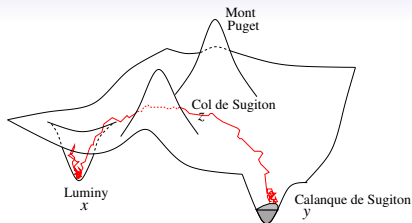
Eigenvalues of Hessian of V at minimum x : $0 < \nu_1 \leq \nu_2 \leq \dots \leq \nu_d$

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

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

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: $\pi(dx) = \frac{1}{Z} e^{-V(x)/\varepsilon} dx \Rightarrow \mathcal{L}^\dagger \pi = 0$

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- ▷ **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:

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

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- ▷ 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

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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]

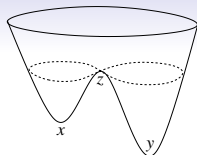
Let $\mathcal{U}_{AB} = \{f: \nabla \cdot f|_{(A \cup B)^c} = 0, \int_{\partial A} f(x) \cdot n_A(x) \sigma(dx) = 1\}$. Then

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

Proof of Eyring–Kramers law

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

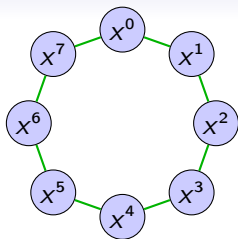
▷ A, B small balls around x, y



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

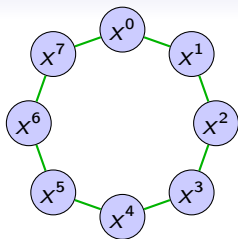


$$dx_t^i = [x_t^i - (x_t^i)^3] dt + \frac{\gamma}{2} [x_t^{i+1} - 2x_t^i + x_t^{i-1}] dt + \sqrt{2\varepsilon} dW_t^i$$

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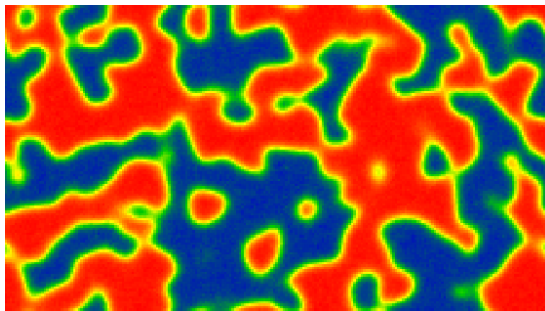
Gradient system $dx_t = -\nabla V(x_t) dt + \sqrt{2\varepsilon} dW_t$

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

Coarsening dynamics with noise

([Link to simulation](#))

5. The stochastic Allen–Cahn PDEs



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)

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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 $\gamma = 2 \frac{N^2}{L^2}$

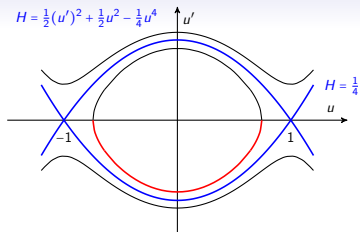
Stationary solutions: $u_0''(x) = -u_0(x) + u_0(x)^3$ critical points of V

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

Stationary solutions

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

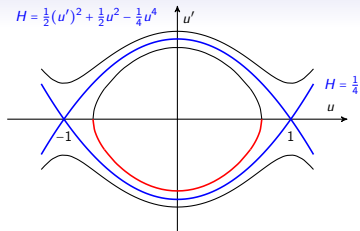
- ▷ $u_{\pm}(x) \equiv \pm 1$
- ▷ $u_0(x) \equiv 0$
- ▷ Nonconstant solutions satisfying b.c.
(expressible in terms of Jacobi elliptic fcts)



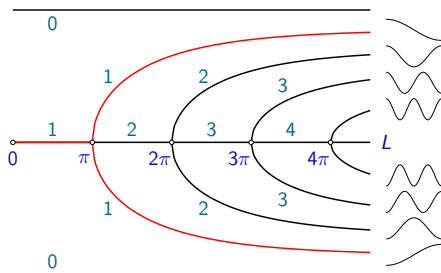
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- ▷ $u_0(x) \equiv 0$
- ▷ Nonconstant solutions satisfying b.c.
(expressible in terms of Jacobi elliptic fcts)
- ▷ Neumann b.c: $2k$ nonconstant solutions when $L > k\pi$



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 $\nu_k = (\frac{\beta k \pi}{L})^2 + 2$

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.)

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

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[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

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

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- ▷ 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**

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

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

- ▷ Spectral Galerkin approximation: $u(t, x) = \sum_{|k| \leq N} z_k(t) e_k(x)$ (Fourier)

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$$\Rightarrow \frac{1}{\varepsilon} V[u_0 + \sqrt{\varepsilon} u_\perp] = \frac{1}{\varepsilon} \underbrace{\left(\frac{1}{4} u_0^4 - \frac{1}{2} u_0^2 \right)}_{V_0(u_0)} + Q_{u_0}[u_\perp] + \sqrt{\varepsilon} R_{u_0}[u_\perp]$$

where

$$\begin{cases} Q_{u_0}[u_\perp] = \frac{1}{2} \int_0^L [u_\perp'(x)^2 - (1 - 3u_0^2) u_\perp(x)^2] dx = \frac{1}{2} \langle u_\perp, [-\Delta - (1 - 3u_0^2)] u_\perp \rangle \\ R_{u_0}[u_\perp] = u_0 \int_0^L u_\perp(x)^3 dx + \sqrt{\varepsilon} \int_0^L u_\perp(x)^4 dx \quad (\text{remainder}) \end{cases}$$

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▷ Dirichlet principle with $h = h(u_0)$ s.t. $h'(u_0) = -\frac{1}{c} e^{V_0(u_0)/\varepsilon}$, $c \simeq \sqrt{\frac{2\pi\varepsilon}{|\lambda_0|}}$

$$\begin{aligned} \text{cap}(A, B) \leq \mathcal{E}(h) &= \frac{\varepsilon^{1+\frac{N}{2}}}{c^2} \int_{-1}^1 e^{V_0(u_0)/\varepsilon} \underbrace{\int e^{-Q_{u_0}[u_\perp]} e^{-\sqrt{\varepsilon} R_{u_0}[u_\perp]} du_\perp}_{=} du_0 \\ &= \sqrt{\frac{(2\pi)^N}{\det[-\Delta_\perp - (1 - 3u_0^2)]}} \mathbb{E} \gamma [e^{-\sqrt{\varepsilon} R_{u_0}}] \end{aligned}$$

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

- ▷ Thomson principle with divergence-free unit flow $f = K^{-1} e^{-Q_0[u_\perp]} e_{u_0}$

$$\text{Normalisation } K = \varepsilon^{\frac{N}{2}} \int e^{-Q_0[u_\perp]} du_\perp = \sqrt{\frac{(2\pi\varepsilon)^N}{\det[-\Delta_\perp - 1]}}$$

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- ▷ Conclusion: $\text{cap}(A, B) = \varepsilon \sqrt{\frac{|\lambda_0|}{2\pi\varepsilon}} \sqrt{\frac{(2\pi\varepsilon)^N}{\det[-\Delta_\perp - 1]}} [1 + \mathcal{O}(\varepsilon)]$

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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:

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

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- ▷ 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 :

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

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- ▷ 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. $|k| \leq N = \delta^{-1}$:

$$w_N(x, t) = \sum_{|k| \leq N} a_k(t) \frac{1}{L} e^{i\Omega k \cdot x} \quad a_k = \int_0^t e^{-\mu_k(t-s)} dW_s^{(k)}$$
$$\mu_k = (\Omega|k|)^2 \quad \Omega = \beta\pi/L$$

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

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

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▷ **Wick powers**

$$:\phi_N^2: = \phi_N^2 - C_N$$

$$:\phi_N^3: = \phi_N^3 - 3C_N \phi_N$$

$$:\phi_N^4: = \phi_N^4 - 6C_N \phi_N^2 + 3C_N^2$$

have zero mean and uniformly bounded variance (when integrated)

Computation of the prefactor

- ▷ Consider for simplicity $L < \beta\pi \Rightarrow$ transition state in 0
- ▷ Galerkin-truncated renormalised potential

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

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

- ▷ Symmetry argument:

$$\int_{B^c} h_{A,B}(z) e^{-V_N(z)/\varepsilon} dz = \frac{1}{2} \int e^{-V_N(z)/\varepsilon} dz = \frac{1}{2} \mathcal{Z}_N(\varepsilon)$$

- ▷ $\mathcal{Z}_N(\varepsilon) \simeq 2 \prod_{|k| \leq N} \sqrt{\frac{2\pi\varepsilon}{\nu_k}} e^{-V_N(L,0)/\varepsilon}$ where $-V_N(L,0) = \frac{1}{4}L^2 + \frac{3}{2}L^2 C_N \varepsilon$

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

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

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Thanks for your attention!