

SPA 2017

Contributed Session: Interacting particle systems

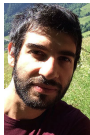
# Metastability for interacting particles in double-well potentials and Allen–Cahn SPDEs

Nils Berglund

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Москва / Moscow, July 28 2017

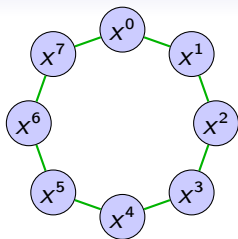
Joint works with Giacomo Di Gesù (Vienna), Bastien Fernandez (Paris),  
Barbara Gentz (Bielefeld) and Hendrik Weber (Warwick)



# Examples of particle systems

Example 1 [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

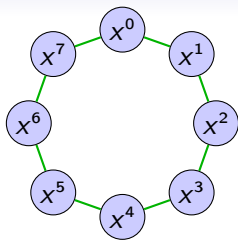


$$dx_t^i = [x_t^i - (x_t^i)^3] dt + \frac{\gamma}{2} [x_t^{i+1} - 2x_t^i + x_t^{i-1}] dt + \sqrt{2\varepsilon} dW_t^i$$

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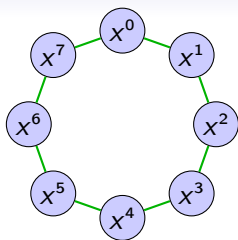
Gradient system  $dx_t = -\nabla V(x_t) dt + \sqrt{2\varepsilon} dW_t$

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

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Example 2 Replace circle by 2D torus  $(\mathbb{Z}/N\mathbb{Z})^2$

Example 3 [B, Dutercq, J Stat Phys 2016]: Same  $V$  + constraint  $\sum_i x^i = 0$

# Coarsening dynamics with noise

([Link to simulation](#))

# General gradient systems with noise

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

$V : \mathbb{R}^N \rightarrow \mathbb{R}$ : confining potential, class  $\mathcal{C}^2$

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- ▷ Stationary points:  $\mathcal{X} = \{x : \nabla V(x) = 0\}$
- ▷ Local minima:  $\mathcal{X}_0 = \{x \in \mathcal{X} : \text{all ev of Hessian } \nabla^2 V(x) \text{ are } > 0\}$
- ▷ Saddles of Morse index 1:  $\mathcal{X}_1 = \{x \in \mathcal{X} : \nabla^2 V(x) \text{ has 1 negative ev } \}$

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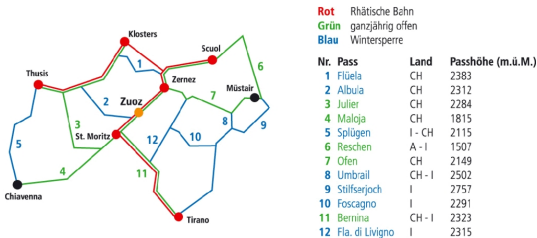
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Dynamics  $\sim$  markovian jump process on  $\mathcal{G} = (\mathcal{X}_0, \mathcal{E})$ ,  $\mathcal{E} \subset \mathcal{X}_1$

[Фрейдлин & Вентцел' / Freidlin & Wentzell 1970], [Bovier et al 2004]





# Eyring–Kramers law

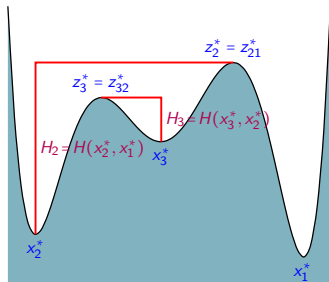
Definition: Communication height

$$\begin{aligned} H(x_i^*, x_j^*) &= \inf_{\gamma: x_i^* \rightarrow x_j^*} \sup_t V(\gamma_t) - V(x_i^*) \\ &= V(z_{ij}^*) - V(x_i^*) \end{aligned}$$

Definition: Metastable hierarchy

$$x_1^* < x_2^* < \dots < x_n^* \Leftrightarrow \exists \theta > 0: \forall k$$

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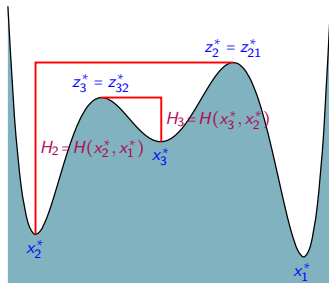
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Theorem: Eyring–Kramers law [Bovier, Eckhoff, Gayraud, Klein 2004]

$\tau_k$  = first-hitting time of nbh of  $\{x_1^*, \dots, x_k^*\}$        $\lambda_k = k^{\text{th}}$  ev of generator

$$\mathbb{E}^{x_k^*}[\tau_{k-1}] = \frac{2\pi}{|\lambda_-(z_k^*)|} \sqrt{\frac{|\det \nabla^2 V(z_k^*)|}{\det \nabla^2 V(x_k^*)}} e^{H_k/\varepsilon} [1 + \mathcal{O}_\varepsilon(1)] \simeq |\lambda_k|^{-1}$$

# Potential landscape for Example 1

$$V(x) = \sum_{i \in \mathbb{Z}/N\mathbb{Z}} U(x^i) + \frac{\gamma}{4} \sum_{i \in \mathbb{Z}/N\mathbb{Z}} (x^{i+1} - x^i)^2 \quad U(\xi) = \frac{1}{4}\xi^4 - \frac{1}{2}\xi^2$$

$\gamma = 0$ :  $\mathcal{X} = \{-1, 0, 1\}^N$ ,  $\mathcal{X}_0 = \{-1, 1\}^N$ ,  $\mathcal{X}_1 = \{x \in \mathcal{X} : \text{one } x^i = 0\}$   
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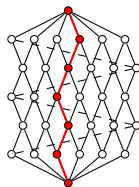
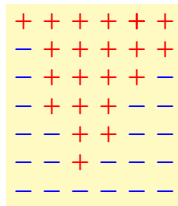
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**Theorem** [BFG, Nonlinearity 2007]

No bifurcation for  $0 \leq \gamma \leq \gamma^*(N)$

where  $\gamma^*(N) > \frac{1}{4} \quad \forall N \geq 2$

$V_\gamma(z_\gamma^*) = V_0(z_0^*) + \gamma(\# \text{ interfaces}) + \dots$   
Ising-like dynamics



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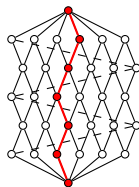
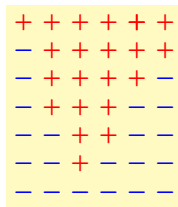
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**Theorem** [BFG, Nonlinearity 2007]

$\gamma > \frac{1}{2 \sin^2(\pi/N)} \asymp N^2 \Leftrightarrow \mathcal{X}_0 = \{\pm(1, \dots, 1)\}$ ,  $\mathcal{X}_1 = \{0\} \Leftrightarrow$  Synchronization

# Limitations of the standard Eyring–Kramers law

▷ **Question 1:**

What happens when  $V$  is invariant under a group of symmetries?

Representation theory of finite groups  $\rightarrow$  clustering of eigenvalues

[B, Dutercq, JoTP 2015]

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What happens when  $V$  has saddles with zero eigenvalues?

( $\det \nabla^2 V(z^*) = 0$  at bifurcations)

Eyring–Kramers law with  $\varepsilon$ -dependent prefactor

[B, Gentz, MPRF 2010]

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## ▷ Question 3:

What happens when  $\gamma \sim N^2$  and  $N \rightarrow \infty$  in Example 1?

One expects convergence to Allen–Cahn SPDE

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

where  $\xi$  is space-time white noise

Is there an Eyring–Kramers law for such SPDEs?



# Deterministic Allen–Cahn PDE

[Chafee & Infante 74, Allen & Cahn 75]

$$\partial_t u(x, t) = \partial_{xx} u(x, t) + f(u(x, t))$$

- ▷  $x \in [0, L]$ ,  $L$ : bifurcation parameter
- ▷  $u(x, t) \in \mathbb{R}$
- ▷ 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 of Example 1 with  $\gamma = 2 \frac{N^2}{L^2}$

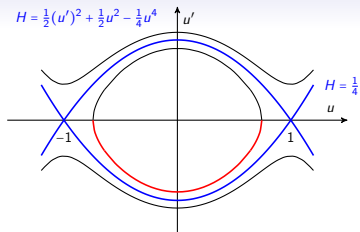
Stationary solutions:  $u_0''(x) = -u_0(x) + u_0(x)^3$  critical points of  $V$

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

# Stationary solutions

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

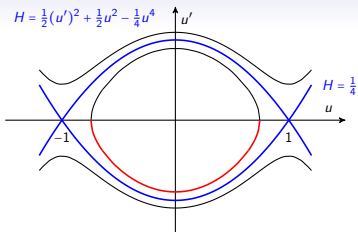
- ▷  $u_{\pm}(x) \equiv \pm 1$
- ▷  $u_0(x) \equiv 0$
- ▷ Nonconstant solutions satisfying b.c.  
(expressible in terms of Jacobi elliptic fcts)



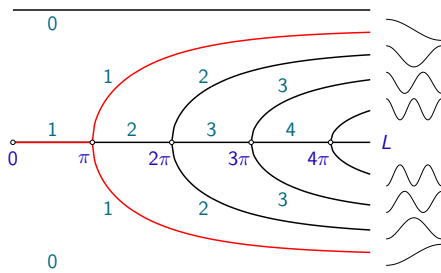
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(expressible in terms of Jacobi elliptic fcts)
- ▷ Neumann b.c:  $2k$  nonconstant solutions when  $L > k\pi$



Number of positive  
eigenvalues  
(= unstable directions)  
Transition state



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

# Eyring–Kramers law for 1D SPDEs: heuristics

$$\dot{u}_t(x) = \Delta u_t(x) + f(u_t(x)) + \sqrt{2\varepsilon} \xi(t, x) \quad (\Delta \equiv \partial_{xx}, f(u) = u - u^3)$$

Initial condition:  $u_{\text{in}}$  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, Elec J Proba 2013]

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

$$\mathbb{E}^{u_{\text{in}}}[\tau_+] = 2\pi \sqrt{\frac{1}{|\lambda_0| \nu_0} \prod_{k=1}^{\infty} \frac{\lambda_k}{\nu_k}} e^{(V[u_{\text{ts}}] - V[u_-])/\varepsilon} [1 + \mathcal{O}(\varepsilon^{1/2} |\log \varepsilon|^{3/2})]$$

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

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

converges because  $(-\Delta_{\perp} + 2)^{-1}$  is **trace class** (limit =  $\frac{\sqrt{2} \sin(L)}{\sinh(\sqrt{2}L)}$ )

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- ▷ Proof uses **spectral Galerkin approx.** and **potential-theoretic** formula

$$\mathbb{E}^{\nu_{A,B}}[\tau_B] = \frac{1}{\text{cap}_A(B)} \int_{B^c} \mathbb{P}^y \{\tau_A < \tau_B\} e^{-V(y)/\varepsilon} dy$$

# The two-dimensional case

([Link to simulation](#))

## The two-dimensional case

- ▷ Large-deviation principle: [Hairer & Weber, Ann. Fac. Sc. Toulouse, 2015]
- ▷ Naive computation of prefactor fails ( $(-\Delta_{\perp} + 2)^{-1}$  is **not** trace class):

$$\begin{aligned}\log \det[1 - 3(-\Delta_{\perp} + 2)^{-1}] &\simeq \sum_{k \in (\mathbb{N}_0^2)^*} \log\left(1 - \frac{3L^2}{|k|^2 \pi^2}\right) \\ &\simeq - \sum_{k \in (\mathbb{N}_0^2)^*} \frac{3L^2}{|k|^2 \pi^2} \simeq -\frac{3L^2}{\pi^2} \int_1^{\infty} \frac{r dr}{r^2} = -\infty\end{aligned}$$

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

**Theorem:** [Da Prato & Debussche 2003]

Let  $\xi^{\delta}$  be a mollification on scale  $\delta$  of white noise. Then

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

with  $C(\delta) = \text{Tr}((-\mathcal{P}_{\delta^{-1}} \Delta_{\perp})^{-1}) \simeq \log(\delta^{-1})$  admits local solution cv 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, Elec J Proba 2016]

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

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

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- ▷ Proof uses absolute continuity of  $e^{-V/\varepsilon}$  wrt Gaussian free field and Nelson argument for Wick powers: if  $X \in n^{\text{th}}$  Wiener chaos then

$$\mathbb{E}[X^{2p}]^{1/2p} \leq C_n (2p - 1)^{n/2} \mathbb{E}[X^2]^{1/2}$$



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**References:** Particle system: [1]; nonquadratic: [2,3]; SPDEs: [4,5]; symmetries: [6,7];

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