

Augsburger Mathematisches Kolloquium

Sharp asymptotics for metastable transition times in one- and two-dimensional Allen–Cahn SPDEs

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

Metastability

A metastable system: supercooled water

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

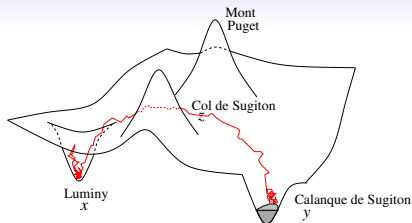
Metastability for finite-dimensional SDEs

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

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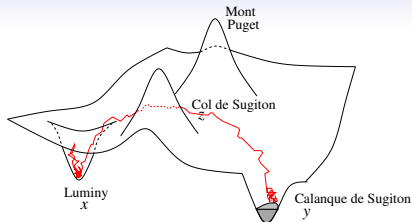
Arrhenius' law (1889): $\mathbb{E}[\tau_y^x] \simeq e^{[V(z)-V(x)]/\varepsilon}$

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

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



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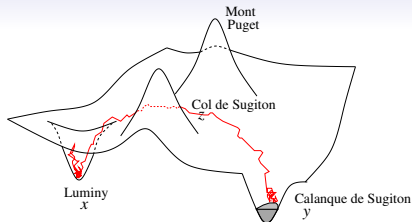
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Arrhenius' law: proved by Freidlin, Wentzell (1979) using large deviations

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



Potential-theoretic proof

“Magic” formula: for $A, B \subset \mathbb{R}^d$ disjoint sets,

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

- ▷ **Equilibrium measure:** $\nu_{A,B}$ proba measure concentrated on ∂A
- ▷ **Committer function:** $h_{A,B}(y) = \mathbb{P}^y\{\tau_A < \tau_B\}$

- ▷ **Capacity:** $\text{cap}_A(B) = \varepsilon \int_{(A \cup B)^c} \|\nabla h_{A,B}(y)\|^2 e^{-V(y)/\varepsilon} dy$

Property: $\text{cap}_A(B) = \varepsilon \inf_{h \in H^1, h|_A=1, h|_B=0} \int_{(A \cup B)^c} \|\nabla h(y)\|^2 e^{-V(y)/\varepsilon} dy$

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Proving Eyring–Kramers formula: A and B small sets around x and y

- ▷ Variational arguments: $\text{cap}_A(B) \simeq \varepsilon \sqrt{\frac{|\lambda_1|}{2\pi\varepsilon}} \sqrt{\frac{(2\pi\varepsilon)^{d-1}}{\lambda_2 \dots \lambda_d}} e^{-V(z)/\varepsilon}$
- ▷ Laplace asymptotics: $\int_{B^c} h_{A,B}(y) e^{-V(y)/\varepsilon} dy \simeq \sqrt{\frac{(2\pi\varepsilon)^d}{\nu_1 \dots \nu_d}} e^{-V(x)/\varepsilon}$
- ▷ Use Harnack inequalities to show that $\mathbb{E}^{\nu_{A,B}}[\tau_B] \simeq \mathbb{E}^x[\tau_B]$

Alternative: coupling argument by [Martinelli, Olivieri & Scoppola]

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 with potential

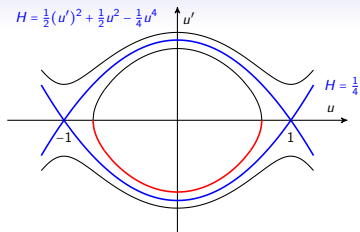
$$V(y) = \frac{N^2}{2L^2} \sum_{i=1}^N (y_{i+1} - y_i)^2 + \sum_{i=1}^N \left[-\frac{1}{2} y_i^2 + \frac{1}{4} y_i^4 \right]$$

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

Stationary solutions

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

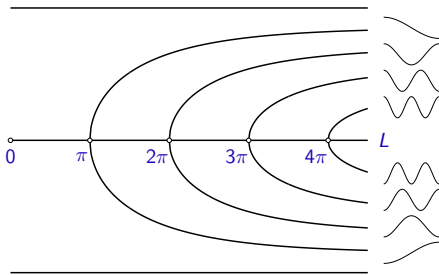
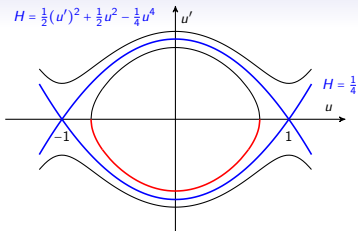
- ▷ $u_{\pm}(x) \equiv \pm 1$
- ▷ $u_0(x) \equiv 0$
- ▷ Nonconstant solutions satisfying b.c.
(expressible in terms of Jacobi elliptic fcts)



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



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

Stability of stationary solutions

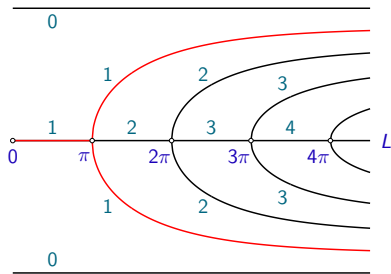
$$u_0''(x) = -u_0(x) + u_0(x)^3$$

Variational eq around u_0 : $\partial_t v_t(x) = v_t''(x) + [1 - 3u_0(x)^2]v_t(x)$

Sturm–Liouville spectrum of RHS determines stability of u_0

- ▷ $u_{\pm} \equiv \pm 1$: always stable (global minima of V)
- ▷ $u_0 \equiv 0$: always unstable, eigenvalues $-\lambda_k = 1 - \left(\frac{\beta k \pi}{L}\right)^2$
(Neumann b.c.: $\beta = 1$, periodic b.c.: $\beta = 2$)

Neumann b.c.:
Number of positive
eigenvalues
(= unstable directions)
Transition state



Coarsening dynamics

[Carr & Pego 89, Chen 04]

([Link to simulation](#))

Stochastic partial differential equations

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

\ddot{W}_{tx} : space-time white noise (formal derivative of Brownian sheet)

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Construction of mild solution via Duhamel formula:

$$\triangleright \dot{u}_t = \Delta u_t \quad \Rightarrow \quad u_t = e^{\Delta t} u_0$$

where $e^{\Delta t} \cos\left(\frac{k\pi x}{L}\right) = e^{-(k\pi/L)^2 t} \cos\left(\frac{k\pi x}{L}\right)$

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$$w_t(x) = \sum_k \int_0^t e^{-(k\pi/L)^2(t-s)} dW_s^{(k)} \cos\left(\frac{k\pi x}{L}\right) \in H^s \cap C^\alpha \quad \forall s, \alpha < \frac{1}{2}$$

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$$\triangleright \dot{u}_t = \Delta u_t + \sqrt{2\varepsilon} \ddot{W}_{tx} + f(u_t)$$

$$\Rightarrow \quad u_t = e^{\Delta t} u_0 + \sqrt{2\varepsilon} w_t + \int_0^t e^{\Delta(t-s)} f(u_s) ds =: F_t[u]$$

\Rightarrow Existence and a.s. uniqueness [Faris & Jona-Lasinio 1982]

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Fourier variables: $u_t(x) = \frac{1}{\sqrt{L}} \sum_{k=-\infty}^{\infty} z_k(t) e^{i\pi kx/L}$

$$\Rightarrow dz_k = -\lambda_k z_k dt - \frac{1}{L} \sum_{k_1+k_2+k_3=k} z_{k_1} z_{k_2} z_{k_3} dt + \sqrt{2\varepsilon} dW_t^{(k)}$$

Itô SDE, $dW_t^{(k)}$: independent Wiener processes

$$\lambda_k = -1 + (\pi k/L)^2$$

Energy functional:

$$V[u] = \frac{1}{2} \sum_{k=-\infty}^{\infty} \lambda_k |z_k|^2 + \frac{1}{4L} \sum_{k_1+k_2+k_3+k_4=0} z_{k_1} z_{k_2} z_{k_3} z_{k_4}$$

$$\Rightarrow dz_t = -\nabla V(z_t) dt + \sqrt{2\varepsilon} dW_t$$

Coarsening dynamics with noise

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Eyring–Kramers law for 1D SPDEs: heuristics

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

Initial condition: u_{in} near $u_- \equiv -1$ with eigenvalues ν_k

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.)

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

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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.

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

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- ▷ Rigorous proof?
- ▷ What happens when $L \rightarrow \beta\pi$ as then $\lambda_1 \rightarrow 0$?

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

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▷ If $\pi - c \leq L \leq \pi$, then

$$\mathbb{E}^{u_{\text{in}}}[\tau_+] = 2\pi \sqrt{\frac{\lambda_1 + \sqrt{3\varepsilon/2L}}{|\lambda_0| \nu_0 \nu_1} \prod_{k=2}^{\infty} \frac{\lambda_k}{\nu_k} \frac{e^{(V[u_{\text{ts}}] - V[u_-])/\varepsilon}}{\Psi_+(\lambda_1/\sqrt{3\varepsilon/2L})}} [1 + R(\varepsilon)]$$

where Ψ_+ explicit, involves Bessel function $K_{1/4}$, $\lim_{\alpha \rightarrow \infty} \Psi_+(\alpha) = 1$

▷ If $\pi \leq L \leq \pi + c$, then same formula, with another function Ψ_- , involving Bessel functions $I_{\pm 1/4}$, $\lim_{\alpha \rightarrow \infty} \Psi_-(\alpha) = 2$

Eyring–Kramers law for 1D SPDEs: comments

- ▷ Periodic b.c.: similar result [B & Gentz, Elec J Proba 2013]
For $L > 2\pi$: extra factor $\sqrt{\varepsilon}$ because saddle is a whole curve
- ▷ Proof: relies on spectral Galerkin approximation
- ▷ Similar results by F. Barret [Annales IHP, 2015]
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- ▷ For Neumann b.c. and $L < \pi$: spectral determinant in prefactor is explicitly computable (Euler product formulas)

$$\frac{1}{|\lambda_0| \nu_0} \prod_{k=1}^{\infty} \frac{\lambda_k}{\nu_k} = \frac{1}{2} \prod_{k=1}^{\infty} \frac{\left(\frac{k\pi}{L}\right)^2 - 1}{\left(\frac{k\pi}{L}\right)^2 + 2} = \frac{1}{2} \prod_{k=1}^{\infty} \frac{1 - \left(\frac{L}{k\pi}\right)^2}{1 + 2\left(\frac{L}{k\pi}\right)^2} = \frac{\sin(L)}{\sqrt{2} \sinh(\sqrt{2}L)}$$

Similar expression for periodic b.c. and $L < 2\pi$

- ▷ For larger L , techniques for Feynman path integrals allow to compute the spectral determinants in prefactors [Maier & Stein]

Sketch of proof: Spectral Galerkin approximation

$$u_t^{(d)}(x) = \frac{1}{\sqrt{L}} \sum_{k=-d}^d z_k(t) e^{i\pi kx/L} \quad \Rightarrow \quad dz_t = -\nabla V(z_t) dt + \sqrt{2\varepsilon} dW_t$$

Theorem [Blömker & Jentzen 13]

For all $\gamma \in (0, \frac{1}{2})$ there exists an a.s. finite r.v. $Z : \Omega \rightarrow \mathbb{R}_+$ s.t. $\forall \omega \in \Omega$

$$\sup_{0 \leq t \leq T} \|u_t(\omega) - u_t^{(d)}(\omega)\|_{L^\infty} < Z(\omega) d^{-\gamma} \quad \forall d \in \mathbb{N}$$

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Proposition (using potential theory)

$\exists \varepsilon_0 > 0 : \forall \varepsilon < \varepsilon_0 \exists d_0(\varepsilon) < \infty : \forall d \geq d_0 \exists \nu_d$ proba measure on $\partial \mathcal{B}_r(u_-)$

$$\int_{\partial \mathcal{B}_r(u_-)} \mathbb{E}^{\nu_0}[\tau_+^{(d)}] \nu_d(d\nu_0) = C(d, \varepsilon) e^{H(d)/\varepsilon} [1 + R(\varepsilon)]$$

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$$\int_{\partial \mathcal{B}_r(u_-)} \mathbb{E}^{\nu_0}[\tau_+^{(d)}] \nu_d(d\nu_0) = C(d, \varepsilon) e^{H(d)/\varepsilon} [1 + R(\varepsilon)]$$

Proposition (using large deviations and lots of other stuff)

$H_0 := V[u_{ts}] - V[u_-]$. $\forall \eta > 0 \exists \varepsilon_0, T_1, H_1 : \forall \varepsilon < \varepsilon_0 \exists d_0 < \infty$ s.t. $\forall d \geq d_0$

$$\sup_{\nu_0 \in \mathcal{B}_r(u_-)} \mathbb{E}^{\nu_0}[\tau_+^2] \leq T_1^2 e^{2(H_0 + \eta)/\varepsilon}, \quad \sup_{d \geq d_0} \sup_{\nu_0 \in \mathcal{B}_r(u_-)} \mathbb{E}^{\nu_0}[(\tau_+^{(d)})^2] \leq T_1^2 e^{2H_1/\varepsilon}$$

Main step of the proof

Set $T_{\text{Kr}} = C(\infty, \varepsilon) e^{H_0/\varepsilon}$

Let $B = \mathcal{B}_\rho(u_+)$ and define nested sets $B_- \subset B \subset B_+$ at L^∞ -distance δ

$$\Omega_{K,d} = \left\{ \sup_{t \in [0, KT_{\text{Kr}}]} \|v_t - v_t^{(d)}\|_{L^\infty} \leq \delta, \tau_{B_-}^{(d)} \leq KT_{\text{Kr}} \right\}$$

$$\mathbb{P}(\Omega_{K,d}^c) \leq \mathbb{P}\{Z > \delta d^\gamma\} + \frac{\mathbb{E}^{v_0^{(d)}}[\tau_{B_-}^{(d)}]}{KT_{\text{Kr}}} \xrightarrow{\text{Cauchy-Schwarz}} \limsup_{d \rightarrow \infty} \mathbb{P}(\Omega_{K,d}^c) = \frac{M(\varepsilon)}{K}$$

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On $\Omega_{K,d}$ one has $\tau_{B_+}^{(d)} \leq \tau_B \leq \tau_{B_-}^{(d)}$

$$\Rightarrow \mathbb{E}^{v_0^{(d)}}[\tau_{B_+}^{(d)} \mathbf{1}_{\{\Omega_{K,d}\}}] \leq \mathbb{E}^{v_0}[\tau_B \mathbf{1}_{\{\Omega_{K,d}\}}] \leq \mathbb{E}^{v_0^{(d)}}[\tau_{B_-}^{(d)} \mathbf{1}_{\{\Omega_{K,d}\}}]$$

$$\Rightarrow \mathbb{E}^{v_0^{(d)}}[\tau_{B_+}^{(d)}] - \mathbb{E}^{v_0^{(d)}}[\tau_{B_+}^{(d)} \mathbf{1}_{\{\Omega_{K,d}^c\}}] \leq \mathbb{E}^{v_0}[\tau_B] \leq \mathbb{E}^{v_0^{(d)}}[\tau_{B_-}^{(d)}] + \mathbb{E}^{v_0}[\tau_B \mathbf{1}_{\{\Omega_{K,d}^c\}}]$$

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Integrate against ν_d and use Cauchy-Schwarz to bound error terms:

$$\mathbb{E}^{v_0}[\tau_B \mathbf{1}_{\{\Omega_{K,d}^c\}}] \leq \sqrt{\mathbb{E}^{v_0}[\tau_B^2] \mathbb{P}(\Omega_{K,d}^c)}, \text{ take } d \rightarrow \infty \text{ and finally } K \text{ large}$$

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:

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

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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])

Renormalisation

Problem: For $d = 2$, stoch. convolution $\int_0^t e^{\Delta(t-s)} \dot{W}_x(ds)$ is a 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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- ▷ $\lim_{t \rightarrow \infty} \int_0^t e^{(\Delta-1)(t-s)} \dot{W}_x(ds) = \phi_N$ 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**

$$\begin{aligned} : \phi_N^2 : &= \phi_N^2 - C_N \\ : \phi_N^3 : &= \phi_N^3 - 3C_N \phi_N \\ : \phi_N^4 : &= \phi_N^4 - 6C_N \phi_N^2 + 3C_N^2 \end{aligned}$$

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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- ▷ 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 $-V_N(L,0) = \frac{1}{4}L^2 + \frac{3}{2}L^2 C_N \varepsilon$

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

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

Main result in dimension 2

Theorem: [B, Di Gesù, Weber 2016]

For 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:

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

Defined whenever T is Hilbert–Schmidt, but not necessarily trace class

Applied here to $T = [(-\Delta + 2) - (-\Delta - 1)](|-\Delta - 1|)^{-1} = 3(|-\Delta - 1|)^{-1}$

Outlook

- ▷ Dim $d = 3$: more difficult because 2 renormalisation constants needed
- ▷ Potentials with more than two wells: understood in $d = 1$
- ▷ Potentials invariant under symmetry group: understood in \mathbb{R}^n
- ▷ More difficult: non-gradient systems

References: For this talk: [1,2,3,5]; Overview: [4]; Non-gradient: [6];

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