DNA Seminar, NTNU Trondheim

Metastable dynamics of stochastic Allen-Cahn PDEs on the torus

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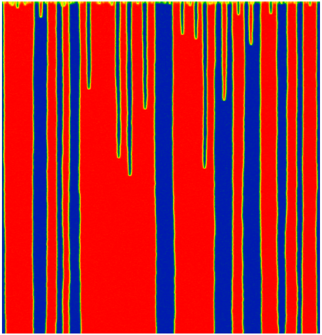
Deterministic Allen–Cahn PDE

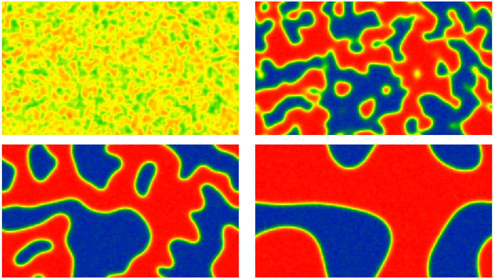
[Chafee & Infante 74, Allen & Cahn 75]

$$\partial_t u = \Delta u + u - u^3$$

▷ $u = u(t,x) \in \mathbb{R}$, $t \geqslant 0$, $x \in \mathbb{T}_L^d = (\mathbb{R}/L\mathbb{Z})^d$, $L > 0$

Phase separation ($d = 1$: [Carr & Pego 89, Chen 04])





Remark: Φ^4 model from QFT: $\partial_t u = \Delta u - u^3$

Deterministic Allen–Cahn PDE

$$\partial_t u = \Delta u + u - u^3$$

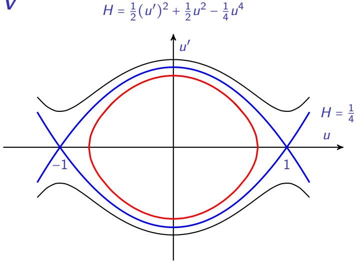
Energy function:

$$V[u] = \int_{\mathbb{T}_L^d} \Big[\frac{1}{2} |\nabla u(x)|^2 - \frac{1}{2} u(x)^2 + \frac{1}{4} u(x)^4 \Big] \mathrm{d}x \qquad \Rightarrow \nabla_v V[u] = -\langle \partial_t u, v \rangle$$

Stationary solutions ($d = 1$):

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

- $u_\pm(x) \equiv \pm 1$
- $u_0(x) \equiv 0$
- Nonconstant solutions if $L > 2\pi$
  (expressible in terms of Jacobi elliptic fcts)



Stability of stationary solutions

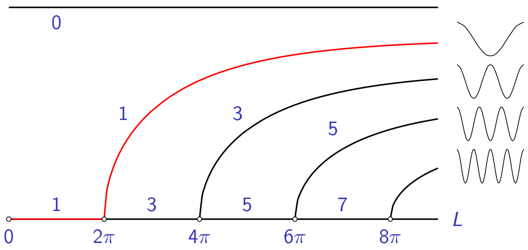
Linearisation at u_0:

$\partial_t v_t(x) = (\mathcal{L}v)(x) := v_t''(x) + [1 - 3u_0(x)^2]v_t(x)$

Stability: Find eigenvalues of $\mathcal{L} \longrightarrow$ Sturm–Liouville problem

- ▷ $u_\pm(x) \equiv \pm 1$: stable
- ▷ $u_0(x) \equiv 0$: unstable
- ▷ Nonconstant solutions: unstable

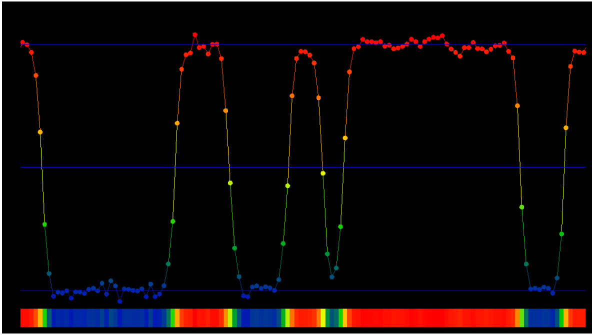
Number of positive eigenvalues
(= unstable directions)
Transition state



Stochastic Allen–Cahn PDE

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

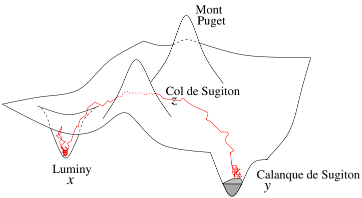
- ξ space-time white noise: centered, Gaussian,
  $\mathbb{E}[\xi(t,x)\xi(s,y)] = \delta(t-s)\delta(x-y)$
- ξ distribution, $\langle \xi, \varphi \rangle \sim \mathcal{N}(0, \|\varphi\|^2_{L^2})$, $\quad \mathbb{E}[\langle \xi, \varphi_1 \rangle \langle \xi, \varphi_2 \rangle] = \langle \varphi_1, \varphi_2 \rangle_{L^2}$



Question: Speed of convergence to equilibrium measure?

Reversible diffusion in a double-well

$$\mathrm{d}x_t = -\nabla V(x_t)\,\mathrm{d}t + \sqrt{2\varepsilon}\,\mathrm{d}W_t$$



$V : \mathbb{R}^d \to \mathbb{R}$ confining 2-well potential

- ▷ Generator:
  $\mathscr{L} = \varepsilon\Delta - \nabla V \cdot \nabla = \varepsilon\,\mathrm{e}^{V/\varepsilon}\,\nabla \cdot \mathrm{e}^{-V/\varepsilon}\,\nabla$
- ▷ Invariant probability: Gibbs measure
  $\pi(\mathrm{d}x) = \frac{1}{Z}\,\mathrm{e}^{-V(x)/\varepsilon}\,\mathrm{d}x \quad \Rightarrow \quad \mathscr{L}^\dagger \pi = 0$
- ▷ Reversible: $\langle f, \mathscr{L} g\rangle_\pi = \langle \mathscr{L} f, g\rangle_\pi$ for $\langle f, g\rangle_\pi = \int_{\mathbb{R}^d} f(x)g(x)\pi(\mathrm{d}x)$

How to characterise convergence to equilibrium?

- ▷ Exponential ergodicity: $|\mathbb{E}^x[f(x_t)] - \langle \pi, f\rangle| \leqslant C(x,f)\,\mathrm{e}^{-\beta t}$
  Possible via Lyapunov functions [Meyn & Tweedie], bad control of β
- ▷ Mean hitting time: Estimate $\mathbb{E}^x[\tau_y]$ where $\tau_y = \inf\{t > 0 \colon x_t \in \mathcal{B}_\varepsilon(y)\}$
- ▷ Spectral gap of $\mathscr{L}$

Mean first hitting time

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

  Proved by [Freidlin, Wentzell, 1979] using large deviations

- Eyring–Kramers law (1935, 1940):
  Eigenvalues of Hessian of V at minimum x: $0 < \nu_1 \leqslant \nu_2 \leqslant \dots \leqslant \nu_d$
  Eigenvalues of Hessian of V at saddle z: $\lambda_1 < 0 < \lambda_2 \leqslant \dots \leqslant \lambda_d$

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

  Spectral gap of $\mathscr{L} = \mathbb{E}^x[\tau_y]^{-1}\big[1 + \mathcal{O}_\varepsilon(1)\big]$

  Proved by [Bovier, Eckhoff, Gayrard, Klein, 2004] using potential theory, by [Helffer, Klein, Nier, 2004] using Witten Laplacian, ...

Potential-theoretic proof of Eyring–Kramers law

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

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

Theorem: $A, B \subset \mathbb{R}^d$ disjoint. $\exists$ proba measure ν_{AB} on ∂A s.t.

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

Proof: $w_B(x) = -\int_{B^c} G_{B^c}(x,y) \,\mathrm{d}y \qquad h_{AB}(y) = -\int_{\partial A} G_{B^c}(y,x) e_{AB}(\mathrm{d}x)$

$\nu_{AB}(\mathrm{d}x) := \frac{1}{\operatorname{cap}(A,B)} \mathrm{e}^{-V(x)/\varepsilon} e_{AB}(\mathrm{d}x) \qquad \operatorname{cap}(A,B) := \int_{\partial A} \mathrm{e}^{-V/\varepsilon} e_{AB}(\mathrm{d}x)$

$$\operatorname{cap}(A,B) \int_{\partial A} w_B(x) \nu_{AB}(\mathrm{d}x) = -\int_{\partial A} \int_{B^c} \underbrace{G_{B^c}(x,y) \,\mathrm{e}^{-V(x)/\varepsilon}}_{= G_{B^c}(y,x) \,\mathrm{e}^{-V(y)/\varepsilon}} e_{AB}(\mathrm{d}x) \,\mathrm{d}y$$

Potential-theoretic proof of Eyring–Kramers law

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Apply to A, B neighbourhoods of x, y

- Laplace asymptotics: $\displaystyle\int_{B^c} h_{A,B}(y)\,\mathrm{e}^{-V(y)/\varepsilon}\,\mathrm{d}y \simeq \sqrt{\frac{(2\pi\varepsilon)^d}{\nu_1 \dots \nu_d}}\,\mathrm{e}^{-V(x)/\varepsilon}$
- Capacity: $\operatorname{cap}(A,B) = \mathscr{E}(h_{AB})$
- Dirichlet form: $\mathscr{E}(f) = \langle f, -\mathscr{L} f\rangle = \varepsilon \displaystyle\int_{\mathbb{R}^d} \mathrm{e}^{-V(x)/\varepsilon} |\nabla f(x)|^2\,\mathrm{d}x$

Theorem: Dirichlet principle

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

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

Appropriate test function yields $\operatorname{cap}(A,B) \simeq \varepsilon \sqrt{\frac{|\lambda_1|}{2\pi\varepsilon}} \sqrt{\frac{(2\pi\varepsilon)^{d-1}}{\lambda_2 \dots \lambda_d}}\,\mathrm{e}^{-V(z)/\varepsilon}$

Stochastic Allen–Cahn PDE

$$\partial_t u = \Delta u + u - u^3 + \sqrt{2\varepsilon}\xi \qquad x \in \mathbb{T}_L$$

- [Faris & Jona-Lasinio '82]: existence/uniqueness of solution
- [Da Prato & Zabczyk '90s]: invariant measure is Gibbs measure associated with

$$V[u] = \int_{\mathbb{T}_L} \Big[\frac{1}{2}|\nabla u(x)|^2 - \frac{1}{2}u(x)^2 + \frac{1}{4}u(x)^4\Big] \mathrm{d}x$$

- [Faris & Jona-Lasinio '82]: Arrhenius law $\mathbb{E}^{u_-}[\tau_{u_+}] \simeq e^{(V[u_{\mathrm{tr}}]-V[u_-])/\varepsilon}$ where u_{tr} transition state, $u_{\mathrm{tr}} = u_0$ if $L < 2\pi$

Question: is there an Eyring–Kramers law? With what prefactor?

Heuristics: $V[u] = \frac{1}{2}\langle u, (-\Delta - 1)u\rangle + \mathcal{O}(u^4)$

- Hessian of V at u_0: $-\Delta - 1$, eigenvalues $\lambda_k = (\frac{2k\pi}{L})^2 - 1$
- Hessian of V at u_-: $-\Delta + 2$, eigenvalues $\nu_k = (\frac{2k\pi}{L})^2 + 2$

Formally, product of ratios of λ_k/ν_k converges [Maier & Stein '01]

Formal computation and Fredholm determinant

Formally (for $L < 2\pi$)

$$\mathbb{E}^{u_-}[\tau_{u_+}] = \frac{2\pi}{|\lambda_1|}\sqrt{\frac{|\det \mathrm{Hess}\, V[u_0]|}{\det \mathrm{Hess}\, V[u_-]}}\, \mathrm{e}^{(V[u_0]-V[u_-])/\varepsilon}\Big[1+\mathcal{O}_\varepsilon(1)\Big]$$

$\Delta_\perp$ Laplacian acting on mean zero functions

$$\begin{aligned}\det\Big([-\Delta_\perp - 1][-\Delta_\perp + 2]^{-1}\Big) &= \det\Big([-\Delta_\perp + 2 - 3][-\Delta_\perp + 2]^{-1}\Big) \\ &= \underbrace{\det\Big(\mathbb{1} - 3[-\Delta_\perp + 2]^{-1}\Big)}_{\text{Fredholm determinant}}\end{aligned}$$

$$\begin{aligned}\log\det\Big(\mathbb{1} - 3[-\Delta_\perp + 2]^{-1}\Big) &= \mathrm{Tr}\log\Big(\mathbb{1} - 3[-\Delta_\perp + 2]^{-1}\Big) \\ &= -\sum_{n\geqslant 1}\frac{3^n}{n}\underbrace{\mathrm{Tr}\Big([-\Delta_\perp + 2]^{-n}\Big)}_{\lesssim\left[\left(\frac{2\pi}{L}\right)^2+2\right]^{-n}} < \infty \qquad (L < 2\pi)\end{aligned}$$

General fact: $\det(\mathbb{1} + T) < \infty$ if T is trace class

Main result for $d = 1$

Theorem: [B & Gentz, Elec. J. Proba 2013]

- If $L < 2\pi - c$ with $c > 0$, then

$$\mathbb{E}^{u_-}[\tau_+] = 2\pi\sqrt{\det(\mathbb{1} - 3[-\Delta + 2]^{-1})}\, e^{(V[u_0]-V[u_-])/\varepsilon}\Big[1 + \mathcal{O}_\varepsilon(1)\Big]$$

- Similar explicit expressions for $L > 2\pi - c$ and $L \simeq 2\pi$
  (with different $u_{\rm tr}$ and slightly different ε-dependence due to 0 eigenvalue)

Remarks:

- Proof relies on spectral Galerkin approximation
- Error more precise than $\mathcal{O}_\varepsilon(1)$
- If $u_{\rm tr} \neq u_0$, Fredholm determinant computed with techniques from path integrals [Maier & Stein]
- Similar results for Neumann b.c.
- Similar results for other nonlinearities than $-u^3$

Allen–Cahn SPDE for $d = 2$

- ▷ Arrhenius law holds via large-deviation principle [Hairer & Weber, 2015]
- ▷ Naive computation of prefactor fails:

$$\operatorname{Tr}\log(\mathbb{1} - 3[-\Delta_\perp + 2]^{-1}) \simeq \sum_{k\in(\mathbb{Z}^2)^*} \log\left(1 - \frac{3L^2}{|k|^2\pi^2}\right)$$

$$\simeq -\sum_{k\in(\mathbb{Z}^2)^*} \frac{3L^2}{|k|^2\pi^2} \simeq -\frac{3L^2}{\pi^2}\int_1^\infty \frac{r\,\mathrm{d}r}{r^2} = -\infty$$

- ▷ 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

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

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

- ▷ $C(\delta)$ ~ variance of mollified Gaussian free field (GFF)
- ▷ Naively, one could expect $u_\pm = \pm\sqrt{1 + 3\varepsilon C(\delta)}$ but this is not the case

Main result in dimension 2

- ▷ Use spectral Galerkin approximation with cut-off N instead of mollification, $L^2 C_N = \mathrm{Tr}(P_N[-\Delta + 2]^{-1}) \sim \log(N)$
- ▷ $V_N[u_0] - V_N[u_-] = \frac{L^2}{4} + \frac{3}{2} L^2 \varepsilon C_N$
- ▷ $(\text{Prefactor})^2 = \det(\mathbb{1} - 3P_N[-\Delta_\perp + 2]^{-1}) \mathrm{e}^{3\,\mathrm{Tr}(P_N[-\Delta_\perp+2]^{-1})}$

  $\det_2(\mathbb{1} - T) = \det(\mathbb{1} - T)\mathrm{e}^{\mathrm{Tr}\,T}$ Carleman–Fredholm determinant

Theorem: [B, Di Gesù, Weber, Elec. J. Proba 2017]

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

$$\limsup_{N\to\infty} \mathbb{E}^{\mu_N}\big[\tau_B\big] \leqslant 2\pi\sqrt{\det_2(\mathbb{1} - 3[-\Delta + 2]^{-1})}\,\mathrm{e}^{(V[u_0]-V[u_-])/\varepsilon}\big[1 + c_+\sqrt{\varepsilon}\big]$$

$$\liminf_{N\to\infty} \mathbb{E}^{\mu_N}\big[\tau_B\big] \geqslant 2\pi\sqrt{\det_2(\mathbb{1} - 3[-\Delta + 2]^{-1})}\,\mathrm{e}^{(V[u_0]-V[u_-])/\varepsilon}\big[1 - c_-\varepsilon\big]$$

- ▷ [Tsatsoulis & Weber, PTRF 2018]: Same result for $\mathbb{E}^{u_-}[\tau_B]$
- ▷ $\det_2$ defined whenever T is only Hilbert–Schmidt (true for $d \leqslant 3$)

References

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Thanks for your attention!