Metastability in a class of parabolic SPDEs

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Metastability in physics

Examples:

- Supercooled liquid
- Supersaturated gas
- Wrongly magnetised ferromagnet

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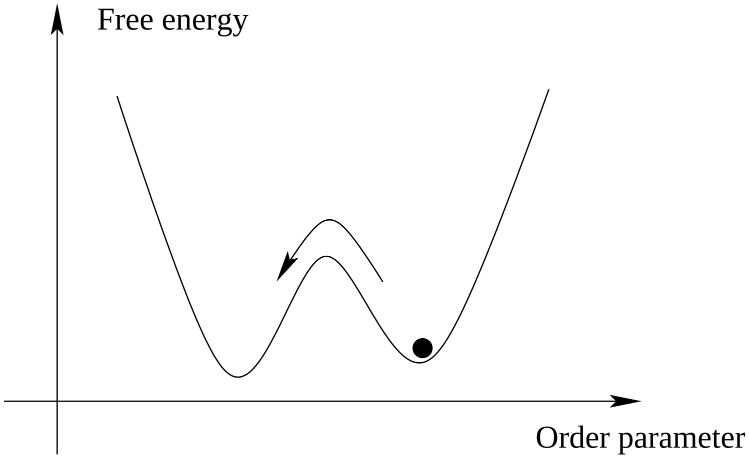
▷ Near first-order phase transition

▷ Nucleation implies crossing energy barrier



Metastability in stochastic lattice models

- ▷ Lattice: $\Lambda \subset\subset \mathbb{Z}^d$
- ▷ Configuration space: $\mathcal{X} = S^\Lambda$, S finite set (e.g. $\{-1, 1\}$)
- ▷ Hamiltonian: $H : \mathcal{X} \to \mathbb{R}$ (e.g. Ising or lattice gas)
- ▷ Gibbs measure: $\mu_\beta(x) = \mathrm{e}^{-\beta H(x)} / Z_\beta$
- ▷ Dynamics: Markov chain with invariant measure μ_β (e.g. Metropolis: Glauber or Kawasaki)

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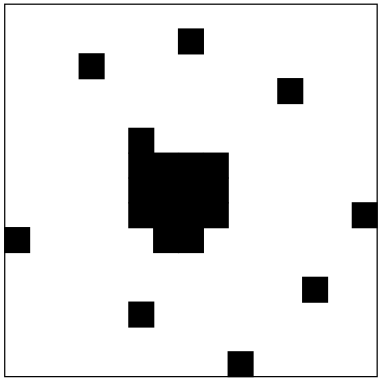
Results (for $\beta \gg 1$) on

- Transition time between $+$ and $-$ or empty and full configuration
- Transition path
- Shape of critical droplet



- ▷ Frank den Hollander, *Metastability under stochastic dynamics*, Stochastic Process. Appl. **114** (2004), 1–26.
- ▷ Enzo Olivieri and Maria Eulália Vares, *Large deviations and metastability*, Cambridge University Press, Cambridge, 2005.

Reversible diffusion

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

- ▷ $V : \mathbb{R}^d \to \mathbb{R}$: potential, growing at infinity
- ▷ W_t: d-dim Brownian motion on $(\Omega, \mathcal{F}, \mathbb{P})$

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invariant measure:

$$\mu_\varepsilon(\mathrm{d}x) = \frac{\mathrm{e}^{-V(x)/\varepsilon}}{Z_\varepsilon}\,\mathrm{d}x$$

(detailed balance)

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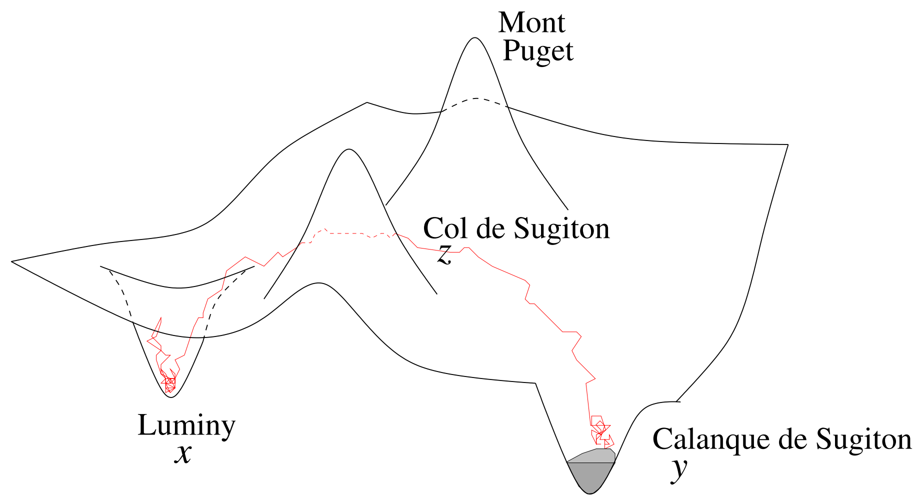

τ_y^x: first-hitting time of small ball $\mathcal{B}_\varepsilon(y)$, starting in x

"Eyring–Kramers law" (Eyring 1935, Kramers 1940)

- • Dim 1: $\mathbb{E}[\tau_y^x] \simeq \dfrac{2\pi}{\sqrt{V''(x)|V''(z)|}}\,\mathrm{e}^{[V(z)-V(x)]/\varepsilon}$
- • Dim$\geqslant 2$: $\mathbb{E}[\tau_y^x] \simeq \dfrac{2\pi}{|\lambda_1(z)|}\sqrt{\dfrac{|\det(\nabla^2 V(z))|}{\det(\nabla^2 V(x))}}\,\mathrm{e}^{[V(z)-V(x)]/\varepsilon}$

Towards a proof of Kramers' law

- Large deviations (Wentzell & Freidlin 1969):

$$\lim_{\varepsilon\to0} \varepsilon \log(\mathbb{E}[\tau_y^x]) = V(z) - V(x)$$

- Analytic (Helffer, Sjöstrand 85, Miclo 95, Mathieu 95, Kolokoltsov 96,...):
  low-lying spectrum of generator
- Potential theory/variational (Bovier, Eckhoff, Gayrard, Klein 2004):

$$\mathbb{E}[\tau_y^x] = \frac{2\pi}{|\lambda_1(z)|}\sqrt{\frac{|\det(\nabla^2 V(z))|}{\det(\nabla^2 V(x))}}\,\mathrm{e}^{[V(z)-V(x)]/\varepsilon}\Big[1+\mathcal{O}(\varepsilon^{1/2}|\log\varepsilon|^{1/2})\Big]$$

  and similar asymptotics for eigenvalues of generator
- Witten complex (Helffer, Klein, Nier 2004):
  full asymptotic expansion of prefactor
- Distribution of τ_y^x (Day 1983, Bovier *et al* 2005):

$$\lim_{\varepsilon\to0} \mathbb{P}\Big\{\tau_y^x > t\mathbb{E}[\tau_y^x]\Big\} = \mathrm{e}^{-t}$$

Allen-Cahn equation

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

where e.g. $f(u) = u - u^3$

$x \in [0, L]$, $u(x,t) \in \mathbb{R}$ represents e.g. magnetisation

- Periodic b.c.
- Neumann b.c. $\partial_x u(0,t) = \partial_x u(L,t) = 0$

Noise: weak, white in space and time

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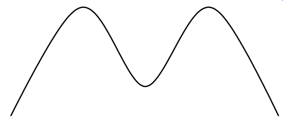
Deterministic system is gradient

$$\partial_{xx} u + u - u^3 = -\frac{\delta V}{\delta u}$$

$$V[u] = \int_0^L \left[\frac{1}{2} u'(x)^2 - \frac{1}{2} u(x)^2 + \frac{1}{4} u(x)^4\right] \mathrm{d}x \qquad \to \quad \text{min}$$

Stationary solutions

$u''(x) = -u(x) + u(x)^3 = -\frac{\mathrm{d}}{\mathrm{d}x}\Big[$  $\Big]$

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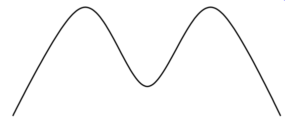
$$u''(x) = -u(x) + u(x)^3 = -\frac{\mathrm{d}}{\mathrm{d}x}\Big[$$  $$\Big]$$

- $u_{\pm}(x) \equiv \pm 1$: global minima of V, stable
- $u_0(x) \equiv 0$: unstable
- Neumann b.c: for $k = 1, 2, \dots$, if $L > \pi k$,
  $u_{k,\pm}(x) = \pm\sqrt{\frac{2m}{m+1}}\,\mathrm{sn}\Big(\frac{kx}{\sqrt{m+1}} + \mathrm{K}(m), m\Big) \qquad 2k\sqrt{m+1}\,\mathrm{K}(m) = L$

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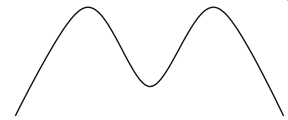
$$u''(x) = -u(x) + u(x)^3 = -\frac{\mathrm{d}}{\mathrm{d}x}\Big[$$  $$\Big]$$

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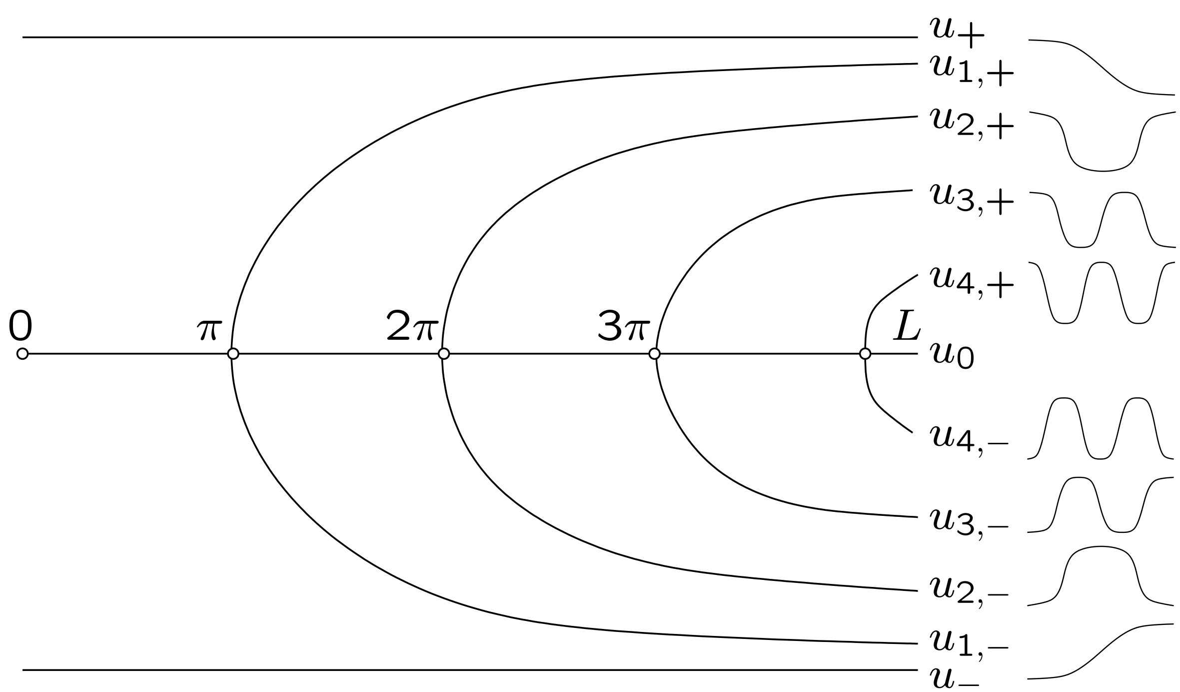

Stability of stationary solutions

Linearisation at $u(x)$: $\partial_t \varphi = A[u]\varphi$, $A[u] = \frac{\mathrm{d}^2}{\mathrm{d}x^2} + 1 - 3u(x)^2$

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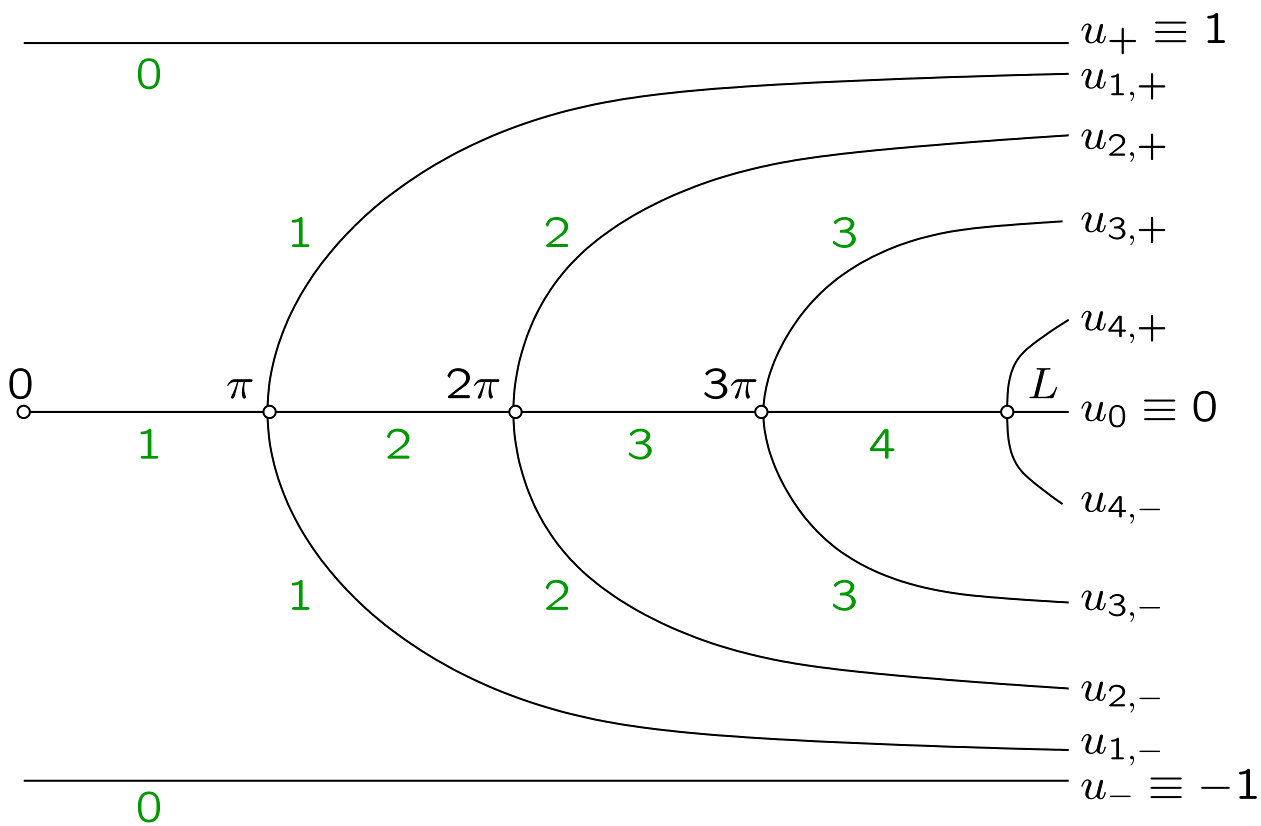
- $u_\pm(x) \equiv \pm 1$: eigenvalues $-(2 + (\pi k/L)^2)$, $k \in \mathbb{N}$
- $u_0(x) \equiv 0$: eigenvalues $1 - (\pi k/L)^2$, $k \in \mathbb{N}$

Number of positive eigenvalues:



Allen-Cahn equation with noise

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

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

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Construction of mild solution:

1. $\dot{u}_t = \Delta u_t \qquad \Rightarrow \qquad u_t = \mathrm{e}^{\Delta t} u_0$

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

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2. $\dot{u}_t = \Delta u_t + \sqrt{2\varepsilon}\,\ddot{W}_{tx}$

   $$\Rightarrow \qquad u_t = \mathrm{e}^{\Delta t}\, u_0 + \sqrt{2\varepsilon}\underbrace{\int_0^t \mathrm{e}^{\Delta(t-s)}\,\dot{W}_x(\mathrm{d}s)}_{=: w_t(x)}$$

   $$w_t(x) = \sum_k \int_0^t \mathrm{e}^{-(k\pi/L)^2(t-s)}\,\mathrm{d}W_s^{(k)}\cos(k\pi x/L)$$

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

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

   $\Rightarrow$ Existence and a.s. uniqueness (Faris & Jona-Lasinio 1982)

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

$$\Rightarrow \qquad \mathrm{d}z_k = -\lambda_k z_k \,\mathrm{d}t - \sum_{k_1+k_2+k_3=k} z_{k_1} z_{k_2} z_{k_3} \,\mathrm{d}t \; + \sqrt{2\varepsilon}\, \mathrm{d}W_t^{(k)}$$

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

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Energy functional:

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

The question

How long does the system take to get from $u_-(x) \equiv -1$ to (a neighbourhood of) $u_+(x) \equiv 1$?

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Large deviations (Faris & Jona-Lasinio 1982)

- $\triangleright$ $L \leqslant \pi$: $\Delta W = V[u_0] - V[u_-] = \frac{L}{4}$
- $\triangleright$ $L > \pi$: $\Delta W = V[u_{1,\pm}] - V[u_-] = \frac{1}{3\sqrt{1+m}} \Big[8\,\mathsf{E}(m) - \frac{(1-m)(3m+5)}{1+m} \mathsf{K}(m) \Big]$

Formal computation for Allen-Cahn (R.S. Maier, D. Stein, 01)

Case $L < \pi$:

Kramers: $\Gamma_0 \simeq \frac{|\lambda_1(u_0)|}{2\pi}\sqrt{\frac{\det(\nabla^2 V[u_-])}{|\det(\nabla^2 V[u_0])|}}$

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Thus formally $\Gamma_0 \simeq \frac{|\lambda_0|}{2\pi}\sqrt{\prod_{k=0}^{\infty}\frac{\mu_k}{|\lambda_k|}} = \frac{1}{2^{3/4}\pi}\sqrt{\frac{\sinh(\sqrt{2}L)}{\sin L}}$

Case $L > \pi$:   Spectral determinant computed by Gelfand's method

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Problems:

1. What happens when $L \to \pi_-$? (bifurcation)
2. Is the formal computation correct in infinite dimension?

Theorem: [Barret, B., Gentz 2010]

$$\mathbb{E}[\tau] = \Gamma_0^{-1}\, \mathrm{e}^{\Delta W/\varepsilon} \Big[1 + \mathcal{O}(\varepsilon^{1/4} |\log \varepsilon|^{5/4}) \Big]$$

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where $\lambda_1 = -1 + (\pi/L)^2$ and

$$\Psi_+(\alpha) = \sqrt{\frac{\alpha(1+\alpha)}{8\pi}} \, \mathrm{e}^{\alpha^2/16} \, K_{1/4}\Big(\frac{\alpha^2}{16}\Big)$$

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$$\lim_{L\to\pi_-}\Gamma_0 = \frac{\Gamma(1/4)}{2(3\pi^7)^{1/4}}\sqrt{\sinh(\sqrt{2}\pi)}\,\varepsilon^{-1/4}$$

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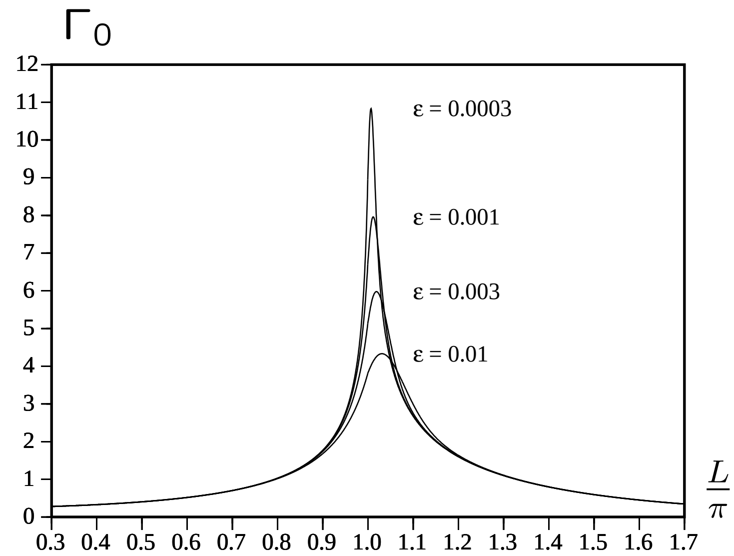
Similar expression for $L > \pi$

(product of eigenvalues computed using

path-integral techniques, cf. Maier and Stein)



Spectral Galerkin approximation

$$u_t^d(x) = \sum_{k=-d}^{d} z_k(t)\, \mathrm{e}^{\mathrm{i}\,\pi k x/L}$$

$z_k(t)$ solution of finite-dimensional SDE

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Theorem: [D. Blömker, A. Jentzen 2009]

Assume

$$\sup_{d\in\mathbb{N}} \sup_{0\leqslant t\leqslant T} \|u_t^d(\omega)\|_{L^\infty} < \infty \qquad \forall \omega \in \Omega$$

Then

$$\sup_{0\leqslant t\leqslant T} \|u_t(\omega) - u_t^d(\omega)\|_{L^\infty} < Z(\omega) d^{-\gamma} \qquad \forall \omega \in \Omega$$

for all $0 < \gamma < 1/2$, with Z a.s. finite r.v.

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Rem: [Liu, 2003] similar result for $\|u\|^2 = \sum_k (1+k^2)^r |z_k|^2, r < \frac{1}{2}$

Potential theory

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

Equilibrium potential : $h_{A,B}(x) = \mathbb{P}^x\{\tau_A < \tau_B\}$

Then

$$\mathbb{E}[\tau_B^x] \simeq \frac{\displaystyle\int_{B^c} h_{\mathcal{B}_\varepsilon(x),B}(y)\,\mathrm{e}^{-V(y)/\varepsilon}\,\mathrm{d}y}{\mathrm{cap}_{\mathcal{B}_\varepsilon(x)}(B)}$$

where

$$\mathrm{cap}_A(B) = \varepsilon \inf_{h\in\mathcal{H}_{A,B}} \int_{(A\cup B)^c} \|\nabla h(x)\|^2\,\mathrm{e}^{-V(x)/\varepsilon}\,\mathrm{d}x$$

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$$\mathbb{E}[\tau_B^x] \simeq \frac{\int_{B^c} h_{\mathcal{B}_\varepsilon(x),B}(y)\,\mathrm{e}^{-V(y)/\varepsilon}\,\mathrm{d}y}{\mathrm{cap}_{\mathcal{B}_\varepsilon(x)}(B)}$$

where

$$\mathrm{cap}_A(B) = \varepsilon \inf_{h\in\mathcal{H}_{A,B}} \int_{(A\cup B)^c} \|\nabla h(x)\|^2\,\mathrm{e}^{-V(x)/\varepsilon}\,\mathrm{d}x$$

Rough a priori bounds on h show that if x potential minimum,

$$\int_{A^c} h_{\mathcal{B}_\varepsilon(x),B}(y)\,\mathrm{e}^{-V(y)/\varepsilon}\,\mathrm{d}y \simeq \frac{(2\pi\varepsilon)^{d/2}\,\mathrm{e}^{-V(x)/\varepsilon}}{\sqrt{\det(\nabla^2 V(x))}}$$

Estimation of capacity

Truncated energy functional: retain only modes with $k \leqslant d$

$$\frac{1}{L}V[u] = -\frac{1}{2}z_0^2 + u_1(z_1) + \frac{1}{2}\sum_{k=2}^{d} \lambda_k |z_k|^2 + \dots$$

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Theorem: For all $L < \pi$,

$$\operatorname{cap}_{\mathcal{B}_\varepsilon(u_-)}(\mathcal{B}_\varepsilon(u_+)) = \varepsilon \frac{\displaystyle\int_{-\infty}^{\infty} \mathrm{e}^{-u_1(z_1)/\varepsilon}\, \mathrm{d}z_1}{\sqrt{2\pi\varepsilon}} \prod_{j=2}^{d} \sqrt{\frac{2\pi\varepsilon}{\lambda_j}} \big[1 + R(\varepsilon)\big]$$

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Corollary:

$$\mathbb{E}_{\mathcal{B}_\varepsilon(u_-)}(\tau_{\mathcal{B}_\varepsilon(u_+)}) = \Gamma_0^{-1}(d,\varepsilon)\,\mathrm{e}^{\Delta W(d)/\varepsilon}[1+R(\varepsilon)]$$

Proposition:

Let $B = \mathcal{B}_\varepsilon(u_+)$. Assume $\sup_{d\in\mathbb{N}} \mathbb{E}[(\tau_B^d)^2], \mathbb{E}[\tau_B^2] < \infty$

Then $\mathbb{E}[\tau_B] = \Gamma_0^{-1}(\infty,\varepsilon)\, \mathrm{e}^{\Delta W(\infty)/\varepsilon}[1 + \mathcal{O}(R(\varepsilon))]$

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Proof: Set $T_{\mathsf{Kr}} = \Gamma_0^{-1}(\infty,\varepsilon)\,\mathrm{e}^{\Delta W(\infty)/\varepsilon}$

Fix sets $B' \subset B \subset B''$ with boundaries at distance δ

Let $\Omega_{K,d} = \left\{ \sup_{t\in[0,KT_{\mathsf{Kr}}]} \|u_t - u_t^d\|_{L^\infty} \leqslant \delta, \tau_{B'}^d \leqslant KT_{\mathsf{Kr}} \right\}$

$\mathbb{P}(\Omega_{K,d}^c) \leqslant \mathbb{P}\{Z > \delta d^\gamma\} + \frac{\mathbb{E}[\tau_{B'}^d]}{KT_{\mathsf{Kr}}} \quad \Rightarrow \quad \lim_{d\to\infty} \mathbb{P}(\Omega_{K,d}^c) \leqslant \frac{2}{K}$

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On $\Omega_{K,d}$ one has $\tau_{B''}^d \leqslant \tau_B \leqslant \tau_{B'}^d$

$\Rightarrow \quad \mathbb{E}[\tau_{B''}^d] - \mathbb{E}[\tau_{B''}^d 1_{\Omega_{K,d}^c}] \leqslant \mathbb{E}[\tau_B] \leqslant \mathbb{E}[\tau_{B'}^d] + \mathbb{E}[\tau_B 1_{\Omega_{K,d}^c}]$

Use $\mathbb{E}[\tau_B 1_{\Omega_{K,d}^c}] \leqslant \sqrt{\mathbb{E}[\tau_B^2]}\sqrt{\mathbb{P}(\Omega_{K,d}^c)}$, take $d \to \infty$ and K large enough

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Potential theory

Consider first Brownian motion $W_t^x = x + W_t$

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$$\begin{aligned} \Delta w_A(x) &= 1 \qquad x \in A^c \\ w_A(x) &= 0 \qquad x \in A \end{aligned}$$

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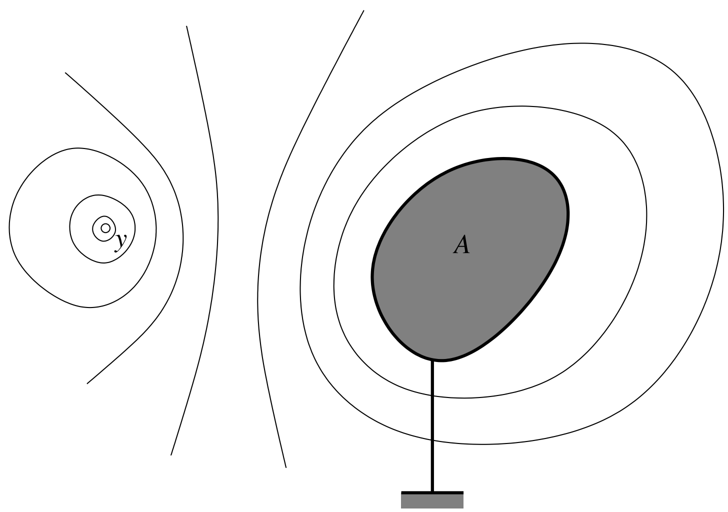

Fact 2: $h_{A,B}(x) = \mathbb{P}[\tau_A^x < \tau_B^x]$ satisfies

$$\begin{aligned} \Delta h_{A,B}(x) &= 0 \qquad && x \in (A \cup B)^c \\ h_{A,B}(x) &= 1 \qquad && x \in A \\ h_{A,B}(x) &= 0 \qquad && x \in B \end{aligned}$$

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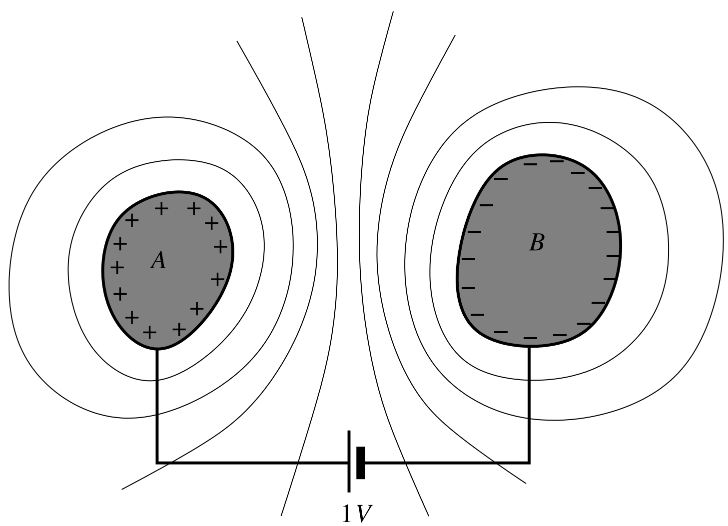
$\rho_{A,B}$: "surface charge density" on ∂A



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Variational representation: Dirichlet form

$$\mathrm{cap}_A(B) = \int_{(A\cup B)^c} \|\nabla h_{A,B}(x)\|^2\,\mathrm{d}x = \inf_{h\in\mathcal{H}_{A,B}} \int_{(A\cup B)^c} \|\nabla h(x)\|^2\,\mathrm{d}x$$

($\mathcal{H}_{A,B}$: set of sufficiently smooth functions satisfying b.c.)

Sketch of proof

Upper bound:

$$\text{cap} = \inf_h \Phi(h) \leqslant \Phi(h_+) \qquad \Phi(h) = \varepsilon \int \|\nabla h(z)\|^2 \, \mathrm{e}^{-V(z)/\varepsilon} \, \mathrm{d}z$$

Let $\delta = \sqrt{c\varepsilon|\log \varepsilon|}$, choose

$$h_+(z) = \begin{cases} 1 & \text{for } z_0 < -\delta \\ f(z_0) & \text{for } -\delta < z_0 < \delta \\ 0 & \text{for } z_0 > \delta \end{cases}$$

where $\varepsilon f''(z_0) + \partial_{z_0} V(z_0, 0) f'(z_0) = 0$ with b.c. $f(\pm\delta) = 0, 1$

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Lower bound:

Bound Dirichlet Φ form below by restricting domain, taking only 1st component of gradient and use for b.c. a priori bound on h