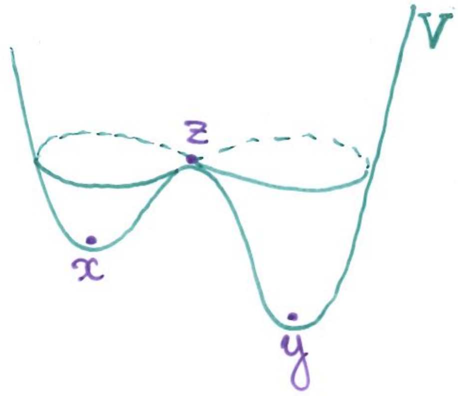
General seminar
IHP, 3/5/17

Metastability in stochastic PDEs

Based on: NB & Barbara Gentz, EJP 18 (24) : 1-58 (2013)
NB, Giacomo Di Gesù & Hendrik Weber, EJP 22 (41): 1-27 (2017)

1. Metastability in gradient SDEs



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

$$\begin{cases} \mathcal{L} = \varepsilon\Delta - \nabla V\cdot\nabla = \varepsilon\, e^{V/\varepsilon}\,\nabla\cdot e^{-V/\varepsilon}\,\nabla \\ \mathcal{L}^\dagger = \varepsilon\,\nabla\cdot e^{-V/\varepsilon}\,\nabla\, e^{V/\varepsilon} \end{cases}$$

- $\mathcal{L}^\dagger(e^{-V/\varepsilon}) = 0 \quad\Rightarrow\quad \pi(x) = \frac{1}{Z}e^{-V(x)/\varepsilon}$ inv. density
- $\mathcal{L}^\dagger e^{-V/\varepsilon} = e^{-V/\varepsilon}\mathcal{L} \quad\Rightarrow\quad (\pi e^{\mathcal{L}t})^\dagger = \pi e^{\mathcal{L}t}$ reversibility (detailed balance)

$\tau := \inf\{t>0 : \|x_t - y\| < \delta\}$ $\qquad \mathbb{E}^x[\tau] = ?$

Arrhenius 1889: $\mathbb{E}^x[\tau] \simeq e^{[V(z)-V(x)]/\varepsilon}$ i.e. $\lim_{\varepsilon\to 0}\varepsilon\log\mathbb{E}^x[\tau] = V(z)-V(x)$

Eyring 1935, Kramers 1940: $\mathbb{E}^x[\tau] = \dfrac{2\pi}{|\lambda_0(z)|}\sqrt{\dfrac{|\det \operatorname{Hess} V(z)|}{\det \operatorname{Hess} V(x)}}\, e^{-[V(z)-V(x)]/\varepsilon}\,[1+o_\varepsilon(1)]$

$\lambda_0(z)$: unique negative ev of Hess $V(z)$

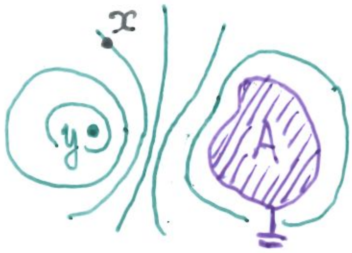
Proofs:
- Arrhenius: large deviations [Freidlin & Wentzell ~ 1970]
- Eyring-Kramers:
  - WKB theory
  - potential theory [Bovier, Eckhoff, Gayrard, Klein 2004]
  - Witten Laplacian [Helffer, Klein, Nier 2005]

Potential theory

$$\tau_A = \inf\{t \geq 0 : x_t \in A\}$$

a) $W_A(x) = \mathbb{E}^x[\tau_A]$ solves $\begin{cases} -\mathcal{L} W_A(x) = 1 & x \in A^c \\ W_A(x) = 0 & x \in A \end{cases}$

Green's function: $\begin{cases} -\mathcal{L} G_{A^c}(x,y) = \delta(x-y) & x \in A^c \\ G_{A^c}(x,y) = 0 & x \in A \end{cases}$



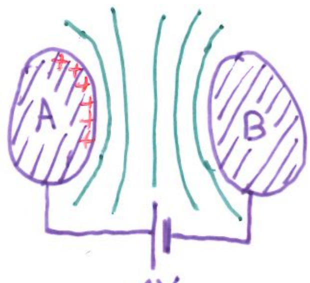
$\varepsilon = 1$, $V=0$: electric potential

$$\Rightarrow \quad W_A(x) = \int_{A^c} G_{A^c}(x-y)\,dy$$

Rem: $e^{-V(x)/\varepsilon} G_{A^c}(x,y) = e^{-V(y)/\varepsilon} G_{A^c}(y,x)$

b) Committor:

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



$$\Rightarrow h_{AB}(x) = \int_{\partial A} G_{B^c}(x,y) \underbrace{\varrho_{AB}(dy)}_{\text{equil. measure on } \partial A}$$

c) Capacity: $\mathrm{cap}(A,B) = \int_{\partial A} e^{-V(y)/\varepsilon} \varrho_{AB}(dy) \quad \Rightarrow \quad \mu_{AB}(dy) = \dfrac{e^{-V(y)/\varepsilon}\varrho_{AB}(dy)}{\mathrm{cap}(A,B)}$

prob. on ∂A

Dirichlet principle: $\mathrm{cap}(A,B) = \varepsilon \int_{(A\cup B)^c} \|\nabla h_{AB}(x)\|^2 e^{-V(x)/\varepsilon}\,dx =: \underbrace{\Phi_{(A\cup B)^c}(h_{AB})}_{\sim \langle h_{AB}, -\mathcal{L} h_{AB}\rangle \text{ Dirichlet form}}$

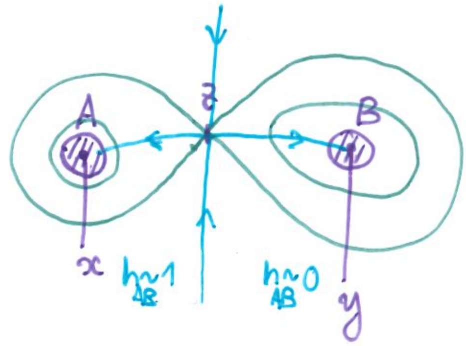
$$\mathrm{cap}(A,B) = \inf_{\substack{h|_A = 1 \\ h|_B = 0}} \Phi_{(A\cup B)^c}(h)$$

d) $\displaystyle\int_{B^c} h_{AB}(x) e^{-V(x)/\varepsilon}\,dx = \int_{B^c}\int_{\partial A} G_{B^c}(x,y) e^{-V(x)/\varepsilon} \varrho_{AB}(dy)\,dx$

$$= \int_{\partial A} e^{-V(y)/\varepsilon} W_B(y)\, \varrho_{AB}(dy) = \mathrm{cap}(A,B)\, \mathbb{E}^{\mu_{AB}}[\tau_B]$$

$$\Rightarrow \quad \boxed{\mathbb{E}^{\mu_{AB}}[\tau_B] = \frac{1}{\mathrm{cap}(A,B)} \int_{B^c} h_{AB}(x) e^{-V(x)/\varepsilon}\,dx}$$

Proof of E-K for double-well potential:



- $\mathrm{cap}(A,B) \simeq \varepsilon \, \frac{|\lambda_0(z)|}{2\pi\varepsilon} \sqrt{\frac{(2\pi\varepsilon)^d}{|\det \mathrm{Hess}\, V(z)|}} \, e^{-V(z)/\varepsilon}$
- $\int_{B^c} h_{AB}(x) e^{-V(x)/\varepsilon} dx \simeq \sqrt{\frac{(2\pi\varepsilon)^d}{\det \mathrm{Hess}\, V(x)}} \, e^{-V(x)/\varepsilon}$
- $\mathbb{E}^{\mu_{AB}}[\tau_B] \simeq \mathbb{E}^{x}[\tau_B]$ (Harnack or coupling)

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2. Allen-Cahn in dimension 1

$$\partial_t \phi = \Delta\phi + \phi - \phi^3 + \sqrt{2\varepsilon}\,\xi \leftarrow \text{space-time white noise:}$$

$\langle \xi, \varphi \rangle$ centred Gaussian r.v.

$\mathbb{E}(\langle \xi, \varphi_1\rangle \langle \xi, \varphi_2\rangle) = \langle \varphi_1, \varphi_2 \rangle$

$\phi = \phi(t,x) \qquad t \geq 0, \quad x \in \mathbb{T} = \mathbb{R}/L\mathbb{Z}$

Potential: $$V(\phi) = \int_0^L \left[\frac{1}{2}\nabla\phi(x)^2 - \frac{1}{2}\phi(x)^2 + \frac{1}{4}\phi(x)^4\right] dx$$

$$\Rightarrow \lim_{h\to 0} \frac{V(\phi + h\psi) - V(\phi)}{h} = \int_0^L \left[\nabla\phi(x)\nabla\psi(x) - \phi(x)\psi(x) + \phi(x)^3\psi(x)\right] dx$$
$$= -\langle \Delta\phi + \phi - \phi^3, \psi \rangle$$

Stationary solutions: $\phi_0(x) \equiv 0$, $\phi_\pm(x) \equiv \pm 1$, additionnal non-const. solutions for $L > 2\pi$

Fourier basis: $\phi(t,x) = \sum_{k\in\mathbb{Z}} z_k(t)\, e_k(x) \Rightarrow \boxed{dz_t = -\nabla\hat{V}(z_t)dt + \sqrt{2\varepsilon}\, dW_t}$

$L < 2\pi$: V = double-well potential with saddle in $\phi_0 = 0$

Hessian at $\phi_0 = 0$: $V(\phi) = \frac{1}{2}\langle \phi, \underbrace{(-\Delta - 1)}_{\mathrm{Hess}V(\phi_0)}\phi \rangle + \mathcal{O}(\phi^4)$

$$\Rightarrow \mathbb{E}^{\phi_-}[\tau_{\phi_+}] \stackrel{?}{=} \frac{2\pi}{|-1|} \underbrace{\sqrt{\frac{|\det(-\Delta - 1)|}{\det(-\Delta + 2)}}}_{\infty/\infty} \underbrace{e^{[V(\phi_0) - V(\phi_-)]/\varepsilon}}_{\text{compatible with LDP by Faris \& Jona-Lasinio}} [1 + O_\varepsilon(1)]$$

ev of $\Delta - 1$: $\lambda_k = \left(k\frac{2\pi}{L}\right)^2 - 1$ $\qquad$ $\Delta_\perp$: projection of Δ on $k \neq 0$

$\Delta + 2$: $\lambda_k + 3$

$$\det\left([-\Delta_\perp - 1][-\Delta_\perp + 2]^{-1}\right) = \det\left([-\Delta_\perp + 2 - 3][-\Delta_\perp + 2]^{-1}\right)$$
$$= \det\left(1 - 3[-\Delta_\perp + 2]^{-1}\right) \qquad \text{Fredholm determinant}$$

$$\log\det\left([-\Delta_\perp - 1][-\Delta_\perp + 2]^{-1}\right) = \operatorname{Tr}\log\left(1 - 3[-\Delta_\perp + 2]^{-1}\right) = -\sum_{n\geq 1}\frac{3^n}{n}\operatorname{Tr}\left([-\Delta_\perp + 2]^{-n}\right)$$
$$\operatorname{Tr}\left([-\Delta_\perp + 2]^{-n}\right) = \sum_{k\neq 0}\frac{1}{\left[\left(\frac{k2\pi}{L}\right)^2 + 2\right]^n} \leqslant \frac{C}{\left[\left(\frac{2\pi}{L}\right)^2 + 2\right]^n}$$

Theorem: [B, Gentz, EJP 2013] E-K formula holds

Proof: uses spectral Galerkin approx. $\qquad$ **Rem:** prefactor $= \dfrac{\sin L}{\sqrt{2}\sinh(\sqrt{2}L)}$ (Euler)

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3. Allen-Cahn in dimension 2

$$\operatorname{Tr}\left[(-\Delta_\perp + 2)^{-1}\right] \sim \sum_{k\neq(0,0)}\frac{1}{\|k\|^2} \sim \int_1^\infty \frac{r\,dr}{r^2} = +\infty$$
$$\operatorname{Tr}\left[(-\Delta_\perp + 2)^{-2}\right] \sim \sum_{k\neq(0,0)}\frac{1}{\|k\|^4} \sim \int_1^\infty \frac{r\,dr}{r^4} < +\infty$$

$(-\Delta_\perp + 2)^{-1}$ is not trace-class but Hilbert-Schmidt

Theorem: [Da Prato, Debussche 2003]

$$\partial_t\phi = \Delta\phi + \phi - [\phi^3 - 3\varepsilon C_N\phi] + \sqrt{2\varepsilon}\,\xi_N$$

mollified on scale $1/N$

with $C_N \sim \log N$ admits limit as $N \to \infty$

$$C_N = \mathbb{E}\,\|\phi_N\|^2_{L^2} = \frac{1}{2}\operatorname{Tr}\left(P_N[-\Delta + 1]^{-1}\right)$$

where ϕ_N is Gaussian free field (GFF): $\Delta\phi_N - \phi_N + \xi_N = 0$

Renormalized potential: $$V_N(\phi) = \frac{1}{2}\int_{\mathbb{T}^2}[\nabla\phi^2 - \phi^2]\,dx + \frac{1}{4}\int_{\mathbb{T}^2}\underbrace{[\phi^4 - 6C_N\phi^2 + 3C_N^2]}_{=:\phi^4:\ \text{(Wick)}}\,dx$$

$$\Rightarrow \text{new prefactor: } \det\left([-\Delta_\perp - 1][-\Delta_\perp + 2]^{-1}e^{3C_N}\right)$$
$$= \det\left(1 - 3[-\Delta_\perp + 2]^{-1}\right)e^{3\operatorname{Tr}[-\Delta + 2]^{-1}} \qquad \text{Carleman-Fredholm det}$$

Theorem: [B, Di Gesù, Weber, EJP 2017] unif. upper/lower bds on EK