SIAM Conference on
Nonlinear Waves and Coherent Structures

The University of Washington, Seattle, WA

13–16 June 2012

Kramers Law – validity and generalizations

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Outline

- Metastability and the Brownian particle in a potential
- Mean first-transition times: Arrhenius and Kramers Law
- Proving Kramers Law: Exponential asymptotics via large deviations
- Proving Kramers Law: Subexponential asymptotics
- Generalizations: Multiwell potentials, non-quadratic saddles, SPDEs
- Limitations: Non-reversible systems

Metastability and Kramers Law

Metastability: A common phenomenon

- Observed in the dynamical behaviour of complex systems
- Related to first-order phase transitions in nonlinear dynamics

Characterization of metastability

- Existence of quasi-invariant subspaces Ω_i, $i \in I$
- Multiple timescales
  - A short timescale on which local equilibrium is reached within the Ω_i
  - A longer metastable timescale governing the transitions between the Ω_i

Important feature

- High free-energy barriers to overcome

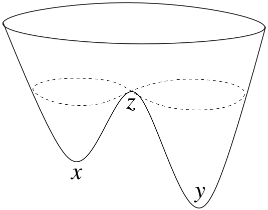
Consequence

- Generally very slow approach to the (global) equilibrium distribution

Brownian particle in a potential landscape

Gradient dynamics (ODE)

$$\dot{x}_t^{\text{det}} = -\nabla V(x_t^{\text{det}})$$



Random perturbation by Gaussian white noise (SDE)

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

Equivalent notation

$$\dot{x}_t^\varepsilon(\omega) = -\nabla V(x_t^\varepsilon(\omega)) + \sqrt{2\varepsilon}\xi_t(\omega)$$

with

- $V : \mathbb{R}^d \to \mathbb{R}$: confining potential, growth condition at infinity
- $\{B_t(\omega)\}_{t\geq 0}$: d-dimensional standard Brownian motion
- $\{\xi_t(\omega)\}_{t\geq 0}$: Gaussian white noise, $\langle \xi_t \rangle = 0$, $\langle \xi_t \xi_s \rangle = \delta(t-s)$

SDEs of gradient type: Properties

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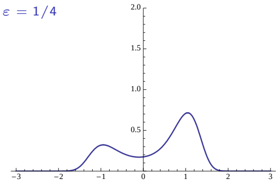

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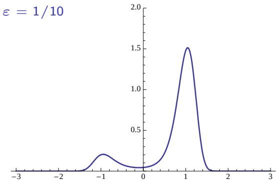

Transition times between potential wells ?

(Random) first-hitting time τ_y of a small ball $B_\delta(y)$

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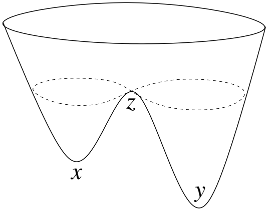

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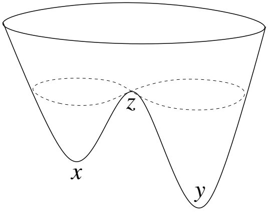

Arrhenius Law [van't Hoff 1885, Arrhenius 1889]

$$\mathbb{E}_x \tau_y \simeq \mathit{const}\ \mathrm{e}^{[V(z)-V(x)]/\varepsilon}$$

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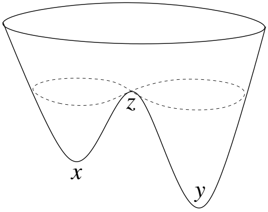

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Eyring–Kramers Law [Eyring 1935, Kramers 1940]

- $d = 1$: $\quad \mathbb{E}_x \tau_y \simeq \dfrac{2\pi}{\sqrt{V''(x)|V''(z)|}}\, \mathrm{e}^{[V(z)-V(x)]/\varepsilon}$

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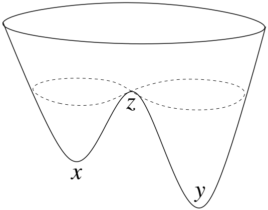

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- $d = 1$: $\mathbb{E}_x \tau_y \simeq \dfrac{2\pi}{\sqrt{V''(x)|V''(z)|}}\, \mathrm{e}^{[V(z)-V(x)]/\varepsilon}$

- $d \geq 2$: $\mathbb{E}_x \tau_y \simeq \dfrac{2\pi}{|\lambda_1(z)|} \sqrt{\dfrac{|\det \nabla^2 V(z)|}{\det \nabla^2 V(x)}}\, \mathrm{e}^{[V(z)-V(x)]/\varepsilon}$

where $\lambda_1(z)$ is the unique negative eigenvalue of $\nabla^2 V$ at saddle z

Proving Kramers Law

Exponential asymptotics via large deviations

- Probability of observing sample paths being close to a given function $\varphi : [0, T] \to \mathbb{R}^d$ behaves like $\sim \exp\{-2I(\varphi)/\varepsilon\}$
- Large-deviation rate function

$$I(\varphi) = I_{[0,T]}(\varphi) = \begin{cases} \frac{1}{2}\int_0^T \|\dot\varphi_s - (-\nabla V(\varphi_s))\|^2 \, ds & \text{for } \varphi \in \mathcal{H}_1 \\ +\infty & \text{otherwise} \end{cases}$$

- Large deviation principle reduces est. of probabilities to variational principle: For any set Γ of paths on $[0, T]$

$$-\inf_{\Gamma^\circ} I \le \liminf_{\varepsilon\to 0} 2\varepsilon \log \mathbb{P}\{(x_t^\varepsilon)_t \in \Gamma\} \le \limsup_{\varepsilon\to 0} 2\varepsilon \log \mathbb{P}\{(x_t^\varepsilon)_t \in \Gamma\} \le -\inf_{\overline{\Gamma}} I$$

- Quasipotential *with respect to* x = "cost to reach z against the flow"

$$V(x,z) := \inf_{t>0} \inf\{I_{[0,t]}(\varphi) \colon \varphi \in \mathcal{C}([0,t],\mathcal{D}),\ \varphi_0 = x,\ \varphi_t = z\}$$

(domain $\mathcal{D}$ with unique asymptotically stable equilibrium point x)

Wentzell–Freidlin theory

Theorem [Wentzell & Freidlin, 1969–72, 1984]

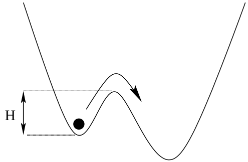
Mean first-exit time from $\mathcal{D}$ satisfies

$$2\varepsilon \log \mathbb{E}\tau_{\mathcal{D}}^{\varepsilon} \to \overline{V} := \inf_{z\in\partial\mathcal{D}} V(x,z) \qquad \text{as } \varepsilon \to 0$$

Gradient case with isotropic noise (reversible diffusion)

- Quasipotential $V(x,z) = 2[V(z) - V(x)]$
- Cost for leaving potential well is

  $\overline{V} = \inf_{z\in\partial\mathcal{D}} V(x,z) = 2H$
- Attained for paths going against the flow: $\dot{\varphi}_t = +\nabla V(\varphi_t)$



Implies Arrhenius Law !

Proving Kramers Law

- Low-lying spectrum of generator of the diffusion
  [Helffer & Sjöstrand 1985; Holley, Kusuoka & Stroock 1989; Mathieu 1995; Miclo 1995; Kolokoltsov 1996; . . .]
- Potential theoretic approach: Relating mean exit times to capacities
  [Bovier, Eckhoff, Gayrard & Klein 2004]
- Two-scale approach and transport techniques
  [Menz & Schlichting 2012]
- Full asymptotic expansion of prefactor
  [Helffer, Klein & Nier 2004; Hérau, Hitrik & Sjöstrand 2008, 2012; . . .]

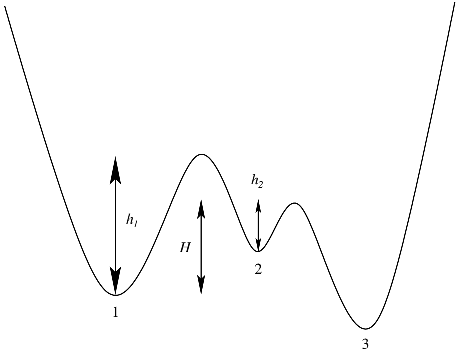
Generalization: Multiwell potentials

Multiwell potentials: Metastable hierarchy

- Order $x_1 \prec x_2 \prec \dots \prec x_n$ of local minima of V according to "depth" $V(x_i)$
- Metastable hierarchy $\mathcal{M}_k = \{x_1, \dots, x_k\}$
- Kramers Law holds for first-hitting time $\mathbb{E}_{x_k} \tau_{\mathcal{M}_{k-1}}$ of neighbourhood of $\mathcal{M}_{k-1}$ [Bovier, Eckhoff, Gayrard & Klein 2004]
- Requires non-degeneracy condition

Example: $3 \prec 1 \prec 2$

- $\mathbb{E}_1 \tau_3 \simeq C_1 \, e^{h_1/\varepsilon}$
- $\mathbb{E}_2 \tau_{\{1,3\}} \simeq C_2 \, e^{h_2/\varepsilon}$
- $\mathbb{E}_2 \tau_3 \simeq C' \, e^{H/\varepsilon} \gg C_2 \, e^{h_2/\varepsilon}$

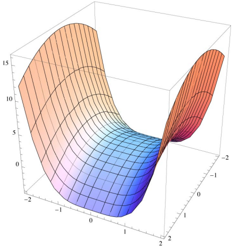


Generalization: Non-quadratic saddles

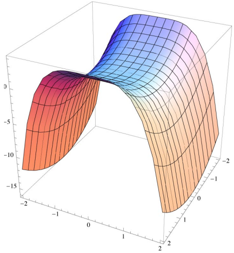
Non-quadratic saddles

What happens if $\det \nabla^2 V(z) = 0$?

$$\det \nabla^2 V(z) = 0 \quad \Rightarrow \quad \text{At least one vanishing eigenvalue at saddle } z$$
$$\Rightarrow \quad \text{Saddle has at least one non-quadratic direction}$$
$$\Rightarrow \quad \text{Kramers Law not applicable}$$



Quartic unstable direction



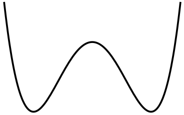
Quartic stable direction

Why do we care about this non-generic situation?

Occurs at bifurcations in parameter-dependent systems

Example: Two harmonically coupled particles

$$V_\gamma(x_1, x_2) = U(x_1) + U(x_2) + \tfrac{\gamma}{2}(x_1 - x_2)^2$$

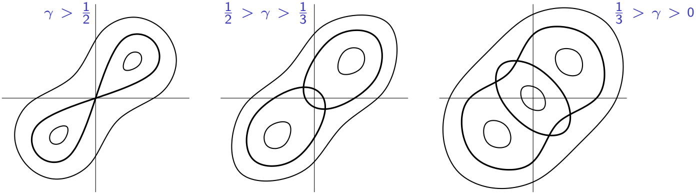


$U(x) = \frac{x^4}{4} - \frac{x^2}{2}$

Change of variable: Rotation by $\pi/4$ yields

$$\widehat{V}_\gamma(y_1, y_2) = -\frac{1}{2}y_1^2 - \frac{1-2\gamma}{2}y_2^2 + \frac{1}{8}\left(y_1^4 + 6y_1^2y_2^2 + y_2^4\right)$$

Note: $\det \nabla^2 \widehat{V}_\gamma(0,0) = 1 - 2\gamma$ $\Rightarrow$ Pitchfork bifurcation at $\gamma = 1/2$



Subexponential asymptotics: Non-quadratic saddles

- $x =$ quadratic local minimum of V (non-quadratic minima possible)
- $y =$ another local minimum of V
- $0 =$ the relevant saddle for passage from x to y
- Normal form near saddle
$$V(z) = -u_1(z_1) + u_2(z_2) + \frac{1}{2}\sum_{j=3}^{d} \lambda_j z_j^2 + \dots$$
- Assume growth conditions on u_1, u_2

Theorem [Berglund & G 2010]

$$\mathbb{E}_x \tau_y = \frac{(2\pi\varepsilon)^{d/2}\,\mathrm{e}^{-V(x)/\varepsilon}}{\sqrt{\det \nabla^2 V(x)}} \Bigg/ \varepsilon \frac{\displaystyle\int_{-\infty}^{\infty} \mathrm{e}^{-u_2(z_2)/\varepsilon}\,\mathrm{d}y_2}{\displaystyle\int_{-\infty}^{\infty} \mathrm{e}^{-u_1(z_1)/\varepsilon}\,\mathrm{d}y_1} \prod_{j=3}^{d} \sqrt{\frac{2\pi\varepsilon}{\lambda_j}}$$
$$\times \left[1 + \mathcal{O}(\varepsilon^{\alpha} |\log \varepsilon|^{1+\alpha})\right]$$

where $\alpha > 0$ is explicitly known (depends on the growth conditions on u_1, u_2)

Corollary: From quadratic saddles to pitchfork bifurcation

Pitchfork bifurcation: $V(z) = -\frac{1}{2}|\lambda_1| z_1^2 + \frac{1}{2}\lambda_2 z_2^2 + C_4 z_2^4 + \frac{1}{2}\sum_{j=3}^{d} \lambda_j z_j^2 + \dots$

- For $\lambda_2 > 0$ (possibly small wrt. ε):

$$\mathbb{E}_x \tau_y = 2\pi \sqrt{\frac{(\lambda_2 + \sqrt{2\varepsilon C_4})\lambda_3 \dots \lambda_d}{|\lambda_1| \det \nabla^2 V(x)}} \, \frac{\mathrm{e}^{[V(0)-V(x)]/\varepsilon}}{\Psi_+(\lambda_2/\sqrt{2\varepsilon C_4})} \, [1 + R(\varepsilon)]$$

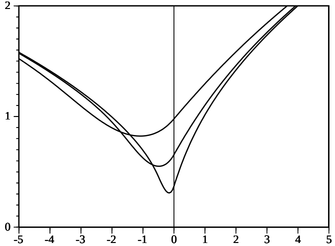
where

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

$$\lim_{\alpha\to\infty} \Psi_+(\alpha) = 1$$

$K_{1/4} =$ modified Bessel fct. of 2*nd* kind

- For $\lambda_2 < 0$: Similar
(involving eigenvalues at new saddles and $I_{\pm 1/4}$)



$\lambda_2 \mapsto$ prefactor

$\varepsilon = 0.5, \ \varepsilon = 0.1, \ \varepsilon = 0.01$

Generalization:

Stochastic partial differential equations

Allen–Cahn SPDE

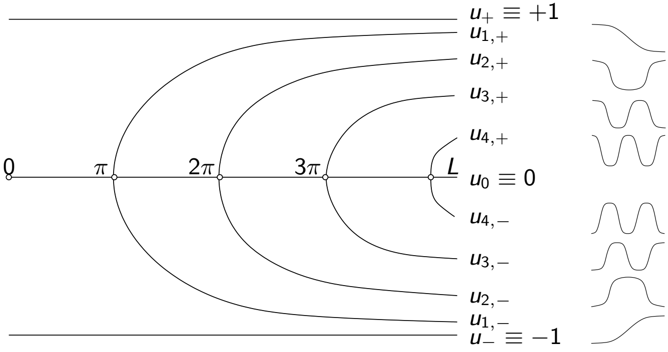
$$\partial_t u(x,t) = \partial_{xx} u(x,t) + u(x,t) - u(x,t)^3 + \sqrt{2\varepsilon}\,\xi(t,x)$$

- $x \in [0,L]$ and $u(x,t) \in \mathbb{R}$
- Weak space–time white noise $\sqrt{2\varepsilon}\,\xi$
- Neumann b.c.: $\partial_x u(0,t) = \partial_x u(L,t) = 0$
- Energy functional $V(u) = V_L(u) = \int_0^L \left[\left(\frac{1}{4}u(x)^4 - \frac{1}{2}u(x)^2\right) + \frac{1}{2}u'(x)^2\right] \mathrm{d}x$
- Stationary states for $L < \pi$:
  - $u_\pm(x) \equiv \pm 1$ (uniform and stable; global minima)
  - $u_0(x) \equiv 0$ (uniform and unstable; transition state)
  - Activation energy $V(u_0) - V(u_\pm) = L/4$
- Stationary states for $L > \pi$:
  - $u_\pm(x) \equiv \pm 1$ (uniform and stable; still global minima)
  - $u_0(x) \equiv 0$ (uniform and unstable; no longer transition state)
  - $u_{\text{inst},\pm}(x)$ of instanton shape (pair of unstable states; transition states)
  - Additional stationary states as L increases; not transition states
- As $L \nearrow \pi$: Pitchfork bifurcation

Stationary states (Neumann b.c.)

For $k = 1, 2, \dots$ and $L > \pi k$:

$$u_{k,\pm}(x) = \pm\sqrt{\frac{2m}{m+1}}\,\mathrm{sn}\Big(\frac{kx}{\sqrt{m+1}} + \mathrm{K}(m), m\Big) \quad \text{where} \quad 2k\sqrt{m+1}\,\mathrm{K}(m) = L$$



Allen–Cahn SPDE: Kramers Law

Results

- Large deviation principle [Faris & Jona-Lasinio 1982] implies Arrhenius Law
- Formal computation of subexponential asymptotics [Maier & Stein 2001]
- Kramers Law away from bifurcation points
  [Barret, Bovier & Méléard 2010, Barret 2012]
- Kramers Law for all finite L [Berglund & G 2012]

Idea of the proof

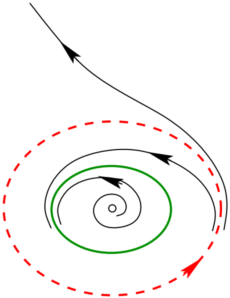
- Spectral Galerkin approximation
- Control of error terms uniformly in dimension
- Use large deviation principle to obtain a priori bounds

Limitations of Kramers Law

New phenomenon in non-reversible case: Cycling

Planar vector field: $d = 2$, $\mathcal{D} \subset \mathbb{R}^2$ s.t. $\partial\mathcal{D} =$ *unstable* periodic orbit

- $\mathbb{E}\tau_{\mathcal{D}} \sim e^{\overline{V}/2\varepsilon}$ still holds
- Quasipotential $V(\Pi, z) \equiv \overline{V}$ is constant on $\partial\mathcal{D}$
- Phenomenon of cycling [Day '90]:
  Distribution of $x_{\tau_{\mathcal{D}}}$ on $\partial\mathcal{D}$ does *not* converge as $\varepsilon \to 0$
  Density is *translated* along $\partial\mathcal{D}$ proportionally to $|\log\varepsilon|$.
- In *stationary regime*: (obtained by reinjecting particle)
  Rate of escape $\frac{d}{dt}\mathbb{P}\{x_t \notin \mathcal{D}\}$ has $|\log\varepsilon|$-periodic prefactor [Maier & Stein '96]



Universality in cycling

Theorem [Berglund & G '04, '05, work in progress]

There exists an explicit parametrization of $\partial\mathcal{D}$ s.t. the exit time density is given by

$$p(t, t_0) = \frac{f_{\text{trans}}(t, t_0)}{\mathcal{N}} \; Q_{\lambda T}\big(\theta(t) - \tfrac{1}{2}|\log\varepsilon|\big) \frac{\theta'(t)}{\lambda T_{\text{K}}(\varepsilon)} \, \mathrm{e}^{-(\theta(t)-\theta(t_0))\,/\,\lambda T_{\text{K}}(\varepsilon)}$$

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- f_{trans} grows from 0 to 1 in time $t - t_0$ of order $|\log\varepsilon|$
- $Q_{\lambda T}(y)$ is a *universal* λT-periodic function
- T is the period of the unstable orbit, λ its Lyapunov exponent

Universality in cycling

Theorem [Berglund & G '04, '05, work in progress]

There exists an explicit parametrization of $\partial\mathcal{D}$ s.t. the exit time density is given by

$$p(t,t_0) = \frac{f_{\text{trans}}(t,t_0)}{\mathcal{N}}\; Q_{\lambda T}\Big(\theta(t) - \tfrac12|\log\varepsilon|\Big)\frac{\theta'(t)}{\lambda T_{\text{K}}(\varepsilon)}\,\mathrm{e}^{-(\theta(t)-\theta(t_0))\,/\,\lambda T_{\text{K}}(\varepsilon)}$$

- f_{trans} grows from 0 to 1 in time $t-t_0$ of order $|\log\varepsilon|$
- $Q_{\lambda T}(y)$ is a *universal* λT-periodic function
- T is the period of the unstable orbit, λ its Lyapunov exponent
- $\theta(t)$ is a "natural" parametrisation of the boundary:
  $\theta'(t) > 0$ is an explicitely known *model-dependent*, T-periodic function;
  $\theta(t+T) = \theta(t) + \lambda T$

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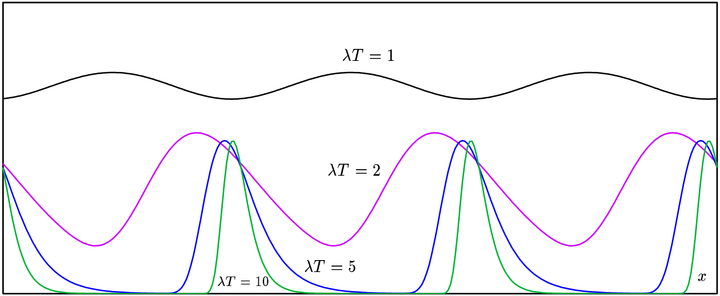
  $\theta'(t) > 0$ is an explicitely known *model-dependent*, T-periodic function;
  $\theta(t+T) = \theta(t) + \lambda T$
- $T_{\text{K}}(\varepsilon)$ is the analogue of Kramers' time: $T_{\text{K}}(\varepsilon) = \dfrac{C}{\sqrt{\varepsilon}}\,\mathrm{e}^{\overline{V}/2\varepsilon}$

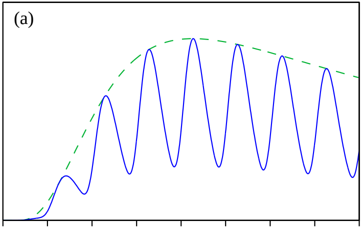
The universal profile

$y \mapsto Q_{\lambda T}(\lambda T y)/2\lambda T$

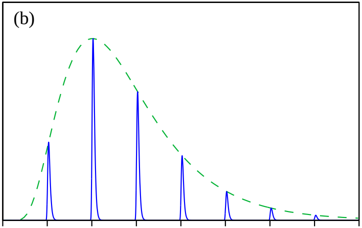


- Profile determines concentration of first-passage times within a period
- Shape of peaks: Gumbel distribution $P(z) = \frac{1}{2} \mathrm{e}^{-2z} \exp\{-\frac{1}{2} \mathrm{e}^{-2z}\}$
- The larger λT, the more pronounced the peaks
- For smaller values of λT, the peaks overlap more

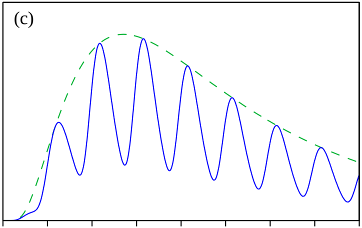
Density of the first-passage time for $\overline{V} = 0.5,\ \lambda = 1$



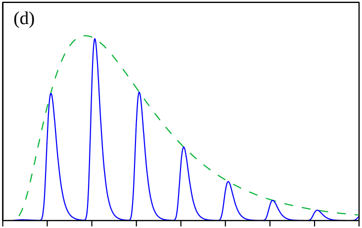
$\varepsilon = 0.4,\ T = 2$



$\varepsilon = 0.4,\ T = 20$



$\varepsilon = 0.5,\ T = 2$



$\varepsilon = 0.5,\ T = 5$

Thank you for your attention !

Relation of first-exit times to PDEs

$$\mathrm{d}x_t^\varepsilon = b(x_t^\varepsilon)\,\mathrm{d}t + \sqrt{2\varepsilon}g(x_t^\varepsilon)\,\mathrm{d}W_t\;, \qquad x_0 \in \mathbb{R}^d$$

Infinitesimal generator $\mathcal{A}^\varepsilon$ of diffusion x_t^ε (adjoint of Fokker–Planck operator)

$$\mathcal{A}^\varepsilon\, v(t,x) = \varepsilon \sum_{i,j=1}^{d} a_{ij}(x)\,\frac{\partial^2}{\partial x_i\,\partial x_j}\,v(t,x) + \langle\, b(x), \nabla v(t,x)\,\rangle$$

Theorem

- Poisson problem:
  $\mathbb{E}_x\{\tau_{\mathcal{D}}^\varepsilon\}$ is the unique solution of
  $$\begin{cases} \mathcal{A}^\varepsilon\, u = -1 & \text{in } \mathcal{D} \\ u = 0 & \text{on } \partial\mathcal{D} \end{cases}$$
- Dirichlet problem:
  $\mathbb{E}_x\{f(x^\varepsilon_{\tau^\varepsilon_{\mathcal{D}}})\}$ is the unique solution of
  (for $f : \partial\mathcal{D} \to \mathbb{R}$ continuous)
  $$\begin{cases} \mathcal{A}^\varepsilon\, w = 0 & \text{in } \mathcal{D} \\ w = f & \text{on } \partial\mathcal{D} \end{cases}$$

Potential theory for Brownian motion I

First-hitting time $\tau_A = \inf\{t > 0 \colon B_t \in A\}$ of $A \subset \mathbb{R}^d$

Fact I: The expected first-hitting time $w_A(x) = \mathbb{E}_x \tau_A$ is a solution to the Dirichlet problem

$$\begin{cases} \Delta w_A(x) = -1 & \text{for } x \in A^c \\ w_A(x) = 0 & \text{for } x \in A \end{cases}$$

and can be expressed with the help of the Green function $G_{A^c}(x, y)$ as

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

Potential theory for Brownian motion II

The equilibrium potential (or capacitor) $h_{A,B}$ is a solution to the Dirichlet problem

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

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

The equilibrium measure (or surface charge density) is the unique measure $\rho_{A,B}$ on ∂A s.t.

$$h_{A,B}(x) = \int_{\partial A} G_{B^c}(x,y)\, \rho_{A,B}(\mathrm{d}y)$$

Capacities

Key observation: For a small ball $C = B_\delta(x)$,

$$\int_{A^c} h_{C,A}(y)\,\mathrm{d}y = \int_{A^c}\int_{\partial C} G_{A^c}(y,z)\,\rho_{C,A}(\mathrm{d}z)\,\mathrm{d}y$$
$$= -\int_{\partial C} w_A(z)\,\rho_{C,A}(\mathrm{d}z) \simeq w_A(x)\,\mathrm{cap}_C(A)$$

where $\mathrm{cap}_C(A) = -\int_{\partial C}\rho_{C,A}(\mathrm{d}y)$ denotes the capacity

$$\Rightarrow \quad \mathbb{E}_x\tau_A = w_A(x) \simeq \frac{1}{\mathrm{cap}_{B_\delta(x)}(A)}\int_{A^c} h_{B_\delta(x),A}(y)\,\mathrm{d}y$$

Variational representation via Dirichlet form

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

where $\mathcal{H}_{C,A}$ = set of sufficiently smooth functions h satisfying b.c.

General case

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

What changes as the generator Δ is replaced by $\varepsilon\Delta - \nabla V \cdot \nabla$?

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

$$\mathbb{E}_x\tau_A = w_A(x) \simeq \frac{1}{\mathrm{cap}_{B_\delta(x)}(A)} \int_{A^c} h_{B_\delta(x),A}(y)\,\mathrm{e}^{-V(y)/\varepsilon}\,\mathrm{d}y$$

It remains to investigate capacity and integral.

Assume, x is a quadratic minimum. Use rough *a priori* bounds on h for cap and

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

Non-quadratic saddles: Worse than quartic . . .

- Quartic unstable direction: $V(z) = -C_4 z_1^4 + \frac{1}{2}\sum_{j=2}^{d} \lambda_j z_j^2 + \dots$

$$\mathbb{E}_x \tau_y = \frac{\Gamma(1/4)}{2C_4^{1/4}\varepsilon^{1/4}} \sqrt{\frac{2\pi\lambda_2 \dots \lambda_d}{\det \nabla^2 V(x)}}\, \mathrm{e}^{[V(0)-V(x)]/\varepsilon}[1 + \mathcal{O}(\varepsilon^{1/4}|\log\varepsilon|^{5/4})]$$

- Degenerate unstable direction: $V(z) = -C_{2p} z_1^{2p} + \frac{1}{2}\sum_{j=2}^{d} \lambda_j z_j^2 + \dots$

$$\mathbb{E}_x \tau_y = \frac{\Gamma(1/2p)}{pC_{2p}^{1/2p}\varepsilon^{1/2(1-1/p)}} \sqrt{\frac{2\pi\lambda_2 \dots \lambda_d}{\det \nabla^2 V(x)}}\, \mathrm{e}^{[V(0)-V(x)]/\varepsilon} \times [1 + \mathcal{O}(\varepsilon^{1/2p}|\log\varepsilon|^{1+1/2p})]$$

Allen–Cahn equation with noise

$$\begin{cases} \partial_t u(x,t) &= \partial_{xx} u(x,t) + u(x,t) - u(x,t)^3 + \sqrt{2\varepsilon}\xi(t,x) \\ u(\cdot,0) &= \varphi(\cdot) \\ \partial_x u(0,t) &= \partial_x u(L,t) = 0 \qquad \text{(Neumann b.c.)} \end{cases}$$

- Space–time white noise $\xi(t,x)$ as formal derivative of Brownian sheet
- Mild / evolution formulation, following [Walsh 1986]:

$$u(x,t) = \int_0^L G_t(x,z)\varphi(z)\,\mathrm{d}z + \int_0^t \int_0^L G_{t-s}(x,z)\big[u(s,z) - u(s,z)^3\big]\,\mathrm{d}z\,\mathrm{d}s$$
$$+ \sqrt{2\varepsilon} \int_0^t \int_0^L G_{t-s}(x,z) W(\mathrm{d}s,\mathrm{d}z)$$

where

- G is the heat kernel
- W is the Brownian sheet

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

Stability of the stationary states: Neumann b.c.

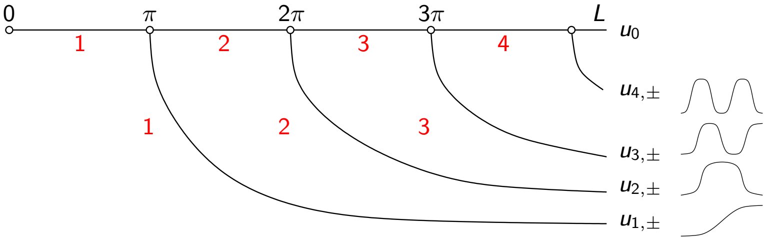
Consider linearization of AC equation at stationary solution $u : [0, L] \to \mathbb{R}$

$$\partial_t v = A[u]v \quad \text{where} \quad A[u] = \frac{\mathrm{d}^2}{\mathrm{d}x^2} + 1 - 3u^2$$

Stability is determined by the eigenvalues of $A[u]$

- $u_\pm(x) \equiv \pm 1$: $A[u_\pm]$ has eigenvalues $-(2 + (\pi k/L)^2)$, $k = 0, 1, 2, \dots$
- $u_0(x) \equiv 0$: $A[u_0]$ has eigenvalues $1 - (\pi k/L)^2$, $k = 0, 1, 2, \dots$

Counting the number of positive eigenvalues: None for $u_\pm$ and ...



Question

How long does a noise-induced transition from the global minimum $u_-(x) \equiv -1$ to (a neighbourhood of) $u_+(x) \equiv 1$ take?

$$\tau_{u_+} = \text{first hitting time of such a neighbourhood}$$

Metastability: We expect $\mathbb{E}_{u_-} \tau_{u_+} \sim e^{\text{const}/\varepsilon}$

We seek

- Activation energy ΔW
- Transition rate prefactor Γ_0^{-1}
- Exponent α of error term

such that

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

Formal computation of the prefactor for the AC equation

Consider $L < \pi$ (and Neumann b.c.)

- Transition state: $u_0(x) \equiv 0$, $V[u_0] = 0$
- Activation energy: $\Delta W = V[u_0] - V[u_-] = L/4$
- Eigenvalues at stable state $u_-(x) \equiv -1$: $\mu_k = 2 + (\pi k/L)^2$
- Eigenvalues at transition state $u_0 \equiv 0$: $\lambda_k = -1 + (\pi k/L)^2$

Thus formally [Maier & Stein 2001, 2003]

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

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

Questions

- What happens when $L \nearrow \pi$? (Approaching bifurcation)
- Is the formal computation correct in infinite dimension?

Allen–Cahn equation: Introducing Fourier variables

- Fourier series

$$u(x,t) = \frac{1}{\sqrt{L}} y_0(t) + \frac{2}{\sqrt{L}} \sum_{k=1}^{\infty} y_k(t) \cos(\pi k x/L) = \frac{1}{\sqrt{L}} \sum_{k\in\mathbb{Z}} \tilde{y}_k(t)\, e^{i\, k\pi x/L}$$

- Rewrite energy functional V in Fourier variables

$$V(y) = \frac{1}{2} \sum_{k=0}^{\infty} \lambda_k y_k^2 + V_4(y)\,, \qquad \lambda_k = -1 + (\pi k/L)^2$$

where

$$V_4(y) = \frac{1}{4L} \sum_{k_1+k_2+k_3+k_4=0} \tilde{y}_{k_1} \tilde{y}_{k_2} \tilde{y}_{k_3} \tilde{y}_{k_4}$$

- Resulting system of SDEs

$$\dot{y}_k = -\lambda_k y_k - \frac{1}{L} \sum_{k_1+k_2+k_3=k} \tilde{y}_{k_1} \tilde{y}_{k_2} \tilde{y}_{k_3} + \sqrt{2\varepsilon}\, \dot{W}_t^{(k)}$$

with i.i.d. Brownian motions $W_t^{(k)}$

Truncating the Fourier series

- Truncate Fourier series (projected equation)

$$u_d(x,t) = \frac{1}{\sqrt{L}} y_0(t) + \frac{2}{\sqrt{L}} \sum_{k=1}^{d} y_k(t) \cos(\pi k x / L)$$

- Retain only modes $k \leq d$ in the energy functional V

$$V^{(d)}(y) = \frac{1}{2} \sum_{k=0}^{d} \lambda_k y_k^2 + V_4^{(d)}(y)$$

where

$$V_4^{(d)}(y) = \frac{1}{4L} \sum_{\substack{k_1+k_2+k_3+k_4=0 \\ k_i \in \{-d,\dots,0,\dots,+d\}}} \tilde{y}_{k_1} \tilde{y}_{k_2} \tilde{y}_{k_3} \tilde{y}_{k_4}$$

- Resulting d-dimensional system of SDEs

$$\dot{y}_k = -\lambda_k y_k - \frac{1}{L} \sum_{\substack{k_1+k_2+k_3=k \\ k_i \in \{-d,\dots,0,\dots,+d\}}} \tilde{y}_{k_1} \tilde{y}_{k_2} \tilde{y}_{k_3} + \sqrt{2\varepsilon}\, \dot{W}_t^{(k)}$$

Reduction to finite-dimensional system

- Show the following result for the projected finite-dimensional systems

$$\varepsilon^\gamma C(d)\,\mathrm{e}^{\Delta W^{(d)}/\varepsilon}[1 - R_d^-(\varepsilon)] \leq \mathbb{E}_{u_-^{(d)}}\tau_{u_+^{(d)}} \leq \varepsilon^\gamma C(d)\,\mathrm{e}^{\Delta W^{(d)}/\varepsilon}[1 + R_d^+(\varepsilon)]$$

(The contribution ε^γ is only present at bifurcation points / non-quadratic saddles)

- The following limits exist and are finite

$$\lim_{d\to\infty} C(d) =: C(\infty) \qquad \text{and} \qquad \lim_{d\to\infty} \Delta W^{(d)} =: \Delta W^{(\infty)}$$

- Important: Uniform control of error terms (uniform in d):

$$R^\pm(\varepsilon) := \sup_d R_d^\pm(\varepsilon) \to 0 \quad \text{as} \quad \varepsilon \to 0$$

Away from bifurcation points, c.f. [Barret, Bovier & Méleard 09]

Taking the limit $d \to \infty$

- For any ε, distance between $u(x,t)$ and solution $u^{(d)}(x,t)$ of the projected equation becomes small on any finite time interval $[0,T]$ [Liu 2003; Blömker & Jentzen 2009]
- Uniform error bounds and large deviation results allow to decouple limits of small ε and large d
- Yielding

$$\varepsilon^{\gamma} C(\infty)\, e^{\Delta W^{(\infty)}/\varepsilon}[1 - R^{-}(\varepsilon)] \leq \mathbb{E}_{u_-}\tau_{u_+} \leq \varepsilon^{\gamma} C(\infty)\, e^{\Delta W^{(\infty)}/\varepsilon}[1 + R^{+}(\varepsilon)]$$

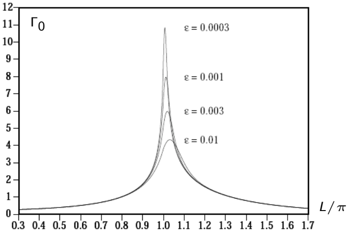
Result for the Allen–Cahn equation (Neumann b.c.)

Theorem [Berglund & G 2012]

For $L < \pi$

$$\mathbb{E}_{u_-}\tau_{u_+} = \frac{1}{\Gamma_0(L)}\,\mathrm{e}^{L/4\varepsilon}[1+\mathcal{O}((\varepsilon|\log\varepsilon|)^{1/4})]$$

where the rate prefactor satisfies
(recall: $\lambda_1 = -1 + (\pi/L)^2$)



$$\Gamma_0(L) = \frac{1}{2^{3/4}\pi}\sqrt{\frac{\sinh(\sqrt{2}L)}{\sin L}}\sqrt{\frac{\lambda_1}{\lambda_1+\sqrt{3\varepsilon/4L}}}\,\Psi_+\Bigl(\frac{\lambda_1}{\sqrt{3\varepsilon/4L}}\Bigr)$$

$$\longrightarrow \frac{\Gamma(1/4)}{2(3\pi^7)^{1/4}}\sqrt{\sinh(\sqrt{2}\pi)}\,\varepsilon^{-1/4} \qquad \text{as } L \nearrow \pi$$

Allen–Cahn equation with periodic b.c.

- Periodic b.c.: $u(0,t) = u(L,t)$ and $\partial_x u(0,t) = \partial_x u(L,t)$
- For $k = 1, 2, \dots$ and $L > 2\pi k$:

  Additional continuous one-parameter family of stationary states, given in terms of Jacobi's elliptic sine by

  $$u_{k,\varphi}(x) = \sqrt{\frac{2m}{m+1}}\,\mathrm{sn}\Big(\frac{kx}{\sqrt{m+1}} + \varphi, m\Big) \quad \text{where} \quad 4k\sqrt{m+1}\mathrm{K}(m) = L$$
- For $L > 2\pi$: Rate prefactor $\Gamma_0(L) \sim L/\sqrt{\varepsilon}$