

Metastability in systems with bifurcations

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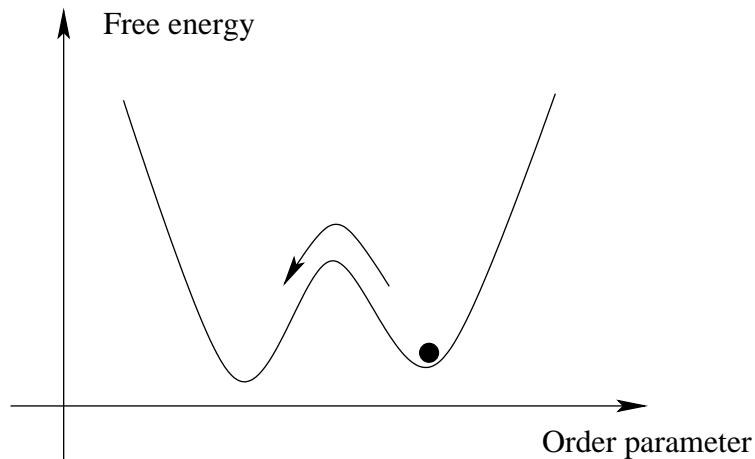
[Bastien Fernandez](#), CPT, CNRS, Marseille

Bielefeld, 18 november 2008

Metastability in physics

Examples:

- Supercooled liquid
 - Supersaturated gas
 - Wrongly magnetised ferromagnet
- ▷ Near first-order phase transition
- ▷ Nucleation implies crossing energy barrier

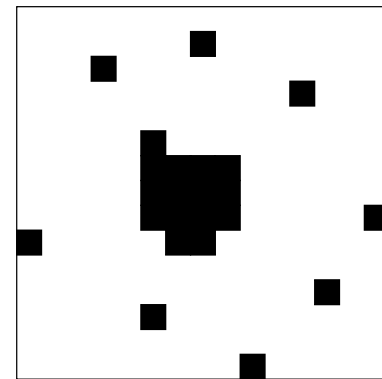


Metastability in stochastic lattice models

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

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

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

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

Reversible w.r.t.
invariant measure:

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

(detailed balance)

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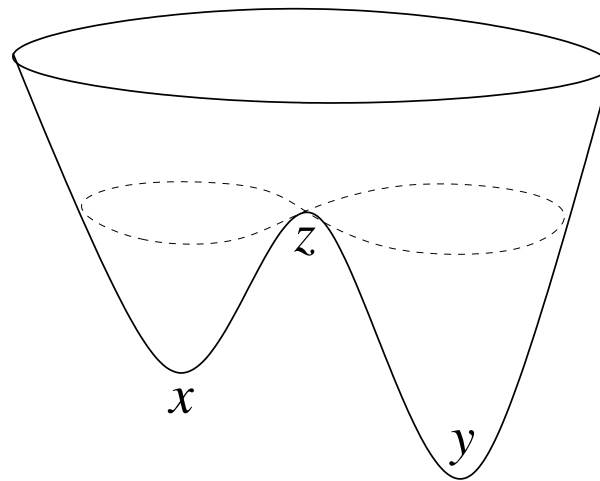
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τ_y^x : first-hitting time of small ball $\mathcal{B}_\varepsilon(y)$, starting in x
“Eyring–Kramers law” (Eyring 1935, Kramers 1940)

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

Towards a proof of Kramers' law

- Large deviations (Wentzell & Freidlin 1969):

$$\lim_{\varepsilon \rightarrow 0} \varepsilon \log(\mathbb{E}[\tau_y^x]) = V(z) - V(x)$$

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

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

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):

$$\lim_{\varepsilon \rightarrow 0} \mathbb{P}\left\{ \tau_y^x > t \mathbb{E}[\tau_y^x] \right\} = e^{-t}$$

The question

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

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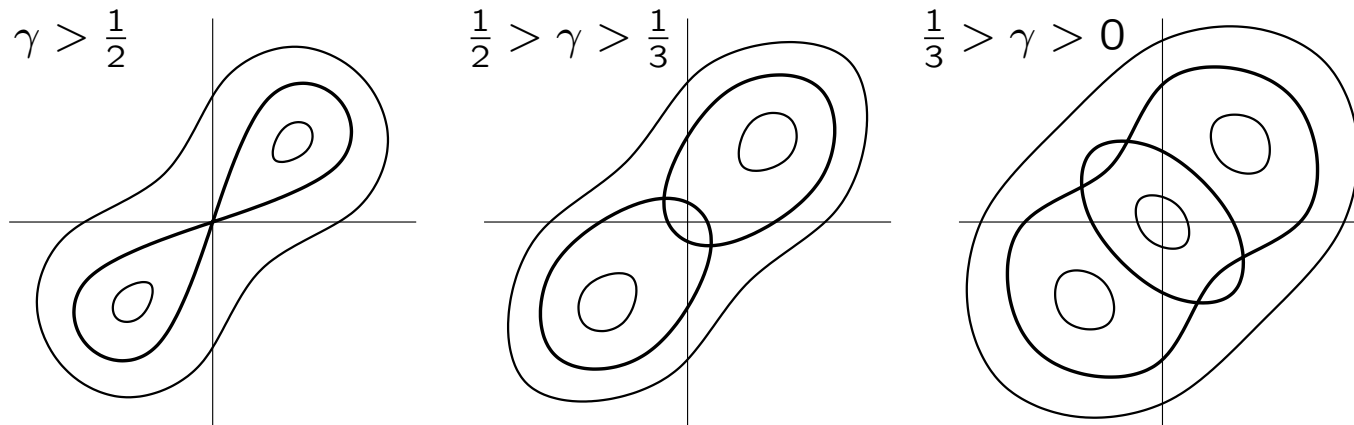
Dependence on parameter \Rightarrow Bifurcations

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

$$U(x) = \frac{1}{4}x^4 - \frac{1}{2}x^2$$

Rotation by $\pi/4$: $\hat{V}_\gamma(y_1, y_2) = -\frac{1}{2}y_1^2 - \frac{1-2\gamma}{2}y_2^2 + \frac{1}{8}(y_1^4 + 6y_1^2y_2^2 + y_2^4)$

$\det \nabla^2 \hat{V}_\gamma(0, 0) = \frac{1-2\gamma}{4}$: Pitchfork bifurcation at $\gamma = \frac{1}{2}$



More examples

- N particles on a circle: $i \in \Lambda = \mathbb{Z} / N\mathbb{Z}$

$$V_\gamma(x) = \sum_{i \in \Lambda} U(x_i) + \frac{\gamma}{4} \sum_{i \in \Lambda} (x_{i+1} - x_i)^2$$

N.B., B. Gentz and B. Fernandez, *Metastability in interacting nonlinear stochastic differential equations I, II*, Nonlinearity 20 (2007), 2551 & 2583

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- Ginzburg-Landau SPDE: $x \in [0, L]$, various b.c.

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

$$V_L(\phi) = \int_0^L \left[U(\phi(x)) + \frac{1}{2} \phi'(x)^2 \right] dx$$

Pitchfork bif. at $L = 2\pi$ (periodic b.c.) or $L = \pi$ (Neumann b.c.)

R.S. Maier and D.L. Stein, *Droplet nucleation and domain wall motion in a bounded interval*, Phys. Rev. Lett. 87 (2001), 270601-1

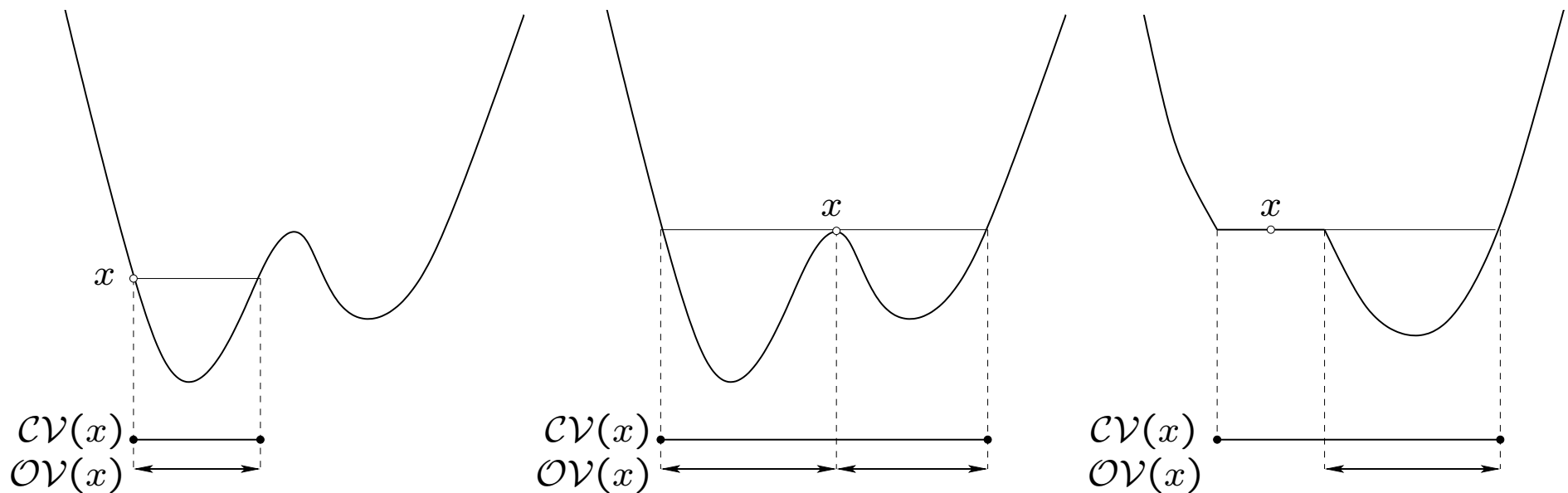
Definition of saddles

- ▷ Communication height $\bar{V}(x, y) = \inf_{\gamma: x \rightarrow y} \sup_{t \in [0, |\gamma|]} V(\gamma(t))$
- ▷ For $A, B \subset \mathbb{R}^d$: $\bar{V}(A, B) = \inf_{x \in A, y \in B} \bar{V}(x, y)$

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▷ Closed valley: $CV(x) = \{y \in \mathbb{R}^d : \bar{V}(x, y) = V(x)\}$

▷ Open valley: $OV(x) = \{y \in CV(x) : V(y) < V(x)\}$

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Definition: z is a **saddle** if

1. $\mathcal{O}\mathcal{V}(z)$ non-empty and not path-connected
2. $(\mathcal{O}\mathcal{V}(z) \cup \{z\})$ path-connected

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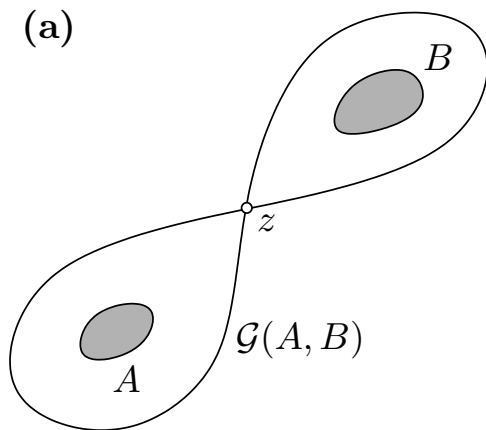
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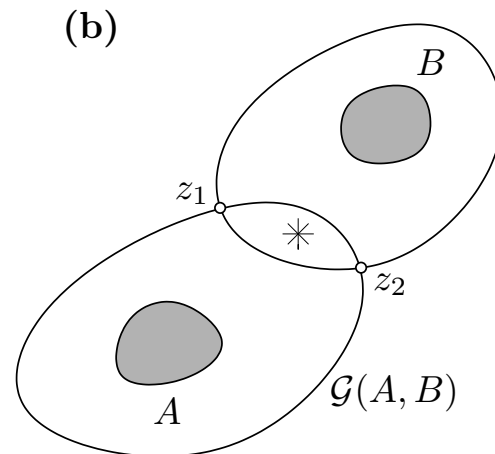
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Saddles can act as **gates** between components of their open valleys

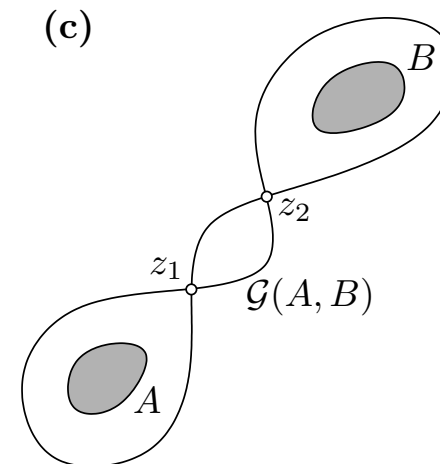
Gate: any minimal subset of $\mathcal{G}(A, B) = \{x : V(x) = \bar{V}(A, B)\}$ that cannot be avoided by minimal paths from A to B



$$\text{gate}(A, B) = \{z\}$$



$$\text{gate}(A, B) = \{z_1, z_2\}$$



$$\text{gate}(A, B) = \{z_1\} \text{ or } \{z_2\}$$

Classification of saddles

Let z be a saddle. Then

- ▷ $V \in \mathcal{C}^1 \Rightarrow \nabla V(z) = 0$
- ▷ $V \in \mathcal{C}^2 \Rightarrow \nabla^2 V(z)$ has at least 1 ev ≤ 0 and at most 1 ev < 0
- ▷ $V \in \mathcal{C}^2, \nabla V(z) = 0, \det \nabla^2 V(z) \neq 0$
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Nonquadratic saddle: $\det \nabla^2 V(z) = 0$

Most generic cases:

- $\nabla^2 V(z)$ has ev $\lambda_1 < 0 = \lambda_2 < \lambda_3 \leq \dots \leq \lambda_d$
- $\nabla^2 V(z)$ has ev $0 = \lambda_1 < \lambda_2 \leq \dots \leq \lambda_d$

Classification of nonquadratic saddles

Assume $V \in \mathcal{C}^4$ and $\nabla^2 V(0)$ has ev $\lambda_1 < 0 = \lambda_2 < \lambda_3 \leq \dots \leq \lambda_d$

$$V(x) = -\frac{1}{2}|\lambda_1|x_1^2 + \frac{1}{2} \sum_{j=3}^d \lambda_j x_j^2 + \sum_{1 \leq i \leq j \leq k \leq d} V_{ijk} x_i x_j x_k + \dots$$

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Normal form: There exists polynomial $g(y) = \mathcal{O}(\|y\|^2)$ s.t.

$$V(y + g(y)) = -\frac{1}{2}|\lambda_1|y_1^2 + \frac{1}{2} \sum_{j=3}^d \lambda_j y_j^2 + C_3 y_2^3 + C_4 y_2^4 + \dots$$

($C_3 = V_{222}$, C_4 explicitly known)

Proposition:

- $C_3 \neq 0$ or $C_4 < 0 \Rightarrow z = 0$ is not a saddle
- $C_3 = 0$ and $C_4 > 0 \Rightarrow z = 0$ is a saddle
- $C_3 = C_4 = 0 \Rightarrow$ depends on higher-order terms

Potential theory

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

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$$\Delta w_A(x) = 1 \quad x \in A^c$$

$$w_A(x) = 0 \quad x \in A$$

$G_{A^c}(x, y)$ Green's function $\Rightarrow w_A(x) = \int_{A^c} G_{A^c}(x, y) \, dy$

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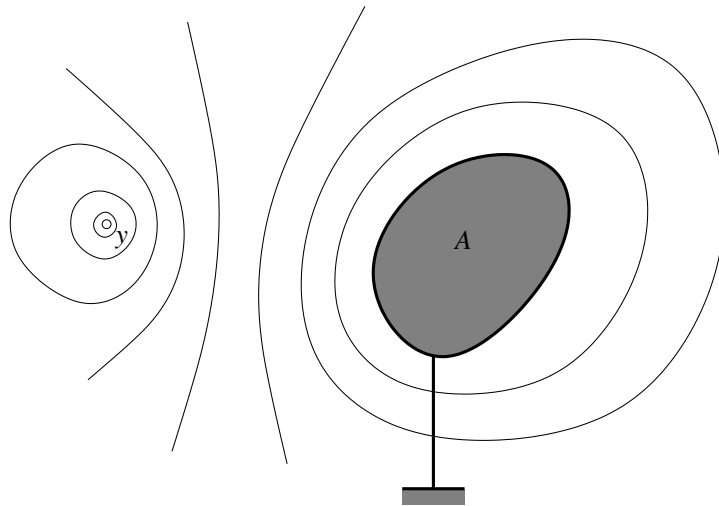
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Potential theory

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

$$\Delta h_{A,B}(x) = 0 \quad x \in (A \cup B)^c$$

$$h_{A,B}(x) = 1 \quad x \in A$$

$$h_{A,B}(x) = 0 \quad x \in B$$

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

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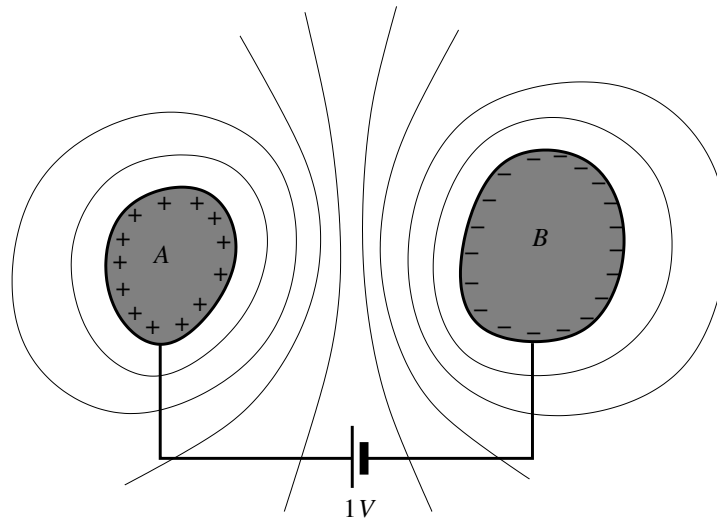
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$\rho_{A,B}$: “surface charge density” on ∂A



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Key observation: let $C = \mathcal{B}_\varepsilon(x)$, then

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Variational representation: Dirichlet form

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

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

Potential theory

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

Generator: $\Delta \mapsto \varepsilon\Delta - \nabla V \cdot \nabla$

Then

$$\mathbb{E}[\tau_A^x] = w_A(x) \simeq \frac{\int_{A^c} h_{\mathcal{B}_\varepsilon(x), A}(y) e^{-V(y)/\varepsilon} dy}{\text{cap}_{\mathcal{B}_\varepsilon(x)}(A)}$$

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

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

Main result

Assume

- $z = 0$ saddle, A, B in different components of $\mathcal{O}\mathcal{V}(z)$
- Normal form $V(y) = -u_1(y_1) + u_2(y_2) + \frac{1}{2} \sum_{j=3}^d \lambda_j y_j^2 + \dots$
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Theorem: For some known $\alpha > 0$ depending on growth cond.

$$\text{cap}_A(B) = \varepsilon \frac{\int_{-\infty}^{\infty} e^{-u_2(y_2)/\varepsilon} dy_2}{\int_{-\infty}^{\infty} e^{-u_1(y_1)/\varepsilon} dy_1} \prod_{j=3}^d \sqrt{\frac{2\pi\varepsilon}{\lambda_j} \left[1 + \mathcal{O}((\varepsilon|\log \varepsilon|)^\alpha) \right]}$$

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Proof:

- ▷ Upper bound: Use $h(y) = f(y_1)$ in Dirichlet form, f solution of $\varepsilon f''(y_1) - u_1'(y_1) f'(y_1) = 0$ with b.c. $f(\pm\delta(\varepsilon)) = 0, 1$
- ▷ Lower bound: Bound Dirichlet form below by restricting domain, taking only 1st component of gradient and use for b.c. a priori bound on $h_{A,B}$

Applications

1. Quadratic case: $V(y) = -\frac{1}{2}|\lambda_1|y_1^2 + \frac{1}{2}\sum_{j=2}^d \lambda_j y_j^2 + \dots$

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Applications

1. Quadratic case: $V(y) = -\frac{1}{2}|\lambda_1|y_1^2 + \frac{1}{2}\sum_{j=2}^d \lambda_j y_j^2 + \dots$

$$\mathbb{E}[\tau_y^x] = 2\pi \sqrt{\frac{\lambda_2 \dots \lambda_d}{|\lambda_1| \det(\nabla^2 V(x))}} e^{\bar{V}(x,y)/\varepsilon} \left[1 + \mathcal{O}((\varepsilon |\log \varepsilon|)^{1/2}) \right]$$

2. Quartic case: $V(y) = -\frac{1}{2}|\lambda_1|y_1^2 + C_4 y_2^4 + \frac{1}{2}\sum_{j=3}^d \lambda_j y_j^2 + \dots$

$$\mathbb{E}[\tau_y^x] = \frac{2C_4^{1/4}}{\Gamma(1/4)} \sqrt{\frac{(2\pi)^3 \lambda_3 \dots \lambda_d}{|\lambda_1| \det(\nabla^2 V(x))}} \varepsilon^{1/4} e^{\bar{V}(x,y)/\varepsilon} \left[1 + \mathcal{O}((\varepsilon |\log \varepsilon|)^{1/4}) \right]$$

3. Pitchfork bif: $V(y) = -\frac{1}{2}|\lambda_1|y_1^2 + \frac{1}{2}\lambda_2 y_2^2 + C_4 y_2^4 + \frac{1}{2}\sum_{j=3}^d \lambda_j y_j^2 + \dots$

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

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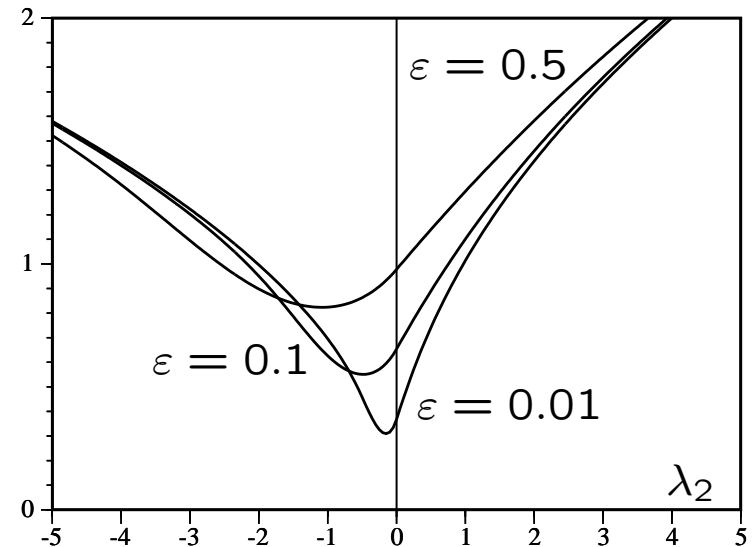
for $\lambda_2 > 0$, where

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

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

Similar expression for $\lambda_2 < 0$

involving $I_{\pm 1/4}$



Applications

4. Ginzburg–Landau equation:

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

Fourier series: $\phi(x, t) = \frac{1}{\sqrt{L}} \sum_{k \in \mathbb{Z}} \phi_k(t) e^{2\pi i k x / L}$

$$d\phi_k = -\lambda_k \phi_k dt - \frac{1}{L} \sum_{k_1 + k_2 + k_3 = k} \phi_{k_1} \phi_{k_2} \phi_{k_3} dt + \sqrt{2\varepsilon} dW_t^{(k)}$$

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

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Kramers rate (Maier & Stein)

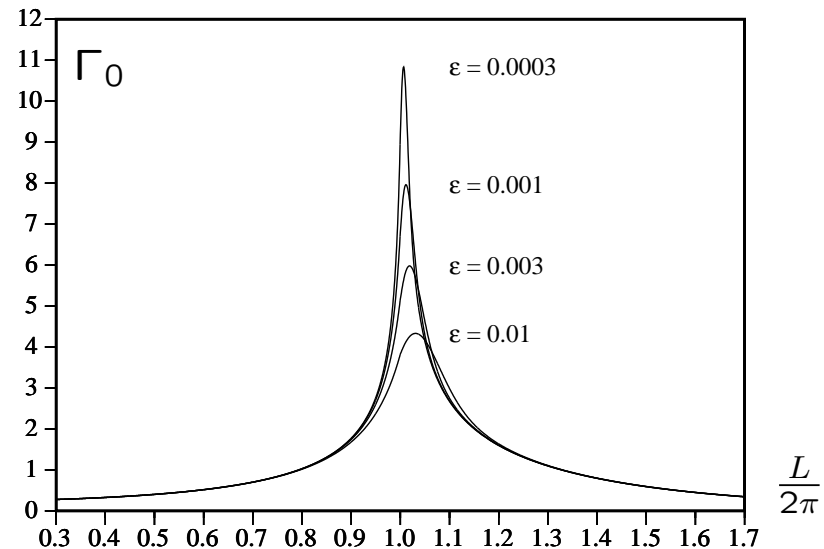
$$\frac{1}{\mathbb{E}\{\tau\}} = \Gamma \simeq \Gamma_0 e^{-\Delta W / \varepsilon}$$

e.g. for $L \ll 2\pi$

$$\Gamma_0 \simeq \frac{\sqrt{2}}{2\pi} \prod_{k=1}^{\infty} \frac{2 + (2\pi k / L)^2}{-1 + (2\pi k / L)^2} = \frac{\sinh(L / \sqrt{2})}{2\pi \sin(L / 2)}$$

For $L \rightarrow 2\pi_-$: multiply by

$$\frac{4\pi^2 - L^2}{4\pi^2 - L^2 + \sqrt{3\varepsilon} L^3 / 2} \Psi + \left(\frac{4\pi^2 - L^2}{\sqrt{3\varepsilon} L^3 / 2} \right)$$



Outlook

- Multiple zero eigenvalues (higher codimension bifurcations)
- Theory directly for SPDE

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References

- Anton Bovier, Michael Eckhoff, Véronique Gayrard and Markus Klein *Metastability in reversible diffusion processes I: Sharp asymptotics for capacities and exit times*, J. Eur. Math. Soc. **6**, 399–424 (2004)
- N. B. and Barbara Gentz, *The Eyring–Kramers law for potentials with non-quadratic saddles*, arXiv/0807.1681 (2008)
- N. B. and Barbara Gentz, *Anomalous behavior of the Kramers rate at bifurcations in classical field theories*, arXiv/0809.2652 (2008)