

Metastable Lifetimes in Coupled Random Dynamical Systems

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SAMSI, 31 August 2009

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

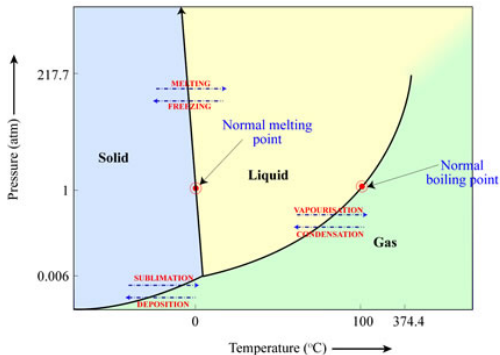
Example: Liquid–crystal transition through nucleation

Change parameters quickly across the line of a first-order phase transition:

- ▶ System remains in metastable equilibrium for long time before undergoing a rapid transition to the new equilibrium state due to (random) perturbations

Example: Supercooled liquid

- ▶ Pure water freezes at about -44°F rather than at its freezing temperature of 32°F if no crystal nuclei are present



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Supercooled water

Reversible diffusions

Gradient dynamics (ODE)

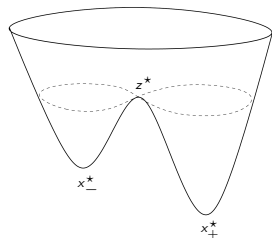
$$\dot{x}_t^{\text{det}} = -\nabla V(x_t^{\text{det}})$$

Random perturbation by Gaussian white noise (SDE)

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

with

- ▷ $V : \mathbb{R}^d \rightarrow \mathbb{R}$: confining potential, growth condition at infinity
- ▷ $\{B_t(\omega)\}_{t \geq 0}$: d -dimensional Brownian motion



Invariant measure or **equilibrium distribution** (for gradient systems)

$$\mu_\varepsilon(dx) = \frac{1}{Z_\varepsilon} e^{-V(x)/\varepsilon} dx \quad \text{with} \quad Z_\varepsilon = \int_{\mathbb{R}^d} e^{-V(x)/\varepsilon} dx$$

μ_ε concentrates in the minima of V

Metastability in reversible diffusions: Timescales

Let V double-well potential as before, start in $x_0^\varepsilon = x_-^* =$ left-hand well

How long does it take until x_t^ε is well described by its invariant distribution?

- ▶ For ε small, paths will stay in the left-hand well for a long time
- ▶ x_t^ε first approaches a Gaussian distribution, centered in x_-^* ,

$$T_{\text{relax}} = \frac{1}{V''(x_-^*)} = \frac{1}{\text{curvature at the bottom of the well}} \quad (d=1)$$

- ▶ With overwhelming probability, paths will remain inside left-hand well, for all times significantly shorter than **Kramers' time**

$$T_{\text{Kramers}} = e^{H/\varepsilon}, \quad \text{where } H = V(z^*) - V(x_-^*) = \text{barrier height}$$

- ▶ Only for $t \gg T_{\text{Kramers}}$, the distribution of x_t^ε approaches p_0

The dynamics is thus very different on the different timescales

Transition times between potential wells

First-hitting time of a small ball $B_\delta(x_+^*)$ around minimum x_+^*

$$\tau_+ = \tau_{x_+^*}^\varepsilon(\omega) = \inf\{t \geq 0: x_t^\varepsilon(\omega) \in B_\delta(x_+^*)\}$$

Eyring–Kramers Law [Eyring 35, Kramers 40]

$$\triangleright d = 1: \quad \mathbb{E}_{x_-^*} \tau_+ \simeq \frac{2\pi}{\sqrt{|V'''(x_-^*)| |V''(z^*)|}} e^{[V(z^*) - V(x_-^*)]/\varepsilon}$$

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$$\triangleright d \geq 2: \quad \mathbb{E}_{x_-^*} \tau_+ \simeq \frac{2\pi}{|\lambda_1(z^*)|} \sqrt{\frac{|\det \nabla^2 V(z^*)|}{\det \nabla^2 V(x_-^*)}} e^{[V(z^*) - V(x_-^*)]/\varepsilon}$$

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

Proving Kramers Law I

- ▶ Exponential asymptotics and optimal transition paths via **large deviations approach** [Wentzell & Freidlin 69–72]

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

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

- ▶ Domain \mathcal{D} with unique asymptotically stable equilibrium point x_-^*
Quasipotential with respect to x_-^* = Cost to reach z against the flow

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

- ▶ Gradient case (reversible diffusion)
 - ▶ Cost for leaving potential well: $\bar{V} := \min_{z \in \partial \mathcal{D}} V(x_-^*, z) = 2[V(z^*) - V(x_-^*)]$
 - ▶ Attained for paths going **against** the flow: $\dot{\varphi}_t = +\nabla V(\varphi_t)$

Proving Kramers Law II

- ▶ Exponential asymptotics depends **only on barrier height**

$$\lim_{\varepsilon \rightarrow 0} \varepsilon \log \mathbb{E}_{x_-^*} \tau_+ = V(z^*) - V(x_-^*)$$

Only 1-saddles are relevant for transitions between wells

- ▶ Low-lying spectrum of generator of the diffusion (analytic approach) [Helffer & Sjöstrand 85, Miclo 95, Mathieu 95, Kolokoltsov 96, ...]
- ▶ Potential theoretic approach [Bovier, Eckhoff, Gayraud & Klein 04]

$$\mathbb{E}_{x_-^*} \tau_+ = \frac{2\pi}{|\lambda_1(z^*)|} \sqrt{\frac{|\det \nabla^2 V(z^*)|}{\det \nabla^2 V(x_-^*)}} e^{[V(z^*) - V(x_-^*)]/\varepsilon} [1 + \mathcal{O}(\varepsilon^{1/2} |\log \varepsilon|)]$$

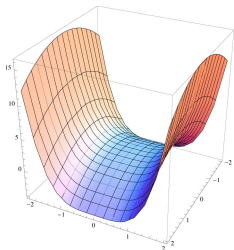
- ▶ Full asymptotic expansion of prefactor [Helffer, Klein & Nier 04]
- ▶ Asymptotic distribution of τ_+ [Day 83, Bovier, Gayraud & Klein 05]

$$\lim_{\varepsilon \rightarrow 0} \mathbb{P}_{x_-^*} \{ \tau_+ > t \cdot \mathbb{E}_{x_-^*} \tau_+ \} = e^{-t}$$

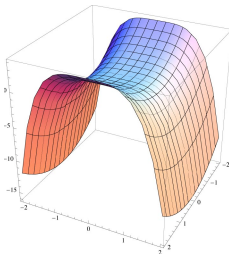
Non-quadratic saddles

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

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



Quartic unstable direction



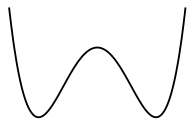
Quartic stable direction

Why do we care about this non-generic situation?

Parameter-dependent systems may undergo **bifurcations**

Example: Two harmonically coupled particles

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

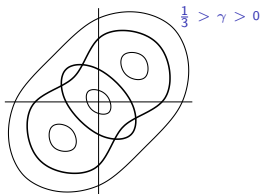
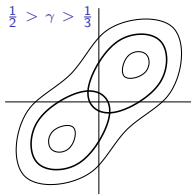
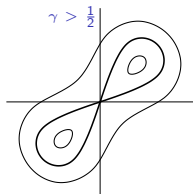


$$U(x) = \frac{x^4}{4} - \frac{x^2}{2}$$

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

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

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



Further examples: More particles

N particles with nearest-neighbour coupling : $i \in \Lambda = \mathbb{Z}/N\mathbb{Z}$

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

Results [Berglund, G. & Fernandez 07]

- ▶ Bifurcation diagram
- ▶ Optimal transition paths
- ▶ Exponential asymptotics of transition times

Weak coupling I

Without coupling $\gamma = 0$:

- ▶ Stationary points of global potential: $\mathcal{S} = \{-1, 0, 1\}^N$
- ▶ Global minima: $\mathcal{S}_0 = \{-1, 1\}^N$

Theorem [Berglund, G. & Fernandez 07]

$\forall N \exists \gamma^*(N) > 0$ s.t.

- ▶ For $k \in \mathbb{N}_0$: k -saddles $x^*(\gamma) \in S_k(\gamma)$ depend continuously on $\gamma \in [0, \gamma^*(N))$
- ▶ $\frac{1}{4} \leq \inf_{N \geq 2} \gamma^*(N) \leq \gamma^*(3) = \frac{1}{3}(\sqrt{3 + 2\sqrt{3}} - \sqrt{3}) = 0.2701\dots$

For $0 < \gamma \ll 1$:

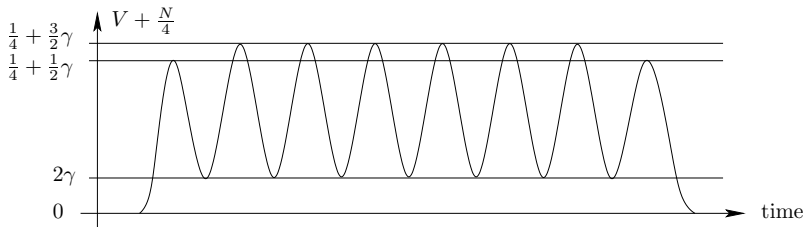
$$V_\gamma(x^*(\gamma)) = V_0(x^*(0)) + \frac{\gamma}{4} \sum_{i \in \Lambda} (x_{i+1}^*(0) - x_i^*(0))^2 + \mathcal{O}(\gamma^2)$$

Dynamics minimizes # of interfaces (cf. Ising spin system with Glauber dynamics)

Weak coupling II

Dynamics like in Ising spin system with Glauber dynamics:

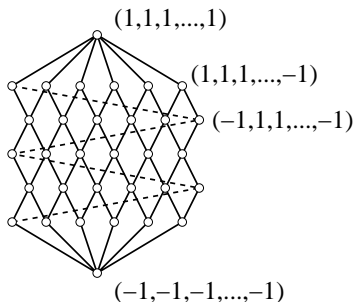
-	-	-	-	-	-	-	-	-	-	-	0	+	+	+	+	+
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-	-	-	-	-	-	-	-	0	+	+	+	+	+	+	+	+
-	-	-	-	-	-	-	-	-	-	-	-	0	+	+	+	+
-	-	-	-	-	-	-	-	-	-	-	-	-	-	0	+	+



Potential seen along an optimal transition path:
Differences in potential height determine transition times

Weak coupling III

Dynamics like in Ising spin system with Glauber dynamics



Partial representation of the hypercube
(showing only edges contained in optimal transition paths)

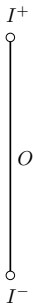
Strong coupling: Synchronisation

For all $\gamma \geq 0$: $I^\pm = \pm(1, 1, \dots, 1) \in \mathcal{S}_0$ and $O = (0, 0, \dots, 0) \in \mathcal{S}$

$$\gamma_1 = \gamma_1(N) := \frac{1}{1 - \cos(2\pi/N)} = \frac{N^2}{2\pi^2} [1 + \mathcal{O}(N^{-2})]$$

Theorem [Berglund, G. & Fernandez 07]

- ▷ Stationary points $\mathcal{S} = \{I^-, I^+, O\} \Leftrightarrow \gamma \geq \gamma_1$
- ▷ 1-saddles $\mathcal{S}_1 = \{O\} \Leftrightarrow \gamma > \gamma_1$



Proof (using Lyapunov function $W(x) = \frac{1}{2} \sum (x_i - x_{i+1})^2 = \frac{1}{2} \|x - Rx\|^2$)

$$\dot{x} = Ax - F(x), \quad A = \begin{pmatrix} 1-\gamma & \gamma/2 & \dots & \gamma/2 \\ \gamma/2 & & \ddots & \vdots \\ \vdots & \ddots & & \gamma/2 \\ \gamma/2 & \dots & \gamma/2 & 1-\gamma \end{pmatrix}, \quad F_i(x) = x_i^3, \quad Rx = (x_2, \dots, x_N, x_1)$$

$$\frac{dW(x)}{dt} = \langle x - Rx, \frac{d}{dt}(x - Rx) \rangle \leq \langle x - Rx, A(x - Rx) \rangle \leq (1 - \frac{\gamma}{\gamma_1}) \|x - Rx\|^2$$

▶ Skip

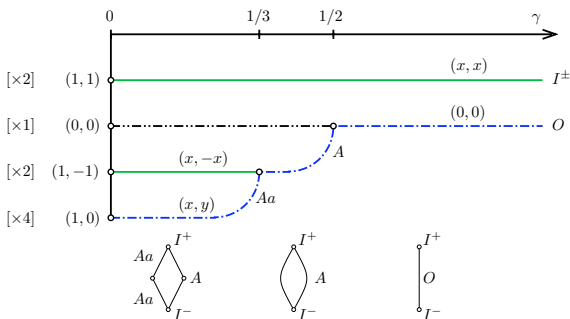
Intermediate coupling

Reduction via symmetry groups: Global potential V_γ is invariant under

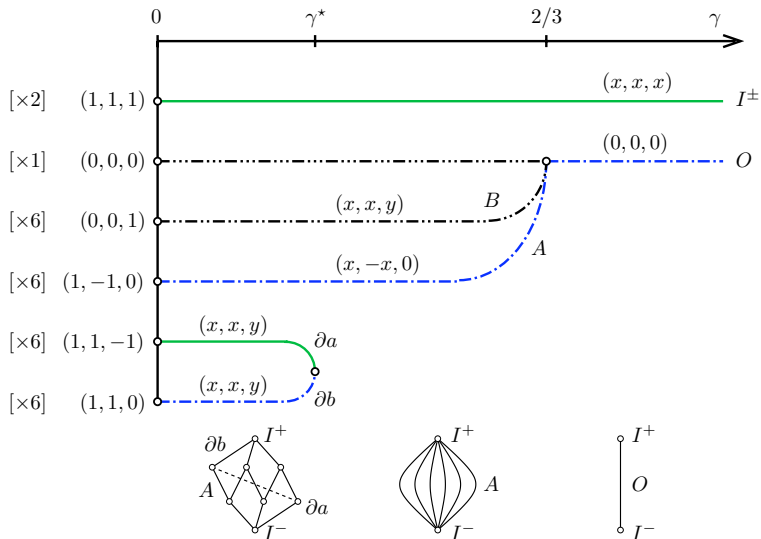
- ▷ $R(x_1, \dots, x_N) = (x_2, \dots, x_N, x_1)$
- ▷ $S(x_1, \dots, x_N) = (x_N, x_{N-1}, \dots, x_1)$
- ▷ $C(x_1, \dots, x_N) = -(x_1, \dots, x_N)$

V_γ invariant under group $G = D_N \times \mathbb{Z}_2$ generated by R, S, C

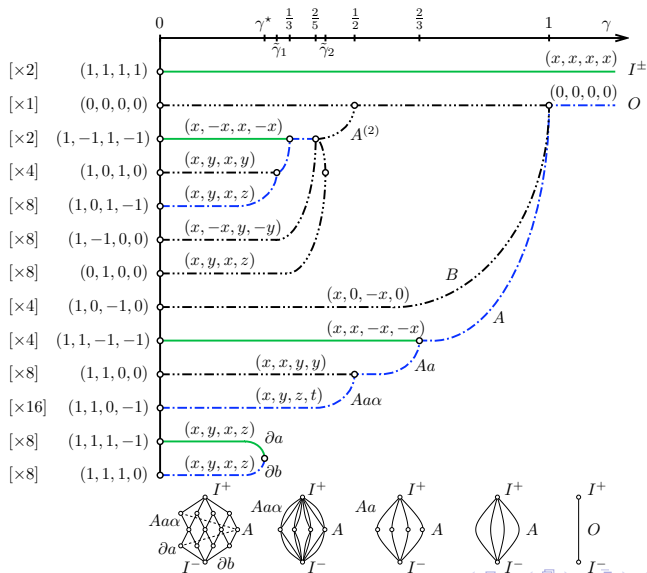
Small lattices: $N = 2$



Small lattices: $N = 3$



Small lattices: $N = 4$



Degenerate saddles

Recall: Only saddles with **one** unstable direction are relevant for transitions

Let z be a stationary point: $\nabla V(z) = 0$

▶ Quadratic case $\det \nabla^2 V(z) \neq 0$:

z saddle $\Leftrightarrow \nabla^2 V(z)$ has **exactly one** e.v. < 0

▶ Non-quadratic case $\det \nabla^2 V(z) = 0$:

z saddle $\Rightarrow \nabla^2 V(z)$ has $\left\{ \begin{array}{l} \text{at least one e.v. } \leq 0 \\ \text{at most one e.v. } < 0 \end{array} \right.$

Most generic cases: One degenerate direction, $\nabla^2 V(z)$ having eigenvalues

▶ $\lambda_1 < 0 = \lambda_2 < \lambda_3 \leq \lambda_4 \leq \dots \leq \lambda_d$ (one stable direction non-quadratic)

▶ $\lambda_1 = 0 < \lambda_2 \leq \lambda_3 \leq \dots \leq \lambda_d$ (the unstable direction non-quadratic)

Degenerate saddles: An example

Assume $z^* = 0$ and eigenvalues $\lambda_1 < 0 = \lambda_2 < \lambda_3 \leq \dots \leq \lambda_d$ of $\nabla^2 V(0)$

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

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

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

$$\begin{array}{l} C_3 = V_{222} \\ C_4 \text{ explicitly known} \end{array} \Rightarrow \begin{cases} C_3 \neq 0 \text{ or } C_4 < 0 & : z = 0 \text{ is not a saddle} \\ C_3 = 0 \text{ and } C_4 > 0 & : z = 0 \text{ is a saddle} \\ C_3 = C_4 = 0 & : \text{higher-order terms relevant} \end{cases}$$

If $z^* = 0$ is a saddle with $C_3 = 0$ and $C_4 > 0$, then

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

Main result

- ▶ Assume x_-^* is a quadratic local minimum of V (non-quadratic minima can be dealt with)
- ▶ Assume x_+^* is another local minimum of V
- ▶ Assume $z^* = 0$ is the **relevant** saddle for passage from x_-^* to x_+^*
- ▶ Normal form near saddle

$$V(y) = -u_1(y_1) + u_2(y_2) + \frac{1}{2} \sum_{j=3}^d \lambda_j y_j^2 + \dots$$

- ▶ Assume growth conditions on u_1, u_2

Theorem [Berglund & G. (to appear in MPRF)]

$$\mathbb{E}_{x_-^*} \tau_+ = \frac{(2\pi\varepsilon)^{d/2} e^{-V(x_-^*)/\varepsilon}}{\sqrt{\det \nabla^2 V(x_-^*)}} \bigg/ \varepsilon \frac{\int_{-\infty}^{\infty} e^{-u_2(y_2)/\varepsilon} dy_2}{\int_{-\infty}^{\infty} e^{-u_1(y_1)/\varepsilon} dy_1} \prod_{j=3}^d \sqrt{\frac{2\pi\varepsilon}{\lambda_j}}$$

$$\times [1 + \mathcal{O}((\varepsilon|\log \varepsilon|)^\alpha)]$$

where $\alpha > 0$ depends on the growth conditions and is explicitly known

Corollaries:

Quadratic saddles, quartic saddles, and worse than that ...

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

$$\mathbb{E}_{x_-^*} \tau_+ = 2\pi \sqrt{\frac{\lambda_2 \dots \lambda_d}{|\lambda_1| \det \nabla^2 V(x_-^*)}} e^{[V(z^*) - V(x_-^*)]/\varepsilon} [1 + \mathcal{O}((\varepsilon |\log \varepsilon|)^{1/2})]$$

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

$$\mathbb{E}_{x_-^*} \tau_+ = \frac{2C_4^{1/4} \varepsilon^{1/4}}{\Gamma(1/4)} \sqrt{\frac{(2\pi)^3 \lambda_3 \dots \lambda_d}{|\lambda_1| \det \nabla^2 V(x_-^*)}} e^{[V(z^*) - V(x_-^*)]/\varepsilon} [1 + \mathcal{O}((\varepsilon |\log \varepsilon|)^{1/4})]$$

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- ▷ Quartic **un**stable direction: $V(y) = -C_4 y_1^4 + \frac{1}{2}\sum_{j=2}^d \lambda_j y_j^2 + \dots$

$$\mathbb{E}_{x_-^*} \tau_+ = \frac{\Gamma(1/4)}{2C_4^{1/4} \varepsilon^{1/4}} \sqrt{\frac{(2\pi)^1 \lambda_2 \dots \lambda_d}{\det \nabla^2 V(x_-^*)}} e^{[V(z^*) - V(x_-^*)]/\varepsilon} [1 + \mathcal{O}((\varepsilon |\log \varepsilon|)^{1/4})]$$

Corollaries: Worse than quartic ...

- ▷ Quartic **unstable** direction: $V(y) = -C_4 y_1^4 + \frac{1}{2} \sum_{j=2}^d \lambda_j y_j^2 + \dots$

$$\mathbb{E}_{x_-^*} \tau_+ = \frac{\Gamma(1/4)}{2C_4^{1/4} \varepsilon^{1/4}} \sqrt{\frac{2\pi \lambda_2 \dots \lambda_d}{\det \nabla^2 V(x_-^*)}} e^{[V(z^*) - V(x_-^*)]/\varepsilon} [1 + \mathcal{O}((\varepsilon |\log \varepsilon|)^{1/4})]$$

- ▷ Degenerate **unstable** direction: $V(y) = -C_{2p} y_1^{2p} + \frac{1}{2} \sum_{j=2}^d \lambda_j y_j^2 + \dots$

$$\mathbb{E}_{x_-^*} \tau_+ = \frac{\Gamma(1/2p)}{p C_{2p}^{1/2p} \varepsilon^{1/2(1-1/p)}} \sqrt{\frac{2\pi \lambda_2 \dots \lambda_d}{\det \nabla^2 V(x_-^*)}} e^{[V(z^*) - V(x_-^*)]/\varepsilon} [1 + \mathcal{O}((\dots)^{1/2p})]$$

Corollaries: Pitchfork bifurcation

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

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

$$\mathbb{E}_{x_-^*} \tau_+ = 2\pi \sqrt{\frac{(\lambda_2 + \sqrt{2\varepsilon C_4}) \lambda_3 \dots \lambda_d}{|\lambda_1| \det \nabla^2 V(x_-^*)}} \frac{e^{[V(z^*) - V(x_-^*)]/\varepsilon}}{\Psi_+(\lambda_2/\sqrt{2\varepsilon C_4})} [1 + R(\varepsilon)]$$

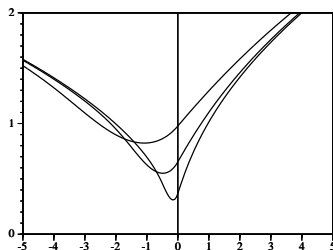
where

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

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

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

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



$\lambda_2 \mapsto$ prefactor

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

Outlook

- ▶ Multiple zero eigenvalues (bifurcations of higher codimension):
Obvious extension under certain assumptions, in progress
- ▶ Expand to SPDEs via Fourier variables:
In progress, first results published [Berglund & G. 09]
- ▶ Develop theory directly for SPDEs



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