Long-Lasting Effects of Random Perturbations on Dynamical Systems

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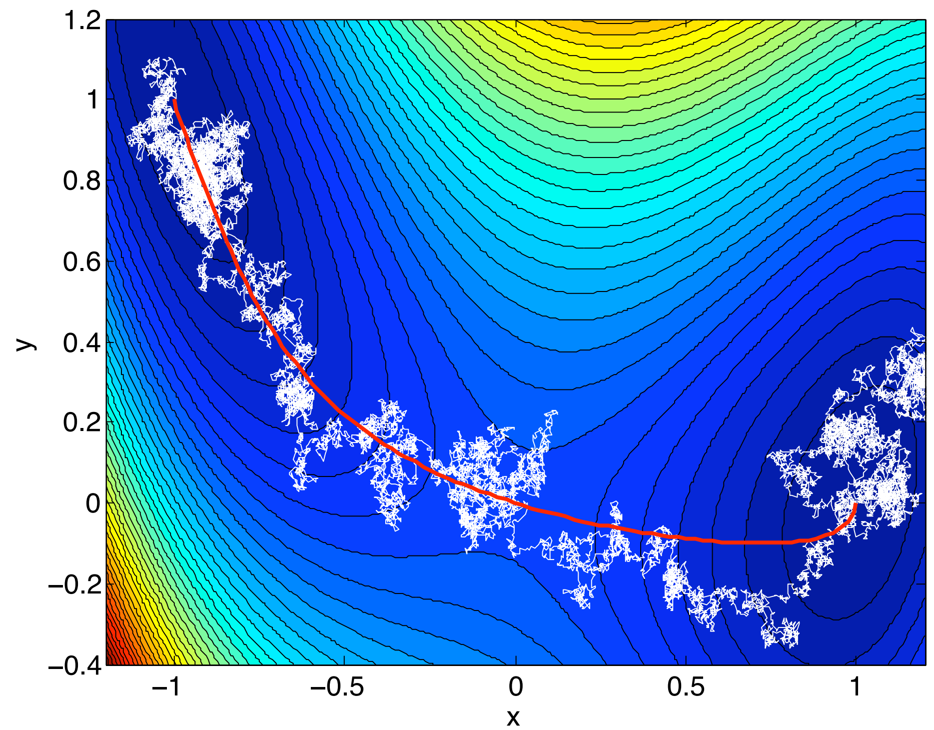
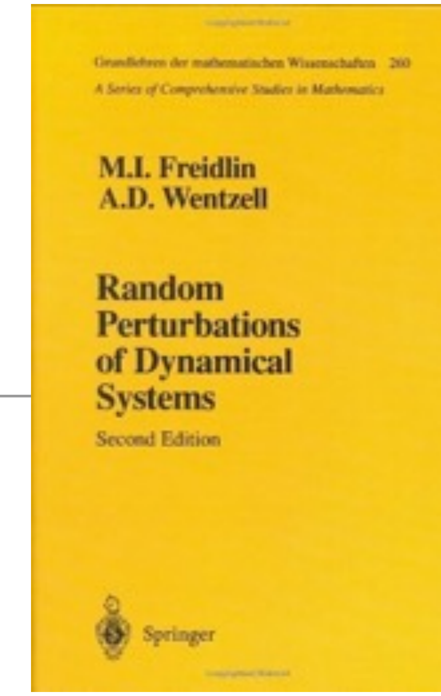


Frontier Probability Days
Salt Lake City, 2016

Joint work with T. Grafke and T. Schaefer

Freidlin-Wentzell approach to LDT



Consider the SDE

$$dX = b(X)dt + \sqrt{\varepsilon}\sigma(X)dW(t)$$

where $W(t)$ is a Wiener process and ε measures the noise amplitude.

The forward Kolmogorov equation associated with this SDE is

$$\partial_t \rho = \nabla \cdot \left(-b\rho + \tfrac{\varepsilon}{2}\nabla(a\rho)\right), \qquad a(x) = (\sigma\sigma^T)(x)$$

Using a WKB-type ansatz $\rho(x,t) = \exp\left(-\varepsilon^{-1}\Phi(x,t)\right)$, to leading order in ε, $\Phi(x,t)$ satisfies the Hamilton-Jacobi equation

$$\partial_t \Phi + H(x, \nabla\Phi) = 0, \qquad H(x,\theta) = b(x)\cdot\theta + \tfrac{1}{2}\theta\cdot a(x)\theta$$

Variational representation formula for the solution

$$\Phi(x,t) = \inf_{\substack{\{\varphi(s), s\in[0,t]\ :\\ \varphi(0)=x_0, \varphi(t)=x\}}} \frac{1}{2}\int_0^t |\dot\varphi - b(\varphi)|_a^2 ds, \qquad |u|_a^2 = u\cdot a^{-1}(\varphi)u$$

The role of the Quasi-Potential (QP)

LDP also important for long time behavior via the solution of $H(x, \nabla\Phi) = 0$, which defines the *quasipotential*

$$\Phi(x,y) = \inf_{T>0} \inf_{\substack{\{\varphi(t), t\in[0,T]\ :\\ \varphi(0)=x, \varphi(T)=y\}}} \frac{1}{2}\int_0^T |\dot{\varphi} - b(\varphi)|_a^2 dt$$

Quasipotential plays roughly the same role as the standard potential, and is important on long time-scales, $T \asymp \exp(\varepsilon^{-1}C)$ for some $C > 0$.

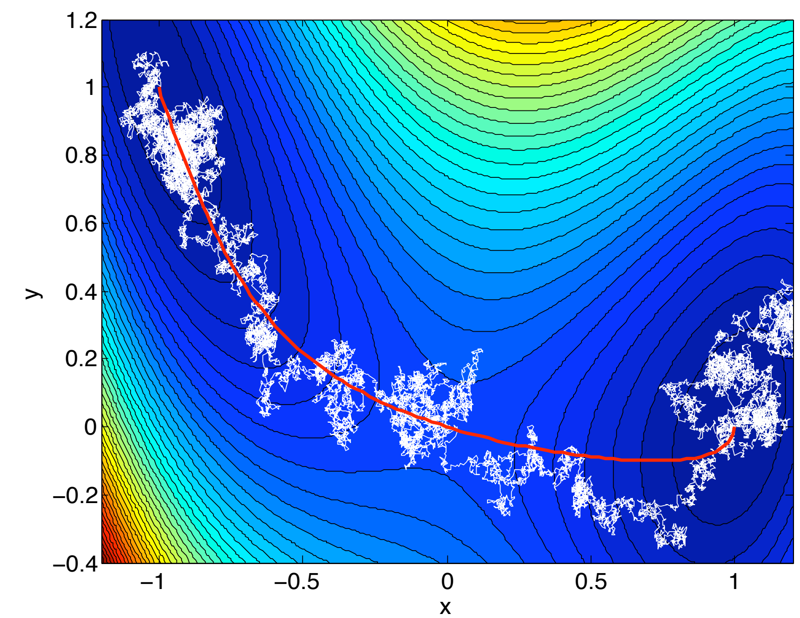
For example, around stable fixed point x_a of $\dot{x} = b(x)$, the nonequilibrium stationary density is

$$\rho(x) \asymp \exp\left(-\varepsilon^{-1}\Phi(x_a, x)\right)$$

and if x_a, x_b are two adjacent stable fixed points of $\dot{x} = b(x)$, the mean first passage time from x_a to x_b is

$$\tau(x_a, x_b) \asymp \exp\left(\varepsilon^{-1}\Phi(x_a, x_b)\right)$$

NB: the case of Systems in Detailed-Balance

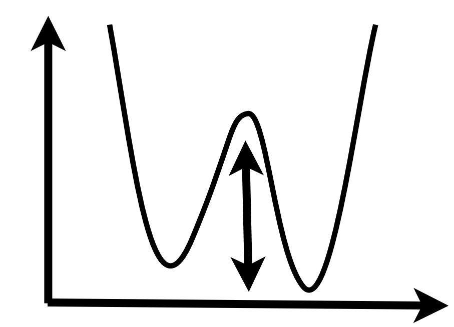


For systems of the type

$$dX = -\nabla U(X)dt + \sqrt{\varepsilon}\, dW(t)$$

• Quasipotential reduces to potential $U(x)$.

• Mimimizer of action (aka maximum likelihood path, MLP) reduces to mimimum energy path (MEP), that is, geometric location of heteroclinic orbits joining two minima via a saddle point.



A MEP can be characterized geometrically as a curve Γ^* satisfying

$$0 = [\nabla U]^{\perp}$$

where $[\cdot]^{\perp}$ denotes the perpendicular projection to the curve.

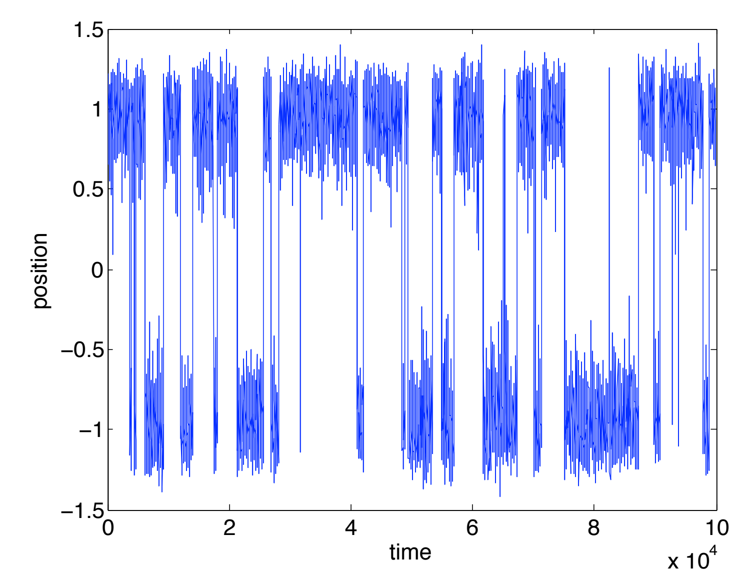


Illustration: Allen-Cahn equation in 2D

Allen-Cahn energy for $u : [0,1]^2 \mapsto \mathbb{R}$:

$$E(u) = \int_{[0,1]^2} \left(\tfrac{1}{2}\delta|\nabla u|^2 + \tfrac{1}{4}\delta^{-1}(1-u^2)^2\right) dx$$

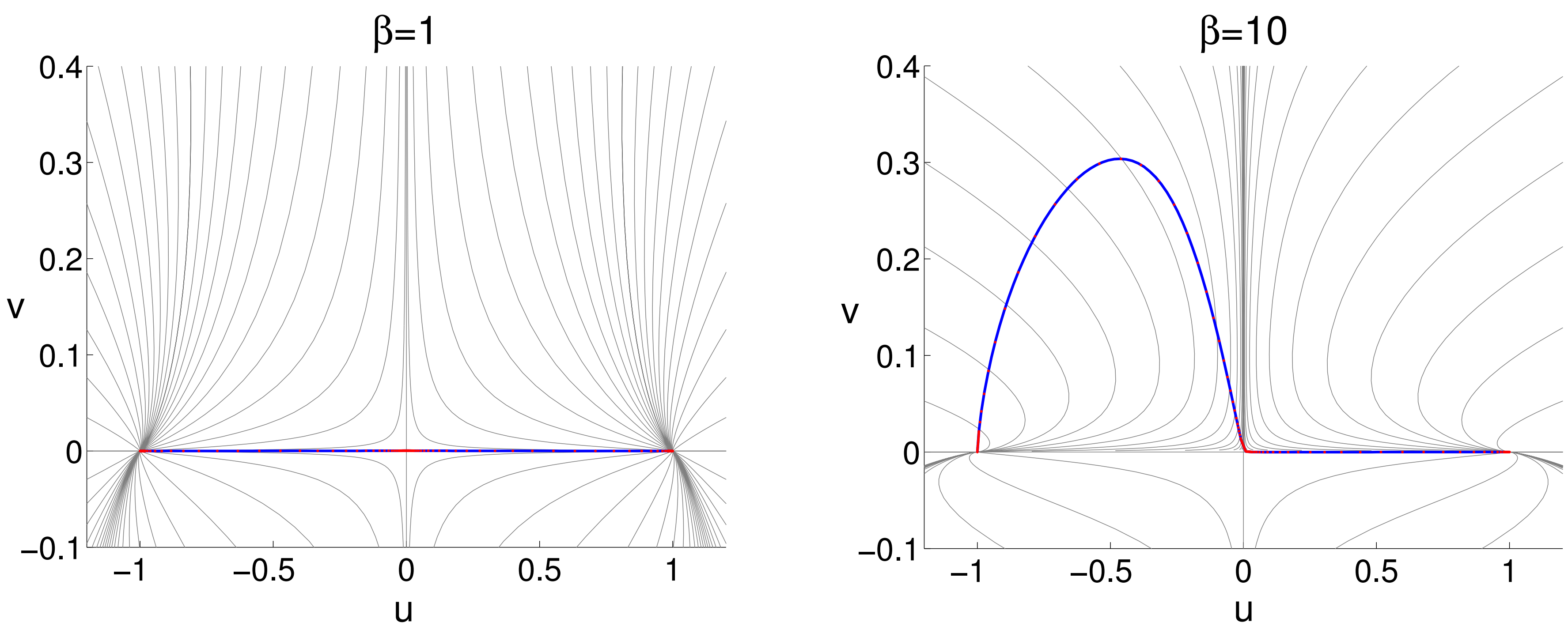
with Dirichlet boundary condition: $u = +1$ on the right and left edges of $[0,1]^2$, $u = -1$ on top and bottom ones.

Simulations by W. Ren

What if the dynamics is not in detailed-balance?

▷ Example from Maier & Stein

$$\begin{cases} du = (u - u^3 - \beta u v^2)dt + \sqrt{\varepsilon}\, dW_u(t) \\ dv = -(1+u^2)v\, dt + \sqrt{\varepsilon}\, dW_v(t) \end{cases}$$



Detailed-balance holds only for $\beta = 1$

For other values, the MLP is no longer the reversed of the deterministic path

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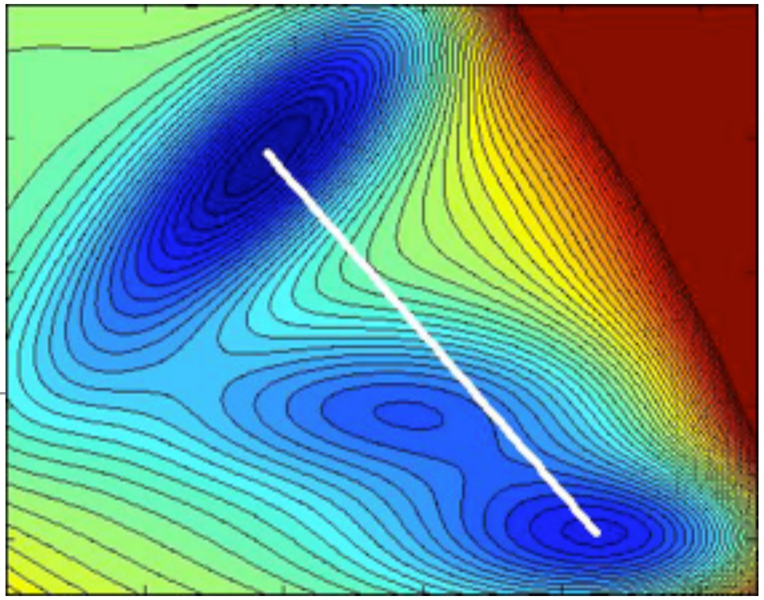
Geometric interpretation and Numerical counterpart



$$\Phi(x,y) = \inf_{T>0} \inf_{\substack{\{\varphi(t), t\in[0,T]\ :\\ \varphi(0)=x, \varphi(T)=y\}}} \frac{1}{2}\int_0^T |\dot\varphi - b(\varphi)|_a^2 dt$$

$$= \inf_{\substack{\{\varphi(t), t\in[0,T]\ :\\ \varphi(0)=x, \varphi(T)=y\}}} \int_0^T \left(|\dot\varphi|_a |b(\varphi)|_a - \langle \dot\varphi, b(\varphi)\rangle_a\right) dt$$

Reduce calculation of the quasipotential to that of a geodesic in a (degenerate) Finsler metric.

Numerical counterpart: geodesic can be identified in practice by moving a parametrized curve in configuration space

$\Rightarrow$ *String method* (gradient systems) and *Minimum action method* (non-gradient systems). (E, Ren & V.-E.; Heymann & V.-E.)

Allen-Cahn/Cahn-Hilliard System

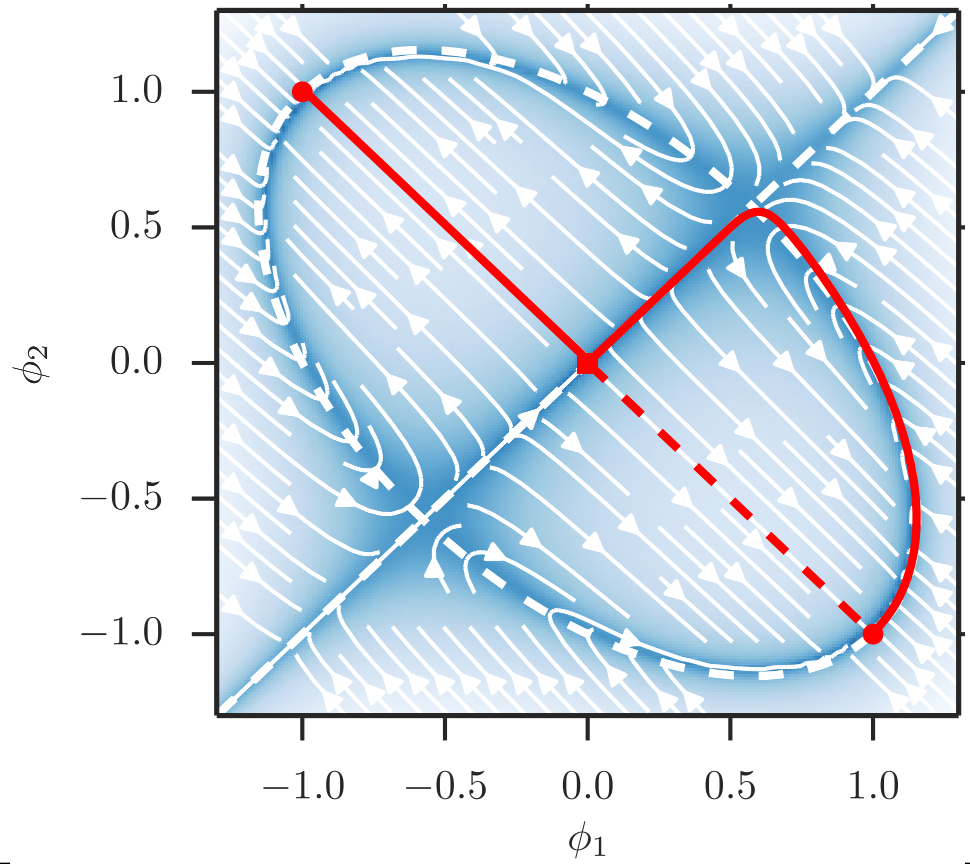
Consider the SDE system

$$d\phi = (\frac{1}{\alpha}Q(\phi - \phi^3) - \phi)dt + \sqrt{\varepsilon}dW$$

with $\phi = (\phi_1, \phi_2)$ and the matrix $Q = ((1, -1), (-1, 1))$.

This system does not satisfy detailed balance, as its drift is made of two gradient terms with incompatible mobility operators (namely Q and Id).

Fig. 2 Allen-Cahn/Cahn-Hilliard toy ODE model, $\alpha = 0.01$. The arrows denote the direction of the deterministic flow, the color its magnitude. The white dashed line corresponds to the slow manifold. The solid line depicts the minimizer, the dashed line the heteroclinic orbit. Markers are located at the fixed points (circle: stable; square: saddle).



Allen-Cahn/Cahn-Hilliard System

Consider next the SPDE

$$\phi_t = \frac{1}{\alpha} P(\kappa \phi_{xx} + \phi - \phi^3) - \phi + \sqrt{\epsilon}\eta(x,t)$$

where P is an operator with zero spatial mean and $\eta(x,t)$ a spatio-temporal white-noise.

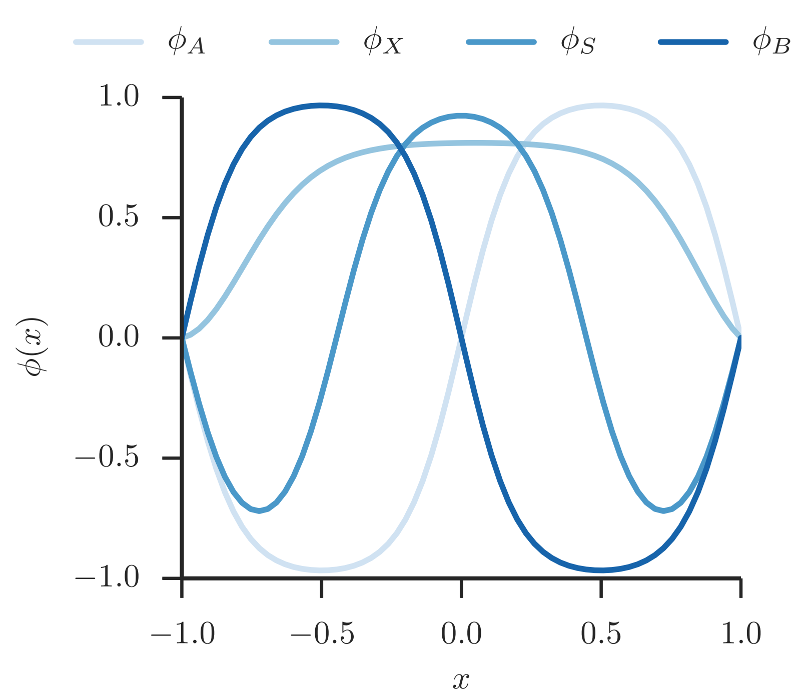


Fig. 4 The configurations A, B, S, X in space: ϕ_A and ϕ_B are the two stable fixed points, ϕ_S is the unstable fixed point on the separatrix in between. At point ϕ_X, the slow manifold intersects the separatrix.

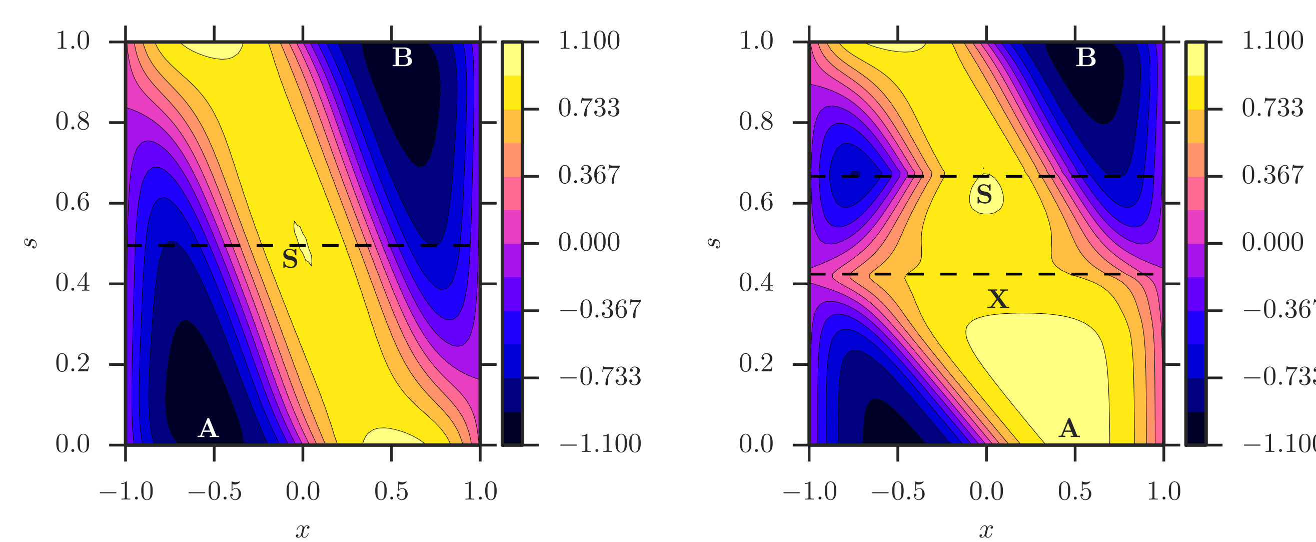
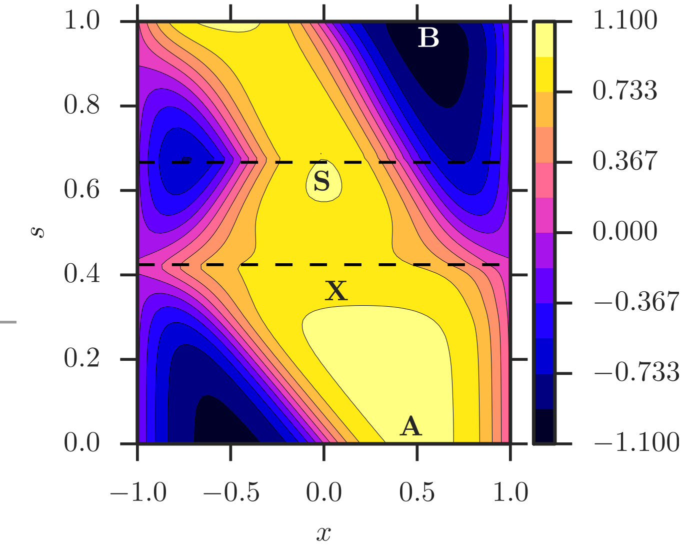


Fig. 5 Transition pathways between two stable fixed points of equation (56) in the limit $\varepsilon \to 0$. Left: heteroclinic orbit, defining the deterministic relaxation dynamics from the unstable point S down to either A or B. Right: Minimizer of the geometric action, defining the most probable transition pathway from A to B, following the slow manifold up to X, where it starts to nearly deterministically travel close to the separatrix into S.

Allen-Cahn/Cahn-Hilliard System



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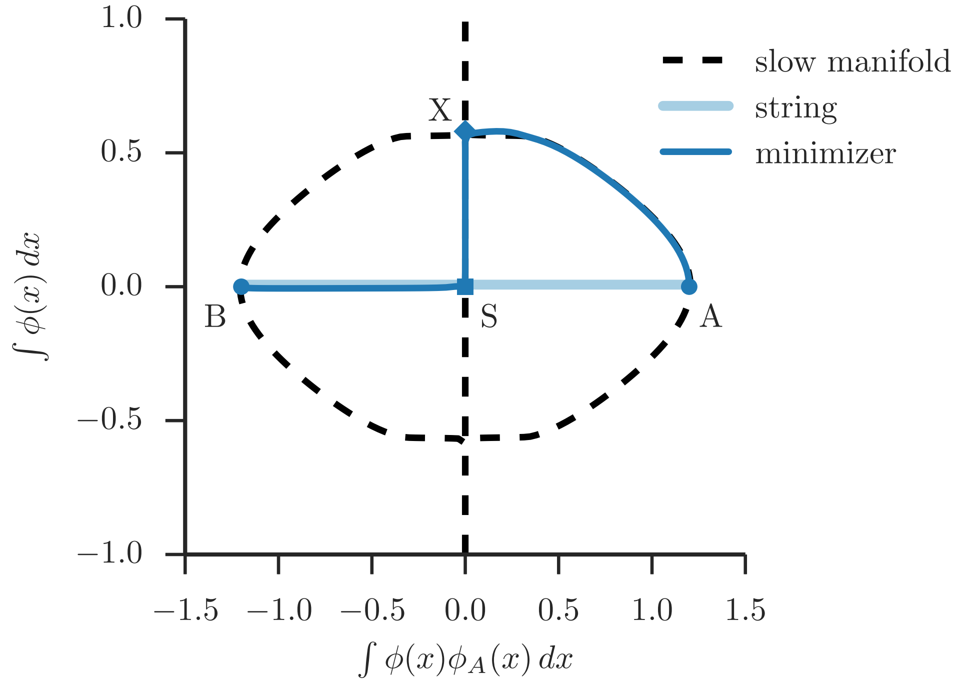
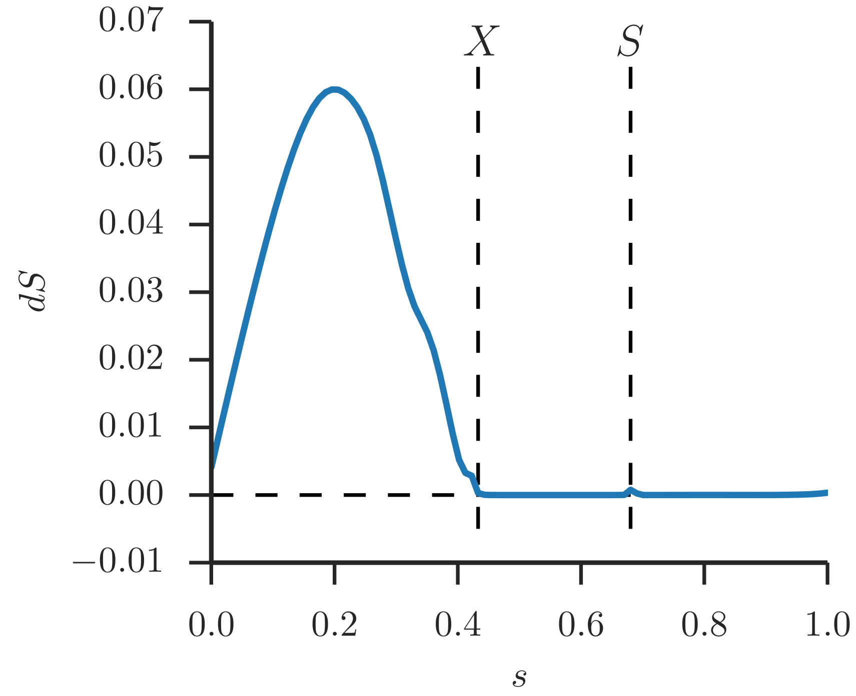




Bistable Reaction Network

Consider the bi-stable chemical reaction network

$$A \underset{k_1}{\overset{k_0}{\rightleftharpoons}} X, \qquad 2X + B \underset{k_3}{\overset{k_2}{\rightleftharpoons}} 3X$$

with rates $k_i > 0$, and where the concentrations of A and B are held constant.

Its dynamics can be modeled as a Markov jump process (MJP) with generator

$$(L^R f)(n) = A_+(n)\,(f(n-1) - f(n)) + A_-(n)\,(f(n+1) - f(n))$$

with the propensity functions

$$\begin{cases} A_+(n) & = k_0 V + (k_2/V)n(n-1) \\ A_-(n) & = k_1 n + (k_3/V^2)n(n-1)(n-2)\,. \end{cases}$$

Bistable Reaction Network

Denote by $c = n/V$ the concentration of X, and normalize it by a typical concentration, $\rho = c/c_0$. Set $\varepsilon = 1/(c_0 V)$ and rescale time by ε:

$$(L_\epsilon^R f)(\rho) = \frac{1}{\epsilon}\Big(a_+(\rho)\,(f(\rho-\epsilon) - f(\rho)) + a_-(\rho)\,(f(\rho+\epsilon) - f(\rho))\Big),$$

where

$$\begin{cases} a_+(\rho) & = \lambda_0 + \lambda_2 \rho^2 \\ a_-(\rho) & = \lambda_1 \rho + \lambda_3 \rho^3 \,. \end{cases}$$

Large deviation principle can be formally obtained via WKB analysis, that is, by setting $f(\rho) = e^{\epsilon^{-1} G(\rho)}$ and expanding in ε. To leading order in ϵ, this gives an Hamilton-Jacobi operator associated with an Hamiltonian that is also the one rigorously derived in LDT:

$$H(\rho, \vartheta) = a_+(\rho)(e^{\vartheta} - 1) + a_-(\rho)(e^{-\vartheta} - 1)\,.$$

Bistable Reaction Network

Consider N neighboring reaction compartments, each well-stirred, but with random jumps possible between neighboring compartments.

Denote by ρ_i the concentration in the i-th compartment and refer to the vector $\boldsymbol{\rho}$ as the complete state, $\boldsymbol{\rho} = \sum_{i=0}^{N} \rho_i \hat{e}_i$. In this case, we obtain a diffusive part of the generator, L^D, coupling neighboring compartments. For a diffusivity D, it is

$$(L^D f)(\boldsymbol{\rho}) = \frac{D}{\epsilon} \sum_{i=1}^{N} \rho_i \Big(f(\boldsymbol{\rho} - \epsilon \hat{e}_i + \epsilon \hat{e}_{i-1}) + f(\boldsymbol{\rho} - \epsilon \hat{e}_i + \epsilon \hat{e}_{i+1}) - 2 f(\boldsymbol{\rho}) \Big) \, .$$

The process associated with this generator also admits a large deviation principle with Hamiltonian

$$H^D(\boldsymbol{\rho}, \boldsymbol{\vartheta}) = D \sum_{i=1}^{N} \rho_i \Big(e^{\vartheta_{i-1} - \vartheta_i} + e^{\vartheta_{i+1} - \vartheta_i} - 2 \Big) \, ,$$

Full Hamiltonian becomes

$$H(\boldsymbol{\rho}, \boldsymbol{\vartheta}) = H^D(\boldsymbol{\rho}, \boldsymbol{\vartheta}) + \sum_{i=1}^{N} H^R(\rho_i, \vartheta_i)$$

Bistable Reaction Network

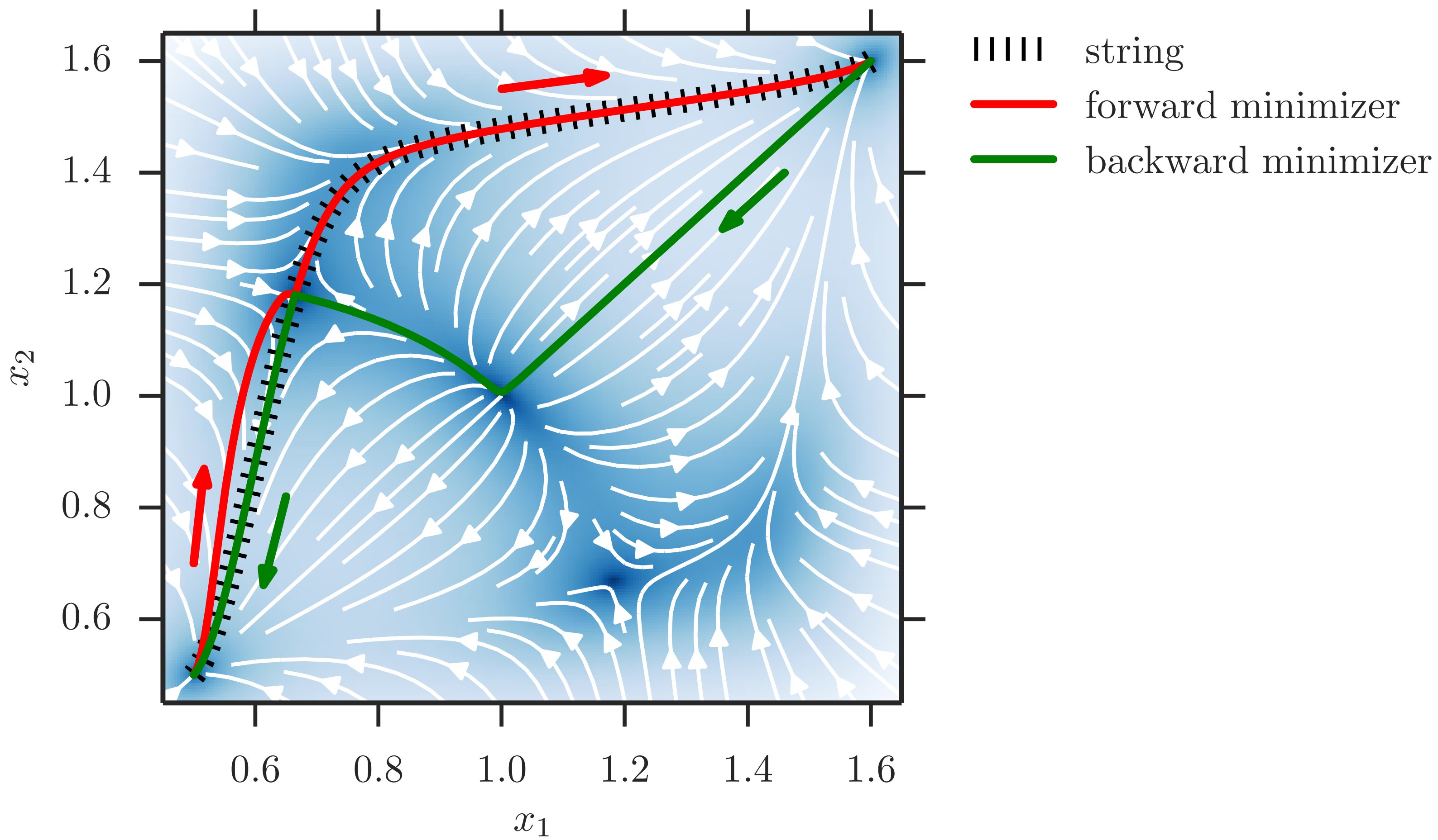


Fig. 15 Bi-Stable reaction-diffusion model with $N = 2$ reaction cells. Show are the forward (red) and backward (green) transitions between the two stable fixed points, in comparison to the hetero-clinic orbit (dashed). The flow-lines depict the deterministic dynamics, their magnitude is indicated by the background shading.

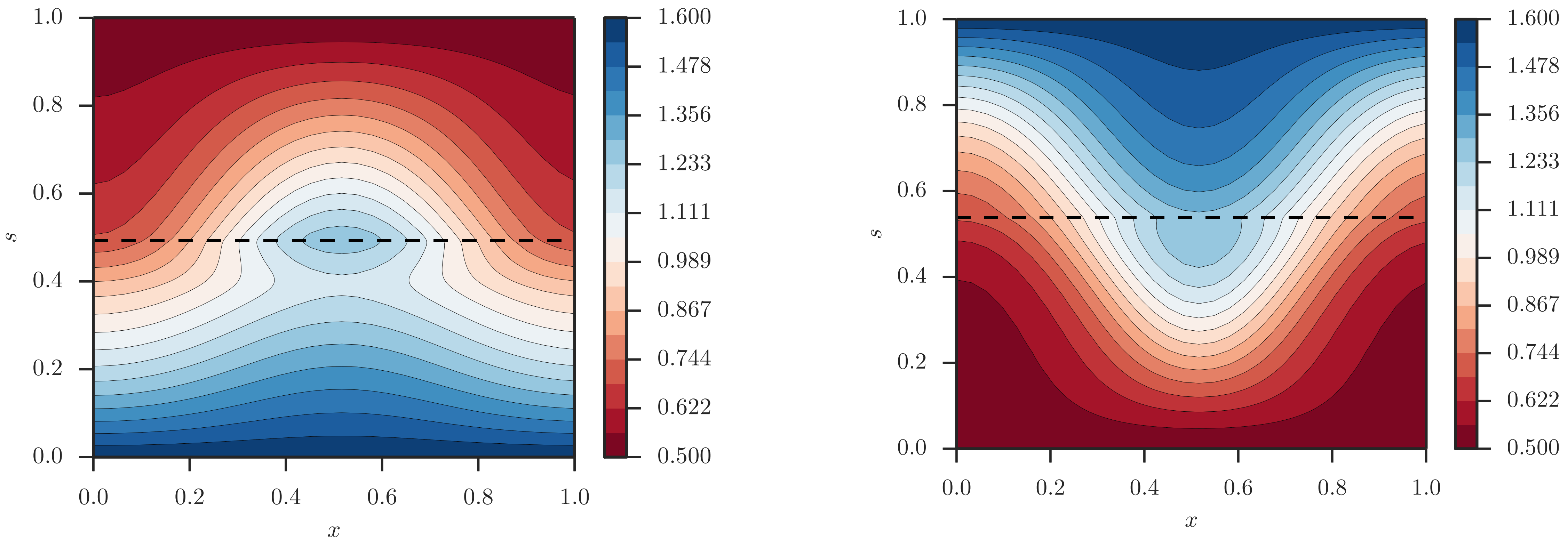
Continuous limit in space

Rescale

$$\rho_j \to h\rho(jh), \qquad \theta_j \to \theta(jh), \qquad a_\pm(\rho_j) \to h a_\pm(\rho(jh))$$

In the limit $h \to 0$, if we scale $D \to Dh^{-2}$ we arrive at

$$H^d(\rho,\theta) = D \int \left(\rho|\partial_x\theta|^2 + \theta\partial_x^2\rho\right) dx\,.$$



forward backward

Fast-Slow Systems

Systems with a slow variable X evolving on a timescale $O(1)$ and a fast variable Y on a time scale $O(\alpha)$:

$$\begin{aligned}\dot{X} &= f(X,Y)\\ dY &= \frac{1}{\alpha}b(X,Y)dt + \frac{1}{\sqrt{\alpha}}\sigma(X,Y)dW.\end{aligned}$$

Limit behavior captured by Law of large numbers (LLN):

$$\dot{\bar{X}} = F(\bar{X}) \quad \text{where} \quad F(x) = \lim_{T\to\infty}\frac{1}{T}\int_0^T f(x, Y_x(\tau))\,d\tau$$

Small deviations captured by Central Limit Theorem (CLT); large deviation captured by LDP with the Hamiltonian

$$H(x,\vartheta) = \lim_{T\to\infty}\frac{1}{T}\log\mathbb{E}\exp\left(\vartheta\int_0^T f(x,Y_x(t))\,dt\right),$$

Fast-Slow Systems - Example

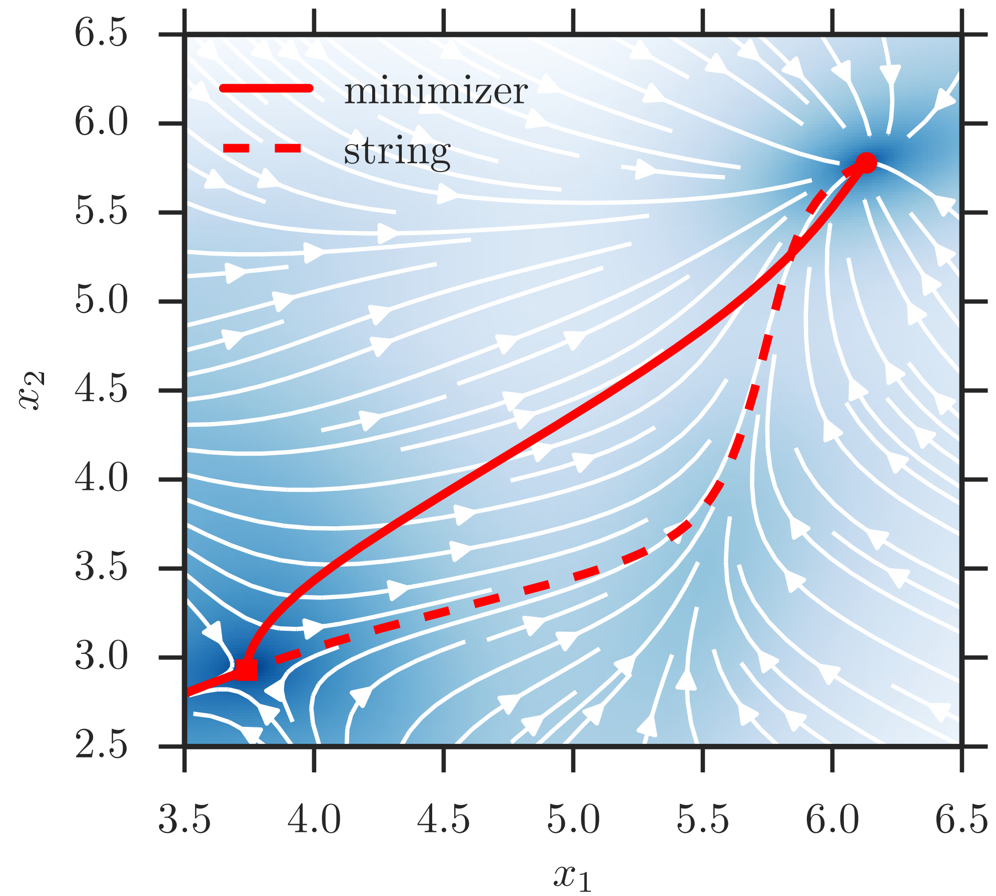
$$
\begin{cases}
\dot{X}_1 = Y_1^2 - \beta_1 X_1 - D(X_1 - X_2) \\
\dot{X}_2 = Y_2^2 - \beta_2 X_2 - D(X_2 - X_1) \\
dY_1 = -\frac{1}{\alpha}\gamma(X_1)Y_1 dt + \frac{\sigma}{\sqrt{\alpha}} dW_1 \\
dY_2 = -\frac{1}{\alpha}\gamma(X_2)Y_2 dt + \frac{\sigma}{\sqrt{\alpha}} dW_2 \,.
\end{cases}
$$

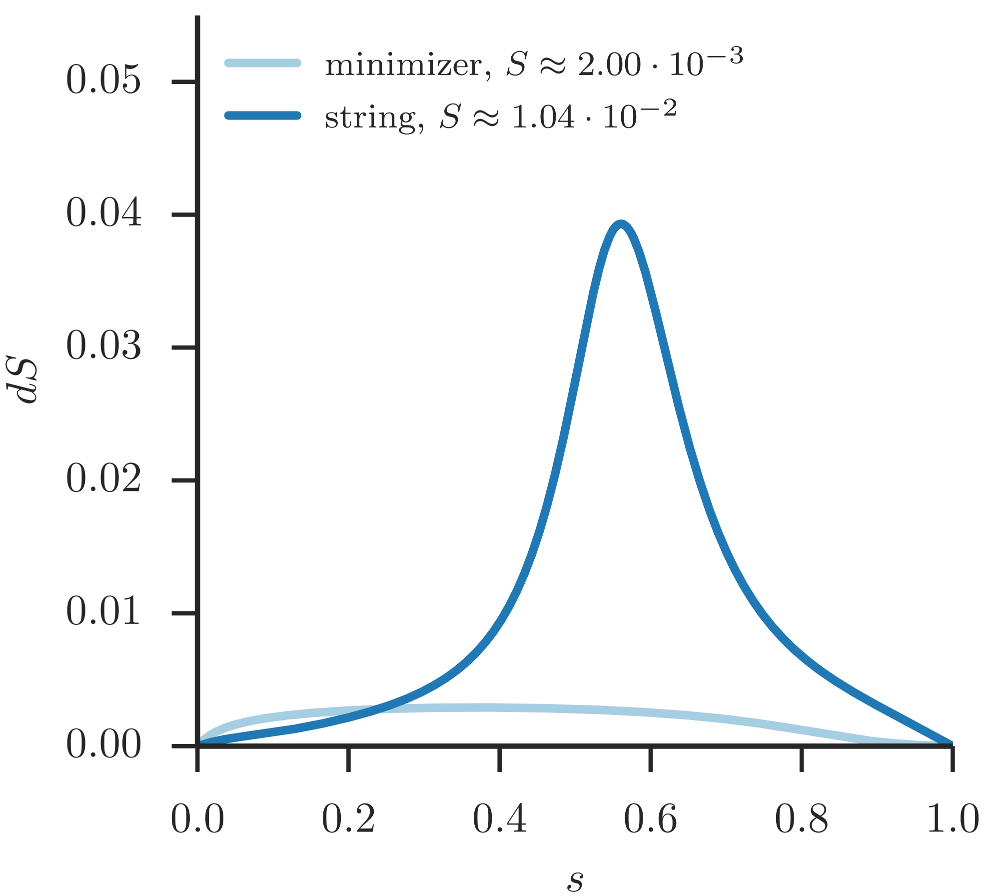
$$H(x_1, x_2, \vartheta_1, \vartheta_2) = h(x_1, \vartheta_1) + h(x_2, \vartheta_2) + \langle -\nabla U(x_1, x_2), \vartheta \rangle \,,$$

$$U(x, y) \;=\; \tfrac{1}{2} D(x-y)^2$$

$$h(x, \vartheta) = -\beta x \vartheta + \tfrac{1}{2}\left(\gamma(x) - \sqrt{\gamma^2(x) - 2\sigma^2 \vartheta}\right) .$$

$$\gamma(X) = (X-5)^2 + 1$$





Conclusions

- LDT can guide the development of numerical tools that bypass the brute-force integration of SPDE.
- Gives rough estimate of probability, along with the path of maximum likelihood by which the event occurs.
- Applicable to systems in detailed-balance or not, on finite or unbounded time intervals.

- *Can be integrated in importance sampling procedures and data assimilation techniques.*
- *Can also be used in other context, e.g. to understand stochastic resonance effects in excitable media, phase transition in unbounded domains, etc.*
- *More challenging are situations where LDT does not apply directly because entropic effects are non-negligible.*

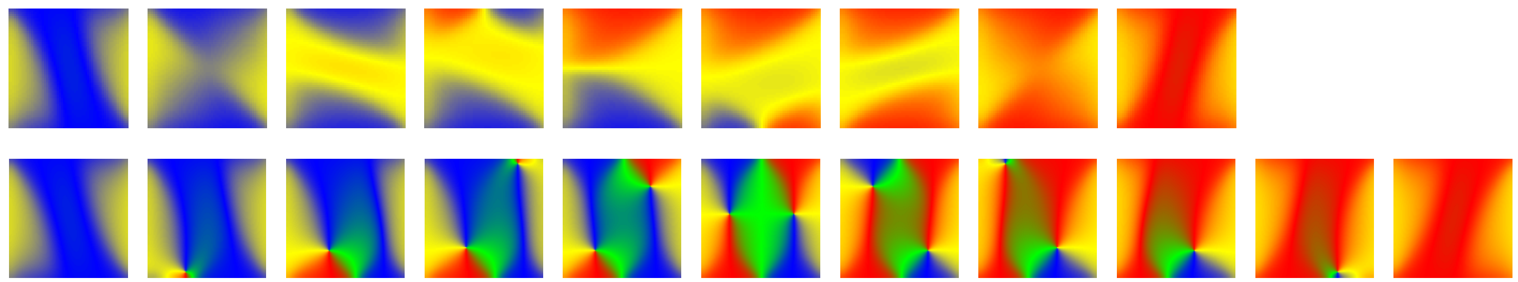
Some other applications

▷ Thermally induced magnetization reversal in submicron ferromagnetic elements

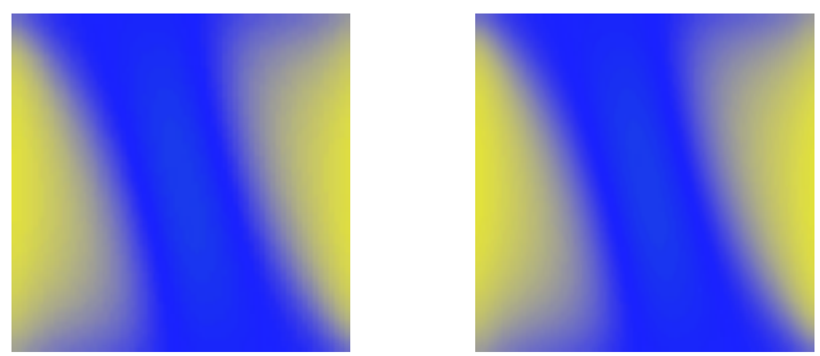
with Weinan E and Weiqing Ren

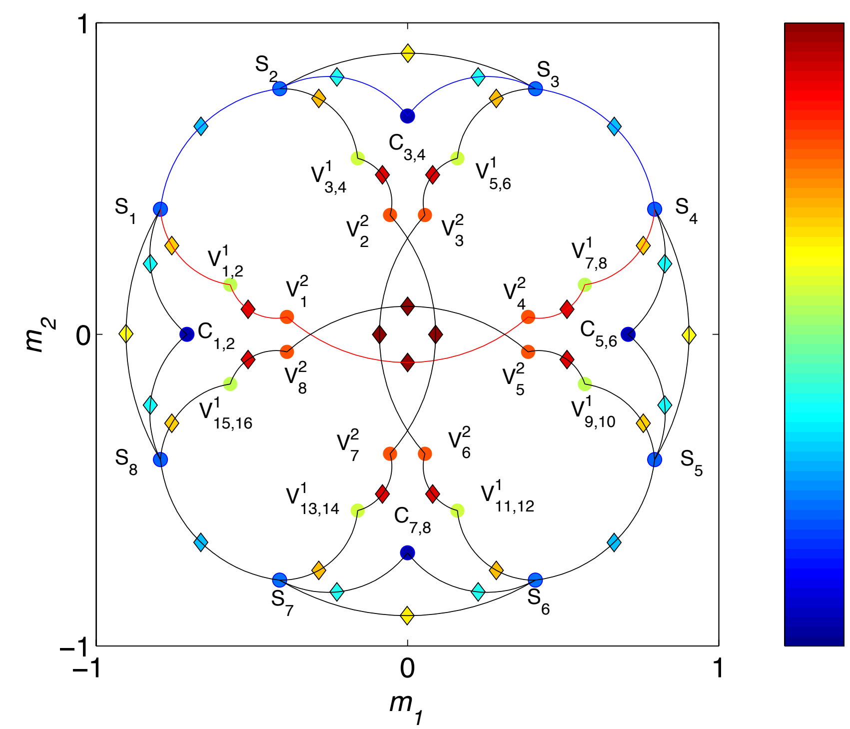
a)

b)



Practical side of LDT - Dynamics can be reduced to a Markov jump process on energy map, whose nodes are the energy minima and whose edges are the minimum energy paths.

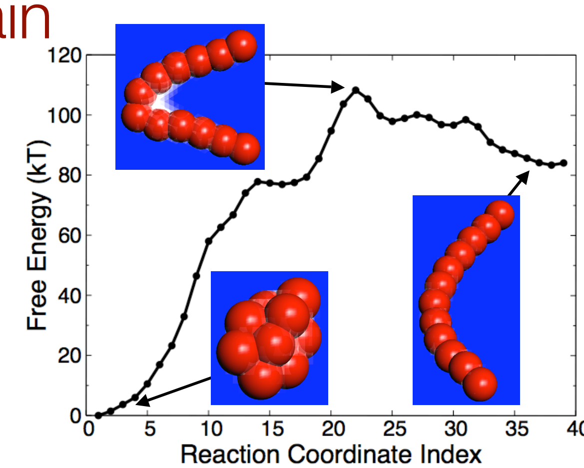


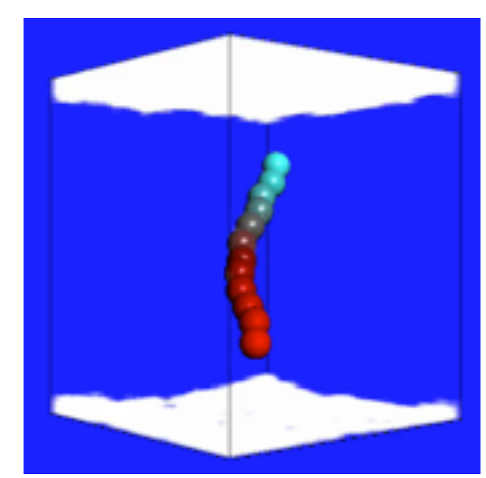


▷ Hydrophobic collapse of a polymeric chain by dewetting transition

with Tommy Miller and David Chandler

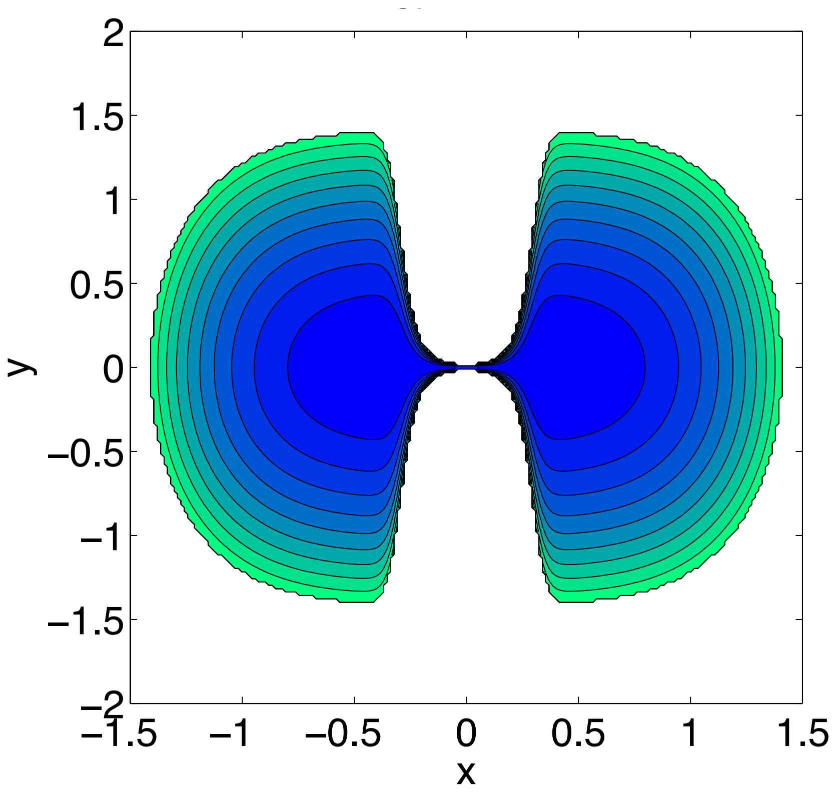
Rate limiting step is entropic - creation of a water bubble

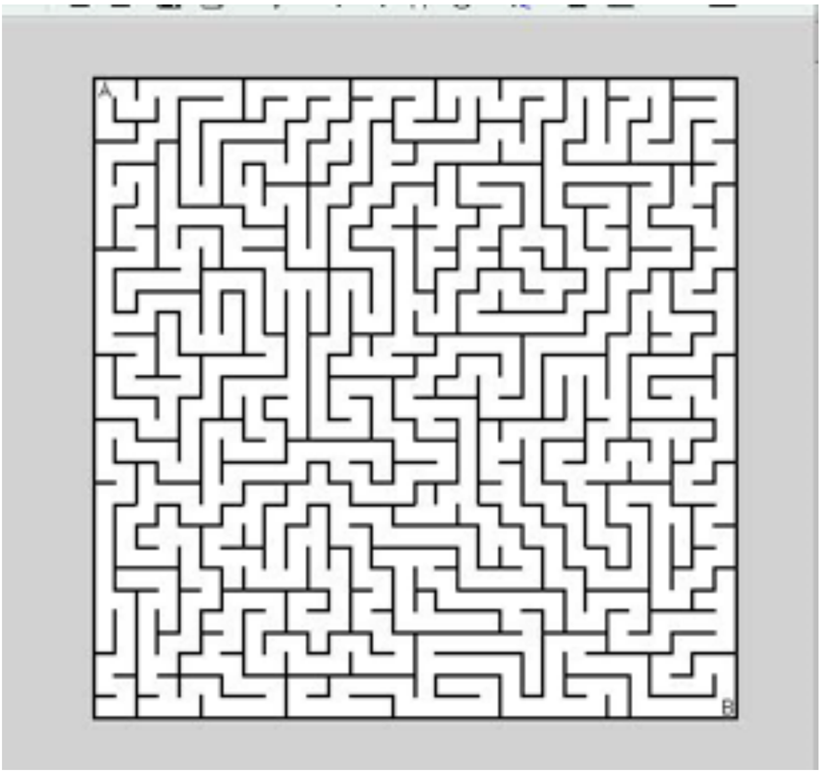


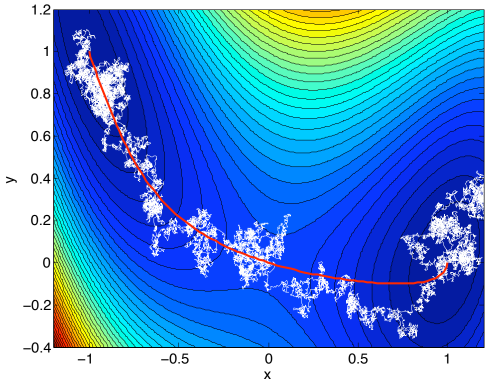


Beyond LDT - when entropy matters

- LDT can fail if entropic effects matter
  - many alternative paths for the event, with lower probability individually, but large one globally.
- These situations require a more general approach to rare event analysis.







Some references

W. E, W. Ren, and and E.V.-E., "String method for the study of rare events," Phys. Rev. B. 66, 052301 (2002).

W. E, W. Ren, and E.V.-E., "Minimum action method for the study of rare events," Comm.Pure Applied Math. 52, 637-656 (2004)

M. Heymann and E.V.-E., "Pathways of Maximum Likelihood for Rare Events in Nonequilibrium Systems: Application to Nucleation in the Presence of Shear," Phys. Rev. Lett. 100, 140601 (2008).

M. Heymann and E.V.-E., "The Geometric Minimum Action Method: A least action principle on the space of curves," Comm. Pure. App. Math. 61(8), 1052-1117 (2008).

T. Grafke, R. Grauer, T. Schafer, E.V.-E. , "Arclength parametrized Hamilton's equations for the calculation of instantons," SIAM Multiscale Modeling & Simulation 12, 566-580 (2014).

F. Bouchet, T. Grafke, T. Tangarife and E V.-E., "Large Deviations in Fast–Slow Systems." J. Stat. Phys. 162, 793-812 (2015).

J. Weare and E.V.-E., "Rare event simulation of small noise diffusions," Comm. Pure App. Math. 65, 1770-1803 (2012).