Schlögl model

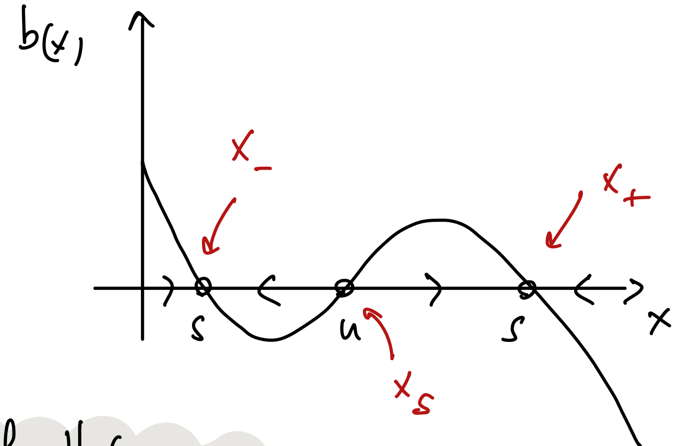
$$A \rightleftharpoons S$$

$$2S + B \rightleftharpoons 3S$$

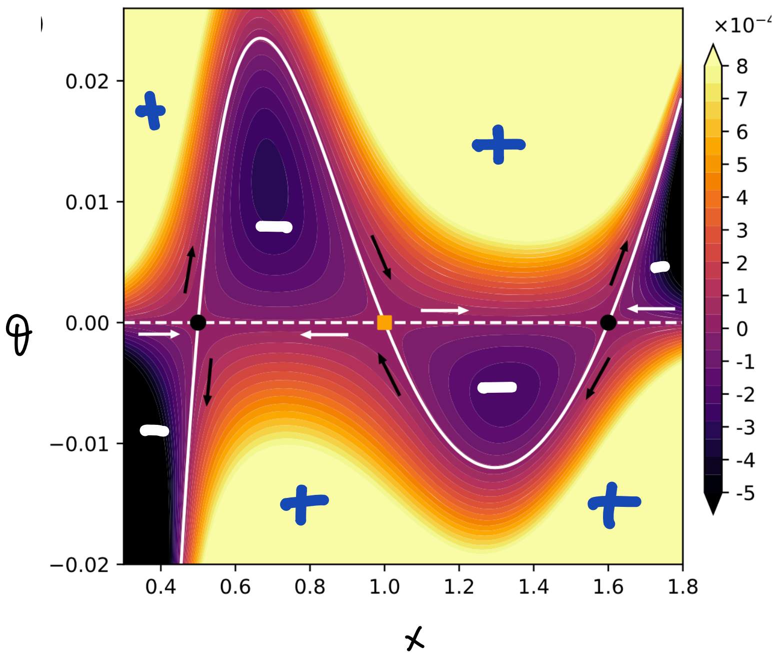
$$\rightsquigarrow \quad H(x,\theta) = \lambda_+(x)\,(e^{\theta} - 1) + \lambda_-(x)\,(e^{-\theta} - 1)$$

$$\begin{cases} \lambda_+(x) = \lambda_0 + \lambda_2 x^2 \\ \lambda_-(x) = \lambda_1 x + \lambda_3 x^3 \end{cases}$$

LLN: $$\dot{x} = \partial_\theta H(x, \theta = 0) = \lambda_+(x) - \lambda_-(x) \equiv b(x)$$



contour plot of $H(x,\theta)$:



white curves = level sets of $H = 0$.

= traj. of Hamiltonian syst

$$\begin{cases} \dot{x} = \partial_\theta H(x,\theta) & x(0) = x_- \quad \text{or} \quad x_+ \\ \dot{\theta} = -\partial_x H(x,\theta) & x(T) = x_+ \quad \text{or} \quad x_- \end{cases}$$

↪ $H = \text{cst}$ along solution.

two heteroclinic orbits going from x_- to x_+ or x_+ to x_- (in infinite time).

$$\boxed{V_T(x_- x_+) = \inf_{\substack{x(0)=x_- \\ x(T)=x_+}} \sup_{\theta} \int_0^T [\underbrace{\dot{x}\cdot\theta}_{\dot\theta \cdot \partial_\theta H \text{ along solution.}} - H(x,\theta)]\, dt \geq 0.}$$

by convexity: $\theta \cdot \partial_\theta H(x,\theta) - H(x,\theta) \geq -H(x,0) = 0$

$= 0$ iff $\theta = 0$

Quasipotential :

$$V(x_- x_+) = \inf_{T>0} V_T(x_- x_+)$$

$$\neq$$

$$V(x_+ x_-) = \inf_{T>0} \inf_{\substack{x \\ x(0)=x_- \\ x(T)=x_+}} \sup_\theta \int_0^T (\dot{x}\cdot\theta - H(x,\theta))\,dt$$

best $T \uparrow \infty$ $H = 0$.

$$= \inf_{\substack{x(0)=x_- \\ x(1)=x_+ \\ H=0}} \sup_\theta \int_0^1 x'\cdot\theta \, ds$$

geometric formulation

can impose $|x'| = cst$

since :

$$\sup_\theta \int_0^T (\dot{x}\cdot\theta - H(x,\theta))\,dt$$

$$\geq \sup_{\substack{\theta \\ H=0}} \int_0^T (\dot{x}\cdot\theta - \cancel{H(x,\theta)})\,dt$$

$$= \sup_{\substack{\theta \\ H=0}} \int_0^T \dot{x}\cdot\theta \, dt$$

= invariant by reparametrization

$t = t(s)$.

quasipotentials $\quad V_{\pm}(x) = V(x_{\pm}, x)$

$\uparrow$ stable fixed pt of LLN

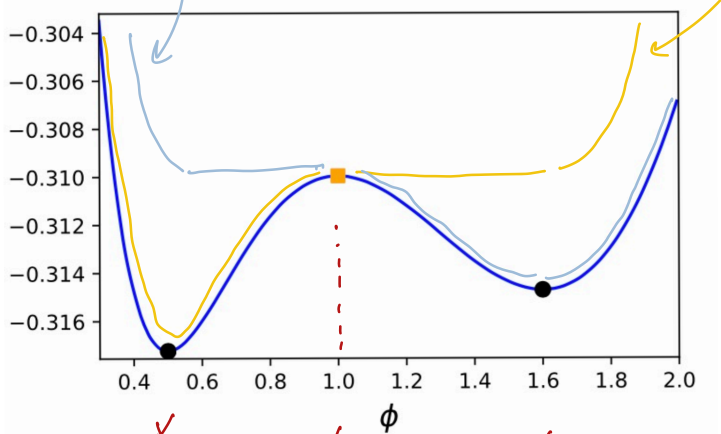
Play similar role as potential in equilibrium systems

- Can be used to construct a global potential.

$V_+(x)$ $\qquad$ $V_-(x)$

$V(x)$

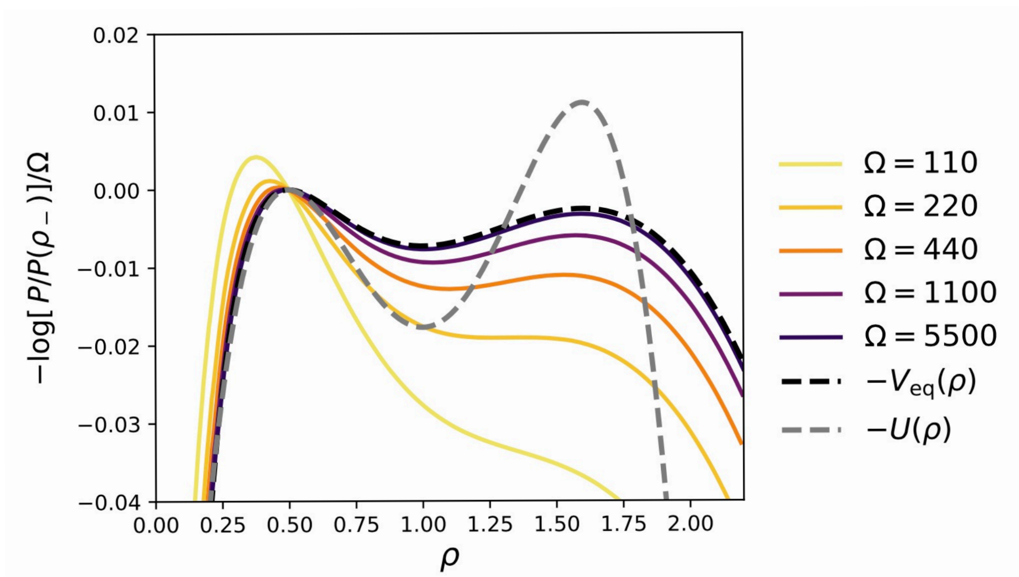
$p(x) \simeq e^{-V(x)/\varepsilon}$



x_- $\qquad$ x_c $\qquad$ x_+

log p(x)

PDF



x

$\Rightarrow$ stable phase is x_- if $V(x_-, x_+) > V(x_+, x_-)$

$\qquad\qquad\qquad\quad\;\; x_+$ if $V(x_-, x_+) < V(x_+, x_-)$

- Can be used to estimate rates.

Asymptotic dynamics = two state MJP with rates

$$\boxed{\begin{aligned} k_{+-} &\asymp e^{-V(x_- x_+)/\varepsilon} \\ k_{-+} &\asymp e^{-V(x_- x_+)/\varepsilon} \end{aligned}}$$

Schlögl with several boxes

$$\begin{cases} H_R(x,\theta) = \sum_{i=1}^{M} \lambda_+(x_i)(e^{\theta_i}-1) + \lambda_-(x_i)(e^{-\theta_i}-1) \\ H_D(x,\theta) = \alpha \sum_{i=1}^{M} x_i \left(e^{\theta_{i+1}-\theta_i} + e^{\theta_{i-1}-\theta_i} - 2\right). \end{cases}$$

continuous:

$$\begin{cases} H_R(x,\theta) = \int_0^1 [\lambda_+(x(s))(e^{\theta(s)}-1) + \lambda_-(x(s))(e^{-\theta(s)}-1)]ds \\ H_D(x,\theta) = \alpha \int_0^1 x(s)\,[\partial_s^2\theta(s) + |\partial_s\theta|^2]\,ds. \end{cases}$$

LLN: $\partial_t x = \alpha\,\partial_s^2 x + \lambda_+(x) - \lambda_-(x).$

$\hookrightarrow$ Allen Cahn / Ginzburg Landau eq.

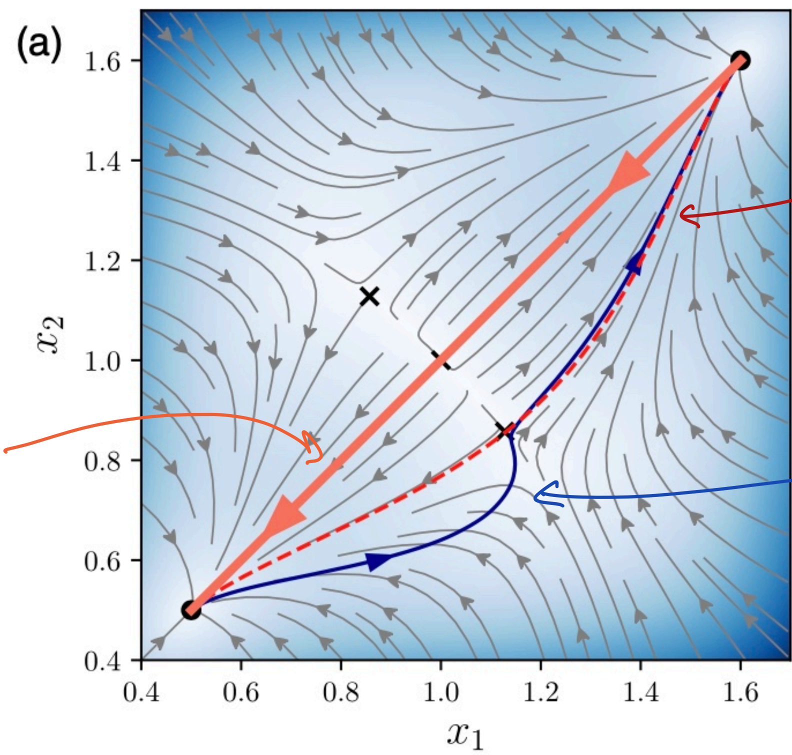
with energy $= \int_0^1 \frac{\alpha}{2}|\partial_s x|^2 + [\Lambda_+(x) - \Lambda_-(x)]\,ds$

$$\Lambda_\pm'(x) = \lambda_\pm(x)$$

⚠ incorrect energy.

Two boxes

Flow lines of $\dot{x} = \partial_\theta H(x,\theta=0)$



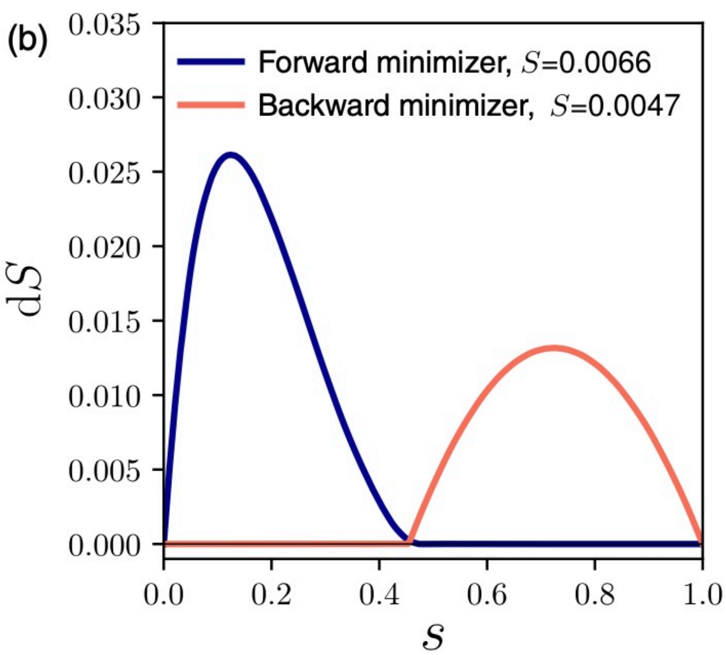
heteroclinic orbit

backward path

forward path

Action along paths

$\Rightarrow$ preferred state = bottom left

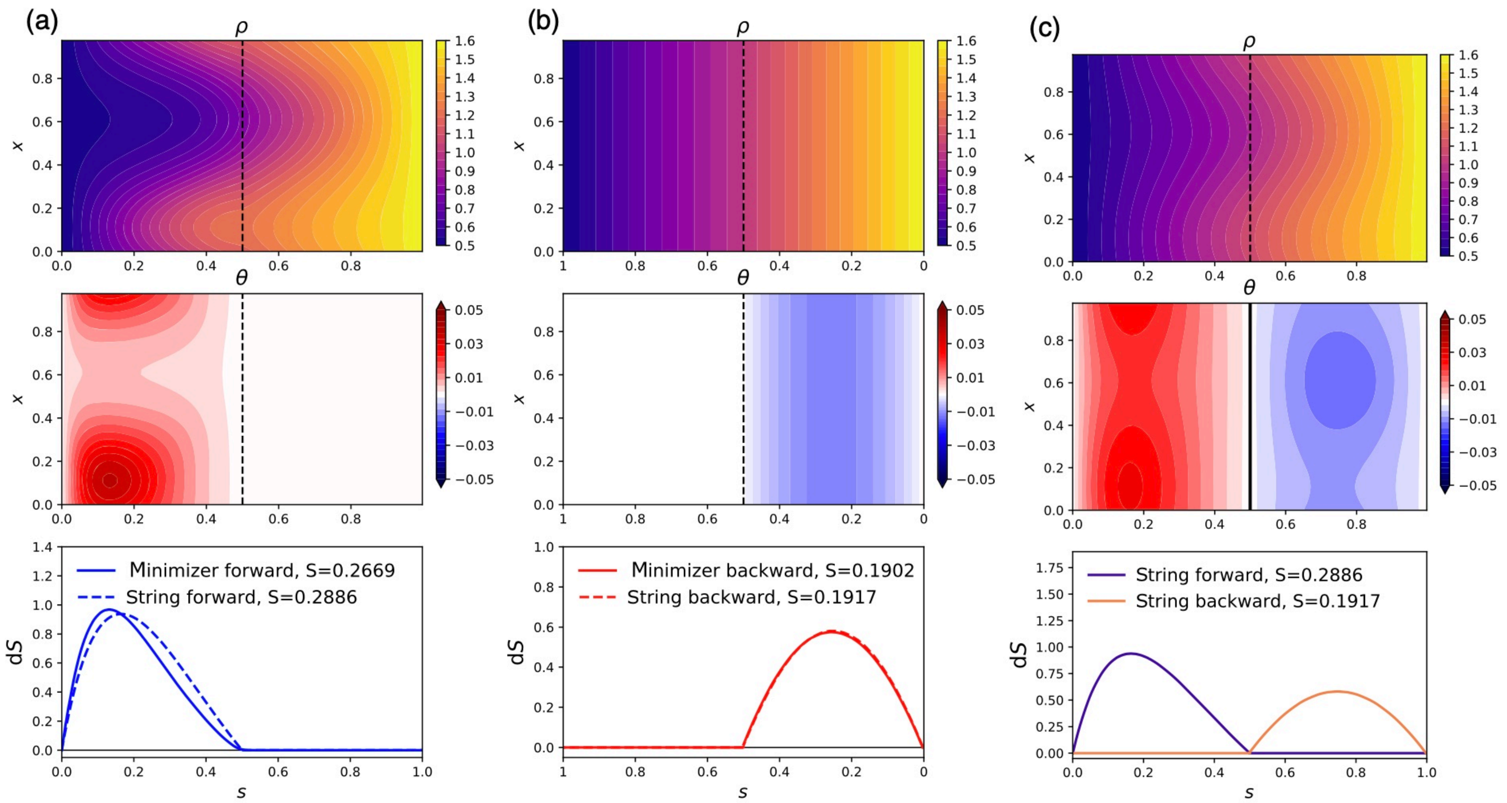


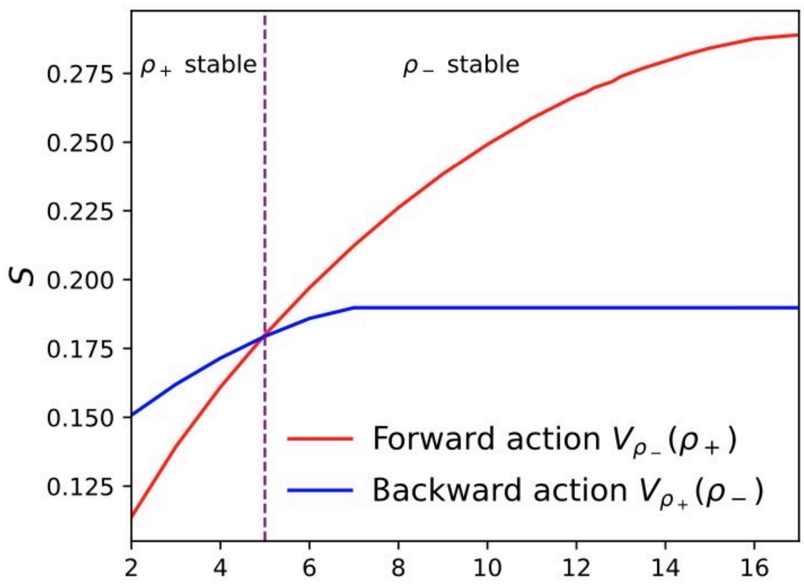
$S(s) = \int_0^s x' \cdot \theta \, ds'$

$|x'| = \underline{cst}$

Many boxes

M = 40

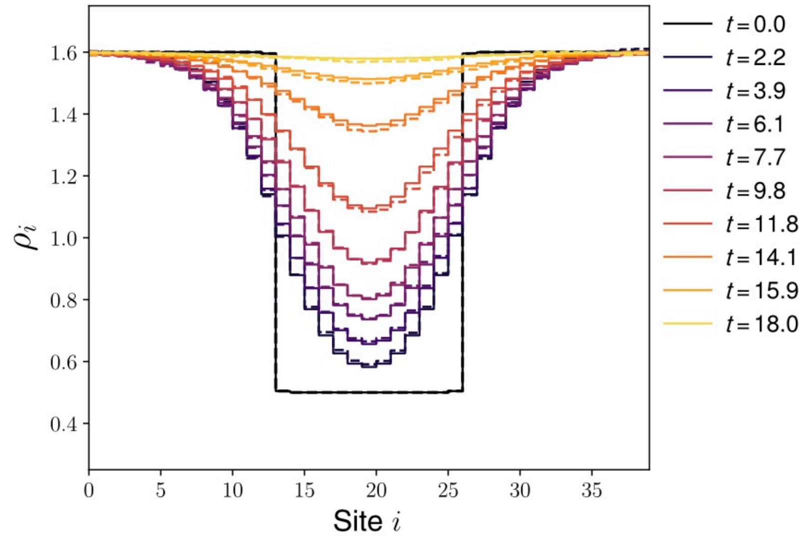




κ = diff. coefficient

ND

Verifying LLN



Verifying rates from LDP