Aggregation Patterns in Non-local Equations: Discrete Stochastic and Continuum Modelling.

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props to: M. Di Francesco, C. Schmeiser

Background

Non-local Fokker-Planck type equation

ρ individual/particle density, mass $\int_{\mathbb{R}} \rho = 1$ conserved

$$\partial_t \rho = \partial_x (\rho \, \partial_x [a(\rho) + W * \rho + V])$$

a: (non-linear) diffusion

$W(x) = W(-x)$: even interaction potential

V: external (confining) potential

- inelastic material $\to W \sim |x|^{1+\varepsilon}$, aggregation
- collective behaviour, swarming/flocking $\to W \sim e^{\pm|x|}, e^{\pm x^2}$ attractive and repulsive/attractive
- chemotaxis $W \sim \log |x|$ 2D: aggregation despite diffusion

Non-local interaction equations

Non-local interaction equation

measure solutions, mass $\int_{\mathbb{R}} \rho = 1$ conserved

$$\frac{\partial \rho}{\partial t} = \frac{\partial}{\partial x}\left[\rho\left(\int_{-\infty}^{+\infty} W'(x-\xi)\rho(\xi,t)d\xi\right)\right],$$

1D: consider $u(z)$ pseudo-inverse[a] of the distribution function $u(z) = \inf\left\{x \in \mathbb{R};\ \int_{-\infty}^{x} \rho\, dx > z\right\}$, for $z \in [0,1]$

$$\partial_t u(z) = \int_0^1 W'(u(\zeta) - u(z))\, d\zeta\,,$$

[a] [Li, Toscani], [Carrillo, Di Francesco, Figalli, Laurent, Slepčev]

Non-local interaction equations

Conservation of (the centre of) mass

Non-local interaction equation

$$\partial_t u(z) = \int_0^1 W'(u(\zeta) - u(z))\, d\zeta\,,$$

Conservation of (the centre of) mass $\int_0^1 u_{in}(z)\, dz$:

$$\frac{d}{dt}\int_0^1 u(t,z)\, dz = \int_0^1 \int_0^1 W'\left(u(\xi) - u(z)\right)\, d\xi\, dz = 0\,,$$

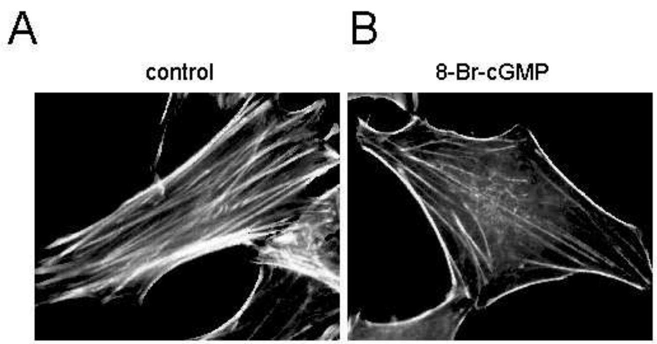
Normalisation

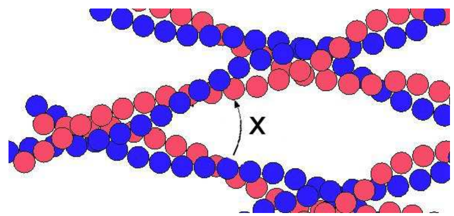
$$\int_0^1 u(z,t)\, dz = \int_0^1 u_{in}(z)\, dz = 0 \qquad t \geq 0\,,$$

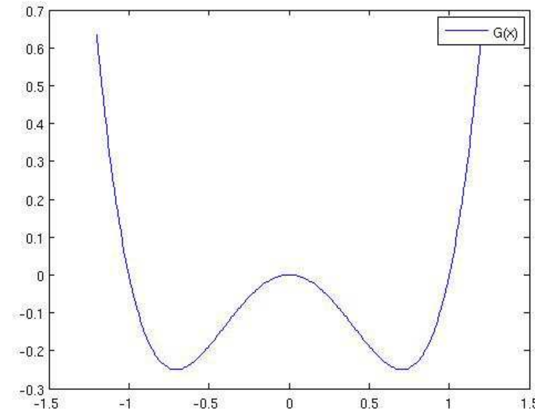
Non-local repulsion-aggregation

A Smooth Double-Well Potential

Actin filaments with or without cross-linking proteins[a]







W double-well potential

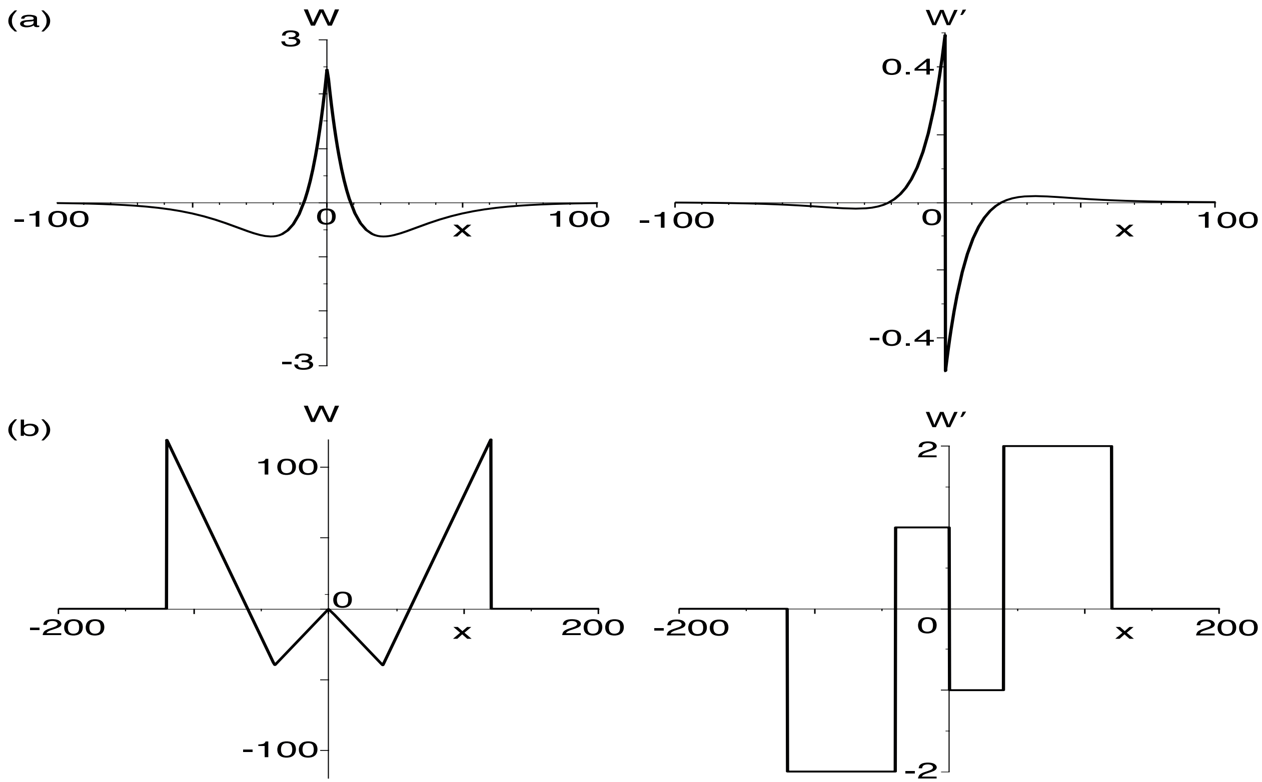
local maximum at $x = 0$: $\beta := -W''(0) > 0$

local minimum at $x = 2x_0$: $\alpha := W''(2x_0) > 0$

[a] [Kang, Perthame, Primi, Stevens, Velazquez]

Non-local repulsion-aggregation

Morse potential, Doubly-singular potential



Morse- (a) and Doubly-singular (b) potentials W with W':

Non-local repulsion-aggregation

Overview

Underlying (immodest) question:

- What is the relation between i) stationary aggregation pattern, ii) the shape and properties of interaction potential W, and iii) the initial data?

Outline:

- Smooth Double-Well Potentials ($\longrightarrow$ Gaël Raoul)
- Morse Potentials
- Douby-Singular Double-Well Potentials

Smooth Double-Well Potential

An explicit example

evenly smoothed modulus $|x|_\varepsilon$ on the interval $(-\varepsilon, \varepsilon)$ for $\varepsilon > 0$

$$W_\varepsilon(x) = x^2 - |x|_\varepsilon, \quad W_\varepsilon'(x) = 2x - \mathrm{sign}_\varepsilon(x), \quad W_\varepsilon''(x) = 2 - 2\delta_\varepsilon(0)$$

where we assume

$$\mathrm{sign}_\varepsilon(0) = 0 \quad \text{and} \quad \mathrm{sign}_\varepsilon(\pm\varepsilon) = \pm 1 \qquad \delta_\varepsilon(0) \approx \frac{1}{\varepsilon}\,.$$

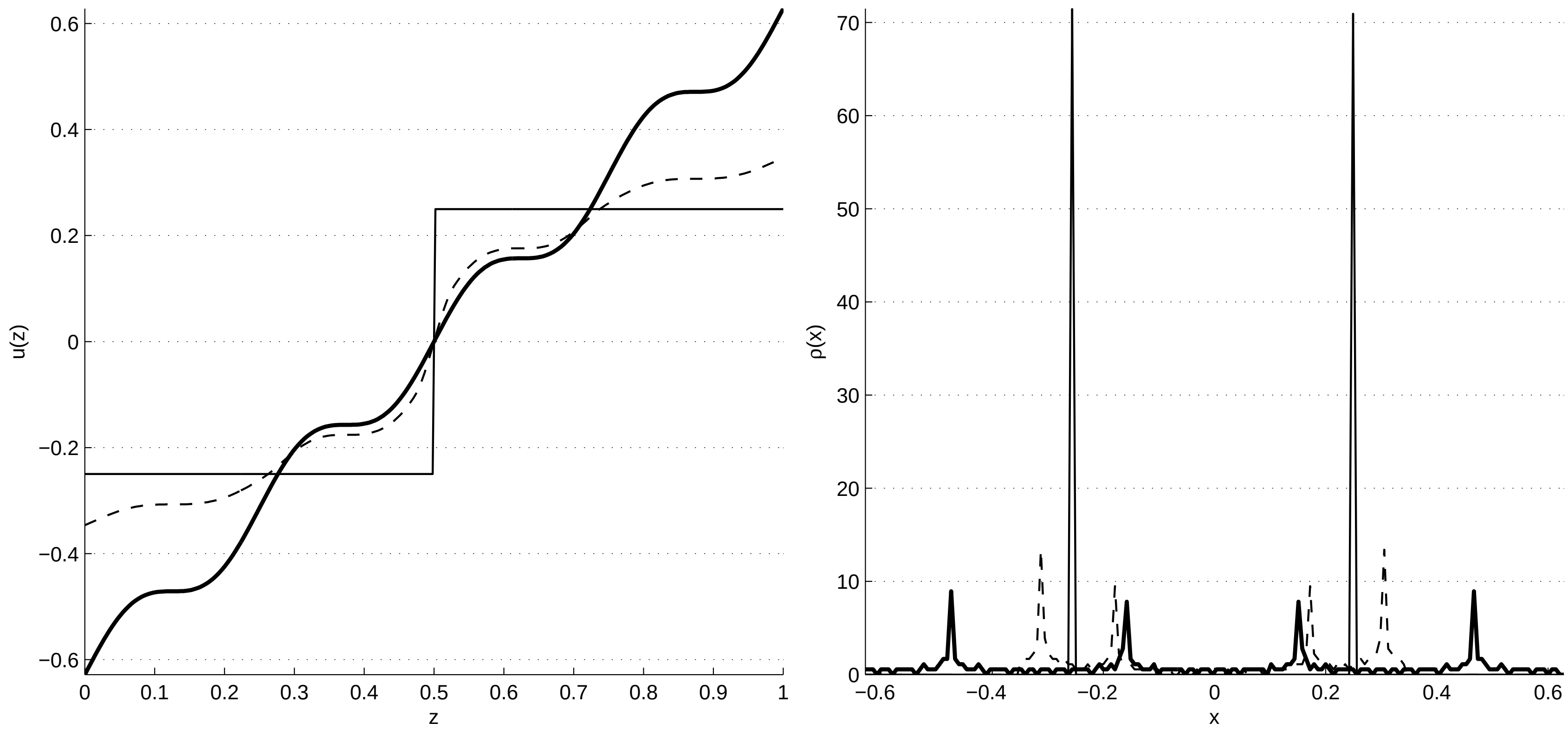
[a]

[a] K.F., G. Raoul, M3AS (2010)

Smooth Double-Well Potential

Numerics: $W_\varepsilon = x^2 - |x|_\varepsilon$ **with** $\varepsilon = 0.4$

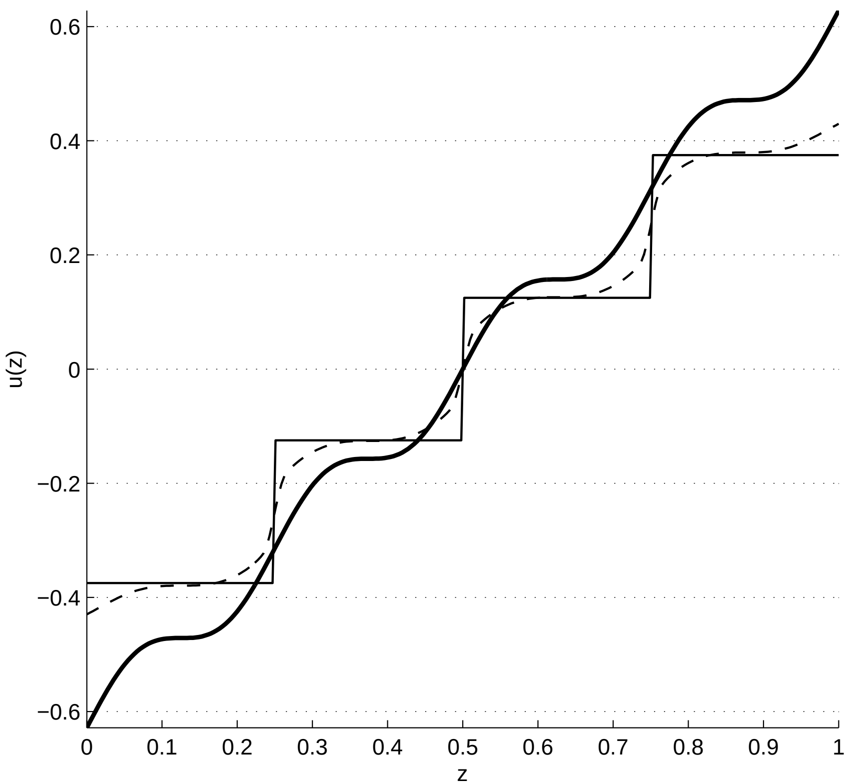
Weak repulsion: Four initial humps converge to two Diracs

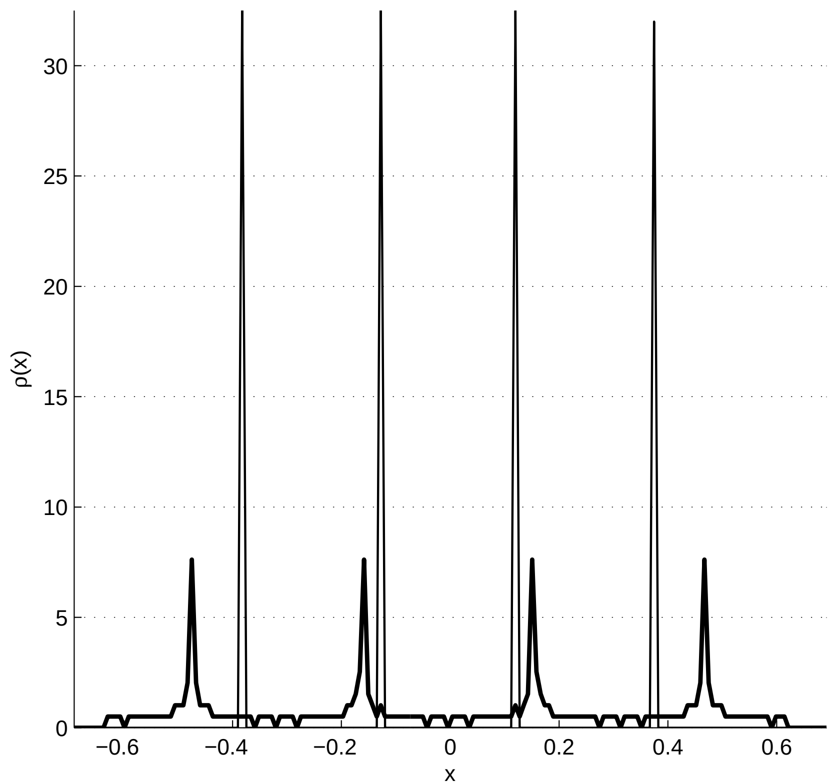


Smooth Double-Well Potential

Numerics: $W_\varepsilon = x^2 - |x|_\varepsilon$ **with** $\varepsilon = 0.18$

More repulsion: Four initial humps converge to four Diracs

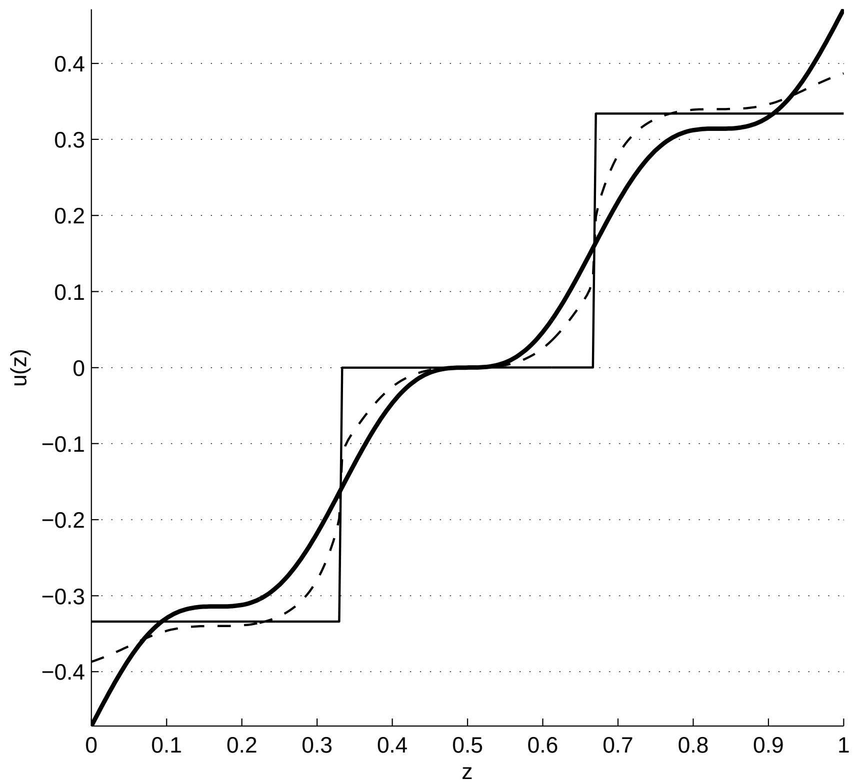


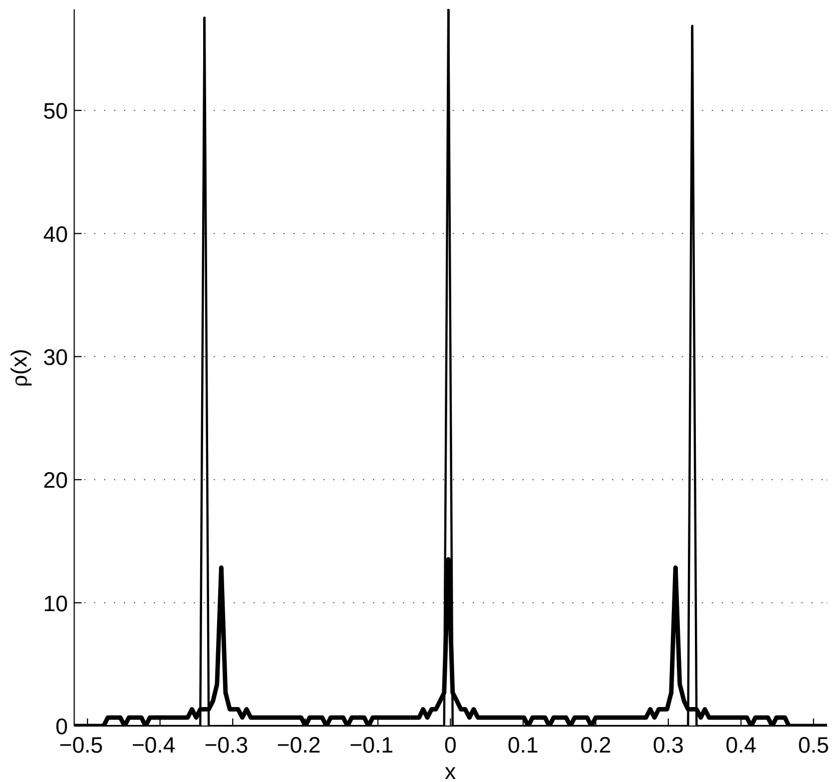


Smooth Double-Well Potential

Numerics: $W_\varepsilon = x^2 - |x|_\varepsilon$ **with** $\varepsilon = 0.18$

More repulsion: Three initial humps converge to three Diracs

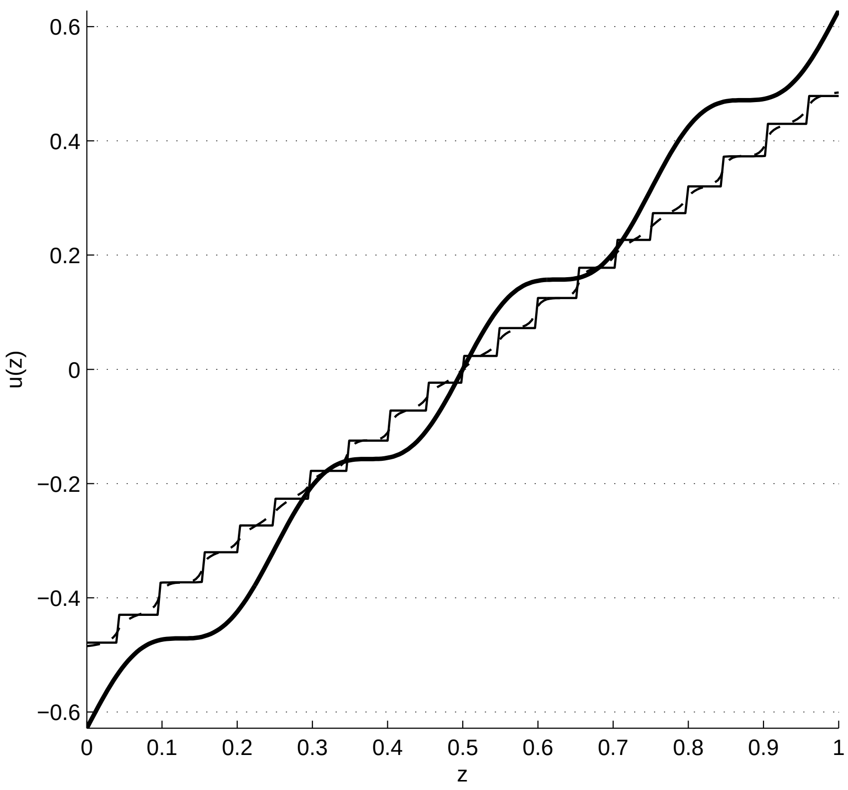


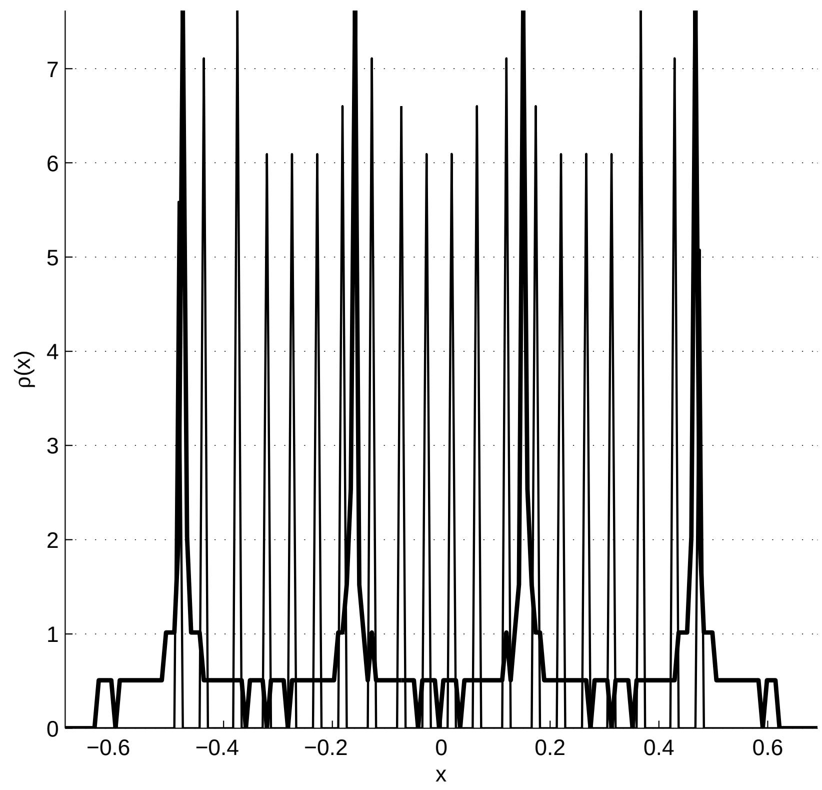


Smooth Double-Well Potential

Numerics: $W_\varepsilon = x^2 - |x|_\varepsilon$ **with** $\varepsilon = 0.03$

Strong repulsion: Convergence to multiple Diracs





Non-local interaction equation

Thm: Stationary States

- W analytic $\Rightarrow$ the stationary states are "discrete" sums of Diracs: $\bar{\rho}(x) = \sum_{i=1}^{n} \rho_i \delta_{u_i}(x)$, $\sum_{i=1}^{n} \rho_i = 1$, $\rho_i > 0$, or $\bar{u}(z) = \sum_{i=1}^{n} u_i \, \mathbb{1}_{I_i}$, $I_i = [\sum_{j<i} \rho_j, \sum_{j\leq i} \rho_j)$, $|I_i| = \rho_i$.
- $W \in C^2 \Rightarrow$ accumulating Diracs have no spectral gap.

A sum of Diracs $\bar{u} = \sum_1^n u_i \mathbb{1}_{I_i}$ with $|I_i| = \rho_i$ is stationary state iff

$$\sum_{j=1}^{n} W'(u_j - u_i)\, \rho_j = V'(u_i), \qquad i = 1, \dots, n\,.$$

Proof: $\partial_t \bar{u} = \int_0^1 W'(\bar{u}(\xi) - u_i)\, d\xi - V'(u_i)$ on $z \in I_i$

Non-local interaction equation

Thm: Linear stability steady state $\bar\rho = \sum_{i=1}^n \rho_i \delta_{u_i}$

- linear stability under small "reallocations" provided

$$0 < m_i := \sum_{j=1}^n W''(u_j - u_i)\rho_j + V''(u_i) \quad \forall i = 1, \dots, n\,.$$

- linear stability under "shifts" of the u_i, if the matrix

$$M = \operatorname{diag}(m_i) - (\rho_i W''(u_j - u_i))$$

has a positive spectrum
iff $V = 0$ then on the hyperspace $\{(w_i) : \sum_{i=1}^n w_i = 0\}$

Non-local interaction equation

Thm: Local nonlinear stability without exchange of mass

$W, V \in C^{2,\alpha} \Rightarrow$ Linearly stable stationary state $\bar{\rho} = \sum_{i=1}^{n} \rho_i \delta_{u_i}$ are locally non-linear stable w.r.t. Wasserstein W_∞, i.e.

$$\|u(0) - \bar{u}\|_\infty \leq \varepsilon \quad \Rightarrow \quad \|u(t) - \bar{u}\|_\infty \leq C\left(1 + t^{n-1}\right) e^{-\eta t},$$

Proof: Consider the vector $w := \left(|v_i|, \int_{I_1} v, \cdots \int_{I_n} v\right)^T$, then

$$\frac{d}{dt}\tilde{w} = \begin{pmatrix} -\mathrm{diag}\,(m_i) & O(1) \\ 0 & -\tilde{M} \end{pmatrix} \tilde{w} + O(\|w\|^2),$$

Stability in higher dimensions via atomisation [CDFLS]

Singular interaction potential

An explicit example

formal: local repulsion $\rightarrow$ Dirac $\Longrightarrow$ quadratic diffusion

Singular locally repulsive example potential: $W(x) = x^2 - |x|$

Unique bounded solution for smooth enough initial data

Unique stationary state: $\bar{\rho} = \mathbb{I}_{[-\frac{1}{2}, \frac{1}{2}]}$

on $\operatorname{supp}(\rho)$:

$$0 = W' * \rho = \int_{\mathbb{R}} 2(x-y)d\rho(y) - \int_{\mathbb{R}} \operatorname{sign}(x-y)d\rho(y)$$

$$= 2x - \int_{-\infty}^{x} d\rho(y) + \int_{x}^{-\infty} d\rho(y) = 2x + 1 - 2\int_{-\infty}^{x} d\rho(y)$$

Singular repulsion

Arbitrary many stable Diracs: an explicit example

Construct stable stationary states with $n \in \mathbb{N}$ Dirac masses:

$\bar{u} = \sum_{i=1}^{n} u_i \mathbb{I}_{I_i}$ with $|I_i| = \rho_i$ and $\max_i\{(u_{i+1} - u_i)\} > \varepsilon > 0$

$$0 = \sum_{j=1}^{n} \rho_j W'_\varepsilon(u_j - u_i) = -2u_i + \sum_{j<i} \rho_j - \sum_{j>i} \rho_j$$

using $\sum_{j=1}^{n} \rho_j = 1$ and $\sum_{j=1}^{n} u_j \rho_j = 0$

For all $n \in \mathbb{N}$, obtain many stationary states

$$(u_{i+1} - u_i) = \frac{\rho_i + \rho_{i+1}}{2} > \varepsilon \quad \Rightarrow \varepsilon < \frac{1}{n}$$

stability: $m_i = \sum_{j=1}^{n} \rho_j W''_\varepsilon(u_j - u_i) = 2 - \frac{\rho_i}{\varepsilon} > 0 \Rightarrow \varepsilon > \frac{\rho_i}{2}$

Singular repulsion

Weak limit towards continuous stationary state, $\varphi \in C$

$u_1 = -\frac{1-\rho_1}{2} \to -\frac{1}{2}$ and $u_n = \frac{1-\rho_n}{2} \to \frac{1}{2}$ since $\rho_i < \frac{2}{n}$ for $n \to \infty$.

$$\int_{\mathbb{R}} \varphi(x)\, d\bar{\rho}(x) = \sum_{i=1}^{n} \varphi(u_i)\, \rho_i = \sum_{i=1}^{n} \int_{u_i-\frac{\rho_i}{2}}^{u_i+\frac{\rho_i}{2}} \varphi(u_i)\, dx$$

$$= \int_{u_1-\frac{\rho_1}{2}}^{u_n+\frac{\rho_n}{2}} \sum_{i=1}^{n} \varphi(u_i) \mathbb{I}_{[u_i-\frac{\rho_i}{2}, u_i+\frac{\rho_i}{2}]}\, dx$$

$$\to \int_{-\frac{1}{2}}^{\frac{1}{2}} \varphi(x)\, dx = \int_{\mathbb{R}} \mathbb{I}_{[-\frac{1}{2},\frac{1}{2}]} \varphi(x)\ dx\,,$$

Theorem: $W_\varepsilon \to W = -|x|$, V strictly convex $\quad \Rightarrow \quad \bar{\rho}_\varepsilon \rightharpoonup \bar{\rho}$

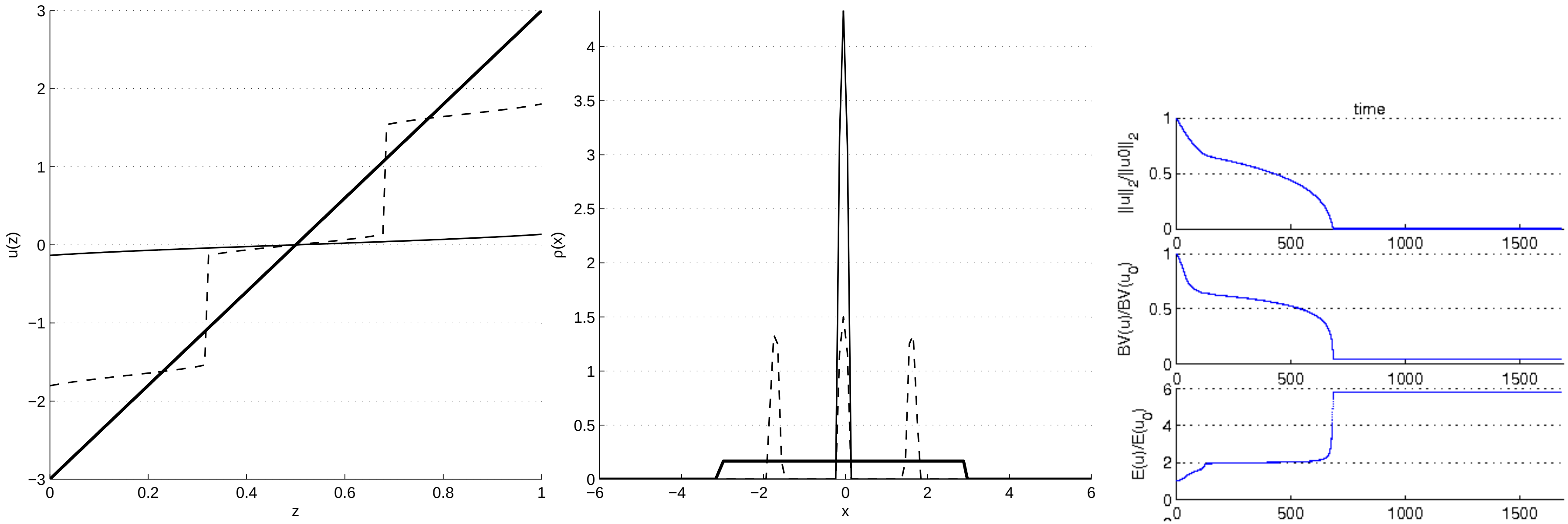
Biology: Reorientation of filament network.

Morse potential

$$W_{F,L_1,L_2}(x) = -FL_1 e^{-\frac{|x|}{L_1}} + L_2 e^{-\frac{|x|}{L_2}} \text{ with } L_2 > L_1, 0 < F < 1$$

Uniform initial support within $[-3, 3]$

Single aggregate as (numerically) stable stationary state[a]



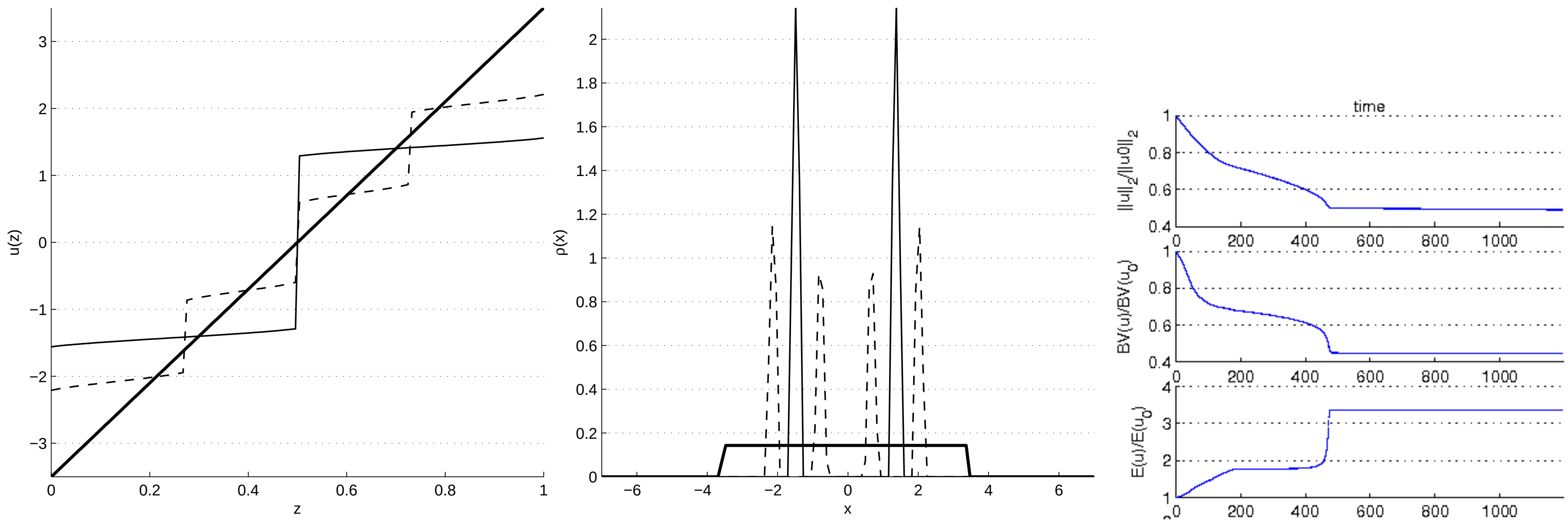
[a] Implicit Newton-iteration scheme for $\partial_t u(z) = \int_0^1 W'(u(\zeta) - u(z))\, d\zeta$

Morse potential

$$W_{F,L_1,L_2}(x) = -FL_1 e^{-\frac{|x|}{L_1}} + L_2 e^{-\frac{|x|}{L_2}} \text{ **with** } L_2 > L_1, 0 < F < 1$$

Uniform initial support within $[-3.5, 3.5]$

Two aggregates as (numerically) stable stationary state



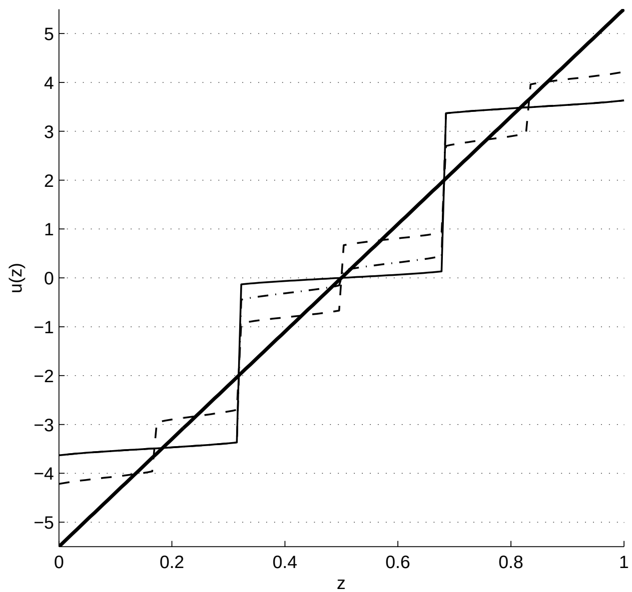
Quasi-stable pattern of 4 aggregates! Coarsening

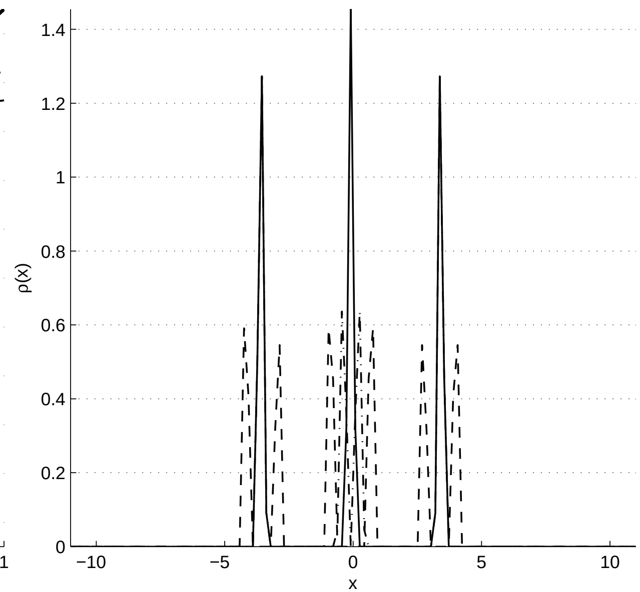
Morse potential

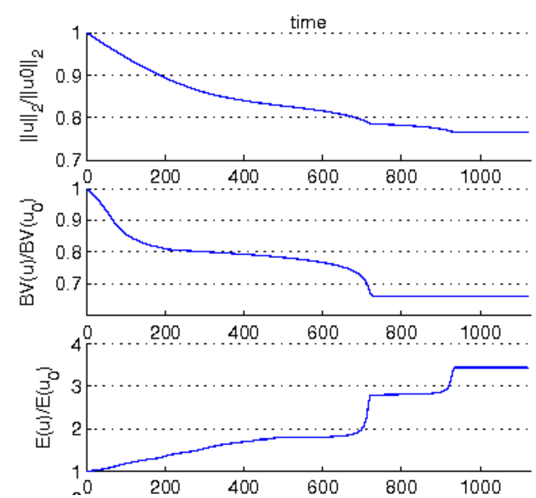
$$W_{F,L_1,L_2}(x) = -FL_1 e^{-\frac{|x|}{L_1}} + L_2 e^{-\frac{|x|}{L_2}}$$ **with** $L_2 > L_1, 0 < F < 1$

Uniform initial support within $[-5.5, 5.5]$

Three aggregates as (numerically) stable stationary state







Slow-Fast Dynamics similar to small diffusion Keller-Segel? [a]

[a] [Dolak, Schmeiser, 2005]

Doubly-singular Double-Well Potential

piecewise linear

λ: relative strength of repulsion and attraction

$r > 0$: range of repulsion

$c \in (r, \infty]$: cut-off

$$W_{r,\lambda,c}(x) = \begin{cases} -|x|, & |x| < r, \\ \lambda|x| - r(\lambda + 1), & r < |x| < c, \\ 0, & |x| > c, \end{cases}$$

disadvantage: by now existence [Carrillo, Ferreira, Precioso]

advantage: simplicity, predicability of pattern

Discrete Stochastic Model

Randon Walk on discrete lattice

Discrete Stochastic Model: does not see singular potential.

N agents on lattice, choose randomly N to move at time step. $\rho_i(k)$: average relative occupancy of site i at the kth time step.

$$\rho_i(k+1) - \rho_i(k) = P\left[\rho_{i-1}(k)\mathrm{R}_{i-1}(k) + \rho_{i+1}(k)\mathrm{L}_{i+1}(k) - \rho_i(k)\left\{\mathrm{R}_i(k) + \mathrm{L}_i(k)\right\}\right],$$

$\mathrm{R}_i(k), \mathrm{L}_i(k)$: step-to-right, step-to-left transition probabilities

$$\frac{\rho_i(k+1) - \rho_i(k)}{\tau} = -\frac{P\Delta}{\tau}\left(\frac{\rho_i(k)\mathrm{R}_i(k) - \rho_{i-1}(k)\mathrm{R}_{i-1}(k)}{\Delta} - \frac{\rho_{i+1}(k)\mathrm{L}_{i+1}(k) - \rho_i(k)\mathrm{L}_i(k)}{\Delta}\right).$$

Discrete Stochastic Model

Continuum Expansion

$I_i = [x_i - \Delta/2, x_i + \Delta/2]$ and $T_k = [(k - \frac{1}{2})\tau, (k + \frac{1}{2})\tau]$:

$$\rho_i(k) \approx \frac{1}{\tau} \int_{T_k} \int_{I_i} \rho(x,t)\; \mathrm{d}x\; \mathrm{d}t \approx \Delta\, \rho(x_i, t_k).$$

Formal Taylor expansion

$$\frac{\partial \rho(x,t)}{\partial t} + \mathcal{O}(\tau) = -\frac{P\Delta}{\tau} \frac{\partial}{\partial x} \Big[\rho(x,t) (\mathrm{R}(x,t) - \mathrm{L}(x,t)) \Big] + \mathcal{O}(\frac{P\Delta^2}{\tau}).$$

with assumption

$$K = \lim_{\Delta \to 0, \tau \to 0} \frac{P\Delta}{\tau}$$

Discrete Stochastic Model

Transition Probabilities

$$r_i(k) = \sum_{j \neq i : W'(\Delta j - \Delta i) > 0} W'(\Delta j - \Delta i)\, \rho_j(k) \geq 0,$$

$$l_i(k) = \sum_{j \neq i : W'(\Delta j - \Delta i) < 0} W'(\Delta j - \Delta i)\, \rho_j(k) \leq 0,$$

$$\mathrm{R}_i(k) = \frac{1}{\|W'\|_\infty} r_i(k), \quad \mathrm{L}_i(k) = -\frac{1}{\|W'\|_\infty} l_i(k).$$

$$\mathrm{R}_i(k) - \mathrm{L}_i(k) = \frac{1}{\|W'\|_\infty} \sum_{j \neq i : j \in L} W'(\Delta j - \Delta i) \rho_j(k)$$

Discrete Stochastic Model

Formal Continuum Limit

$$\frac{\partial \rho}{\partial t} = \frac{K}{\|W'\|_\infty} \frac{\partial}{\partial x} \left[\rho \left(\int_{-\infty}^{+\infty} W'(x-\xi)\rho(\xi,t)d\xi \right) \right].$$

Alternative Transition Probabilities

$$\mathrm{R}_i(k) = \frac{1}{\|W'\|_\infty} \left[r_i(k) + l_i(k) \right] H\Big(r_i(k) + l_i(k) \Big),$$

$$\mathrm{L}_i(k) = -\frac{1}{\|W'\|_\infty} \left[r_i(k) + l_i(k) \right] \Big[1 - H\Big(r_i(k) + l_i(k) \Big) \Big],$$

Fast Simulation Transition Probabilities

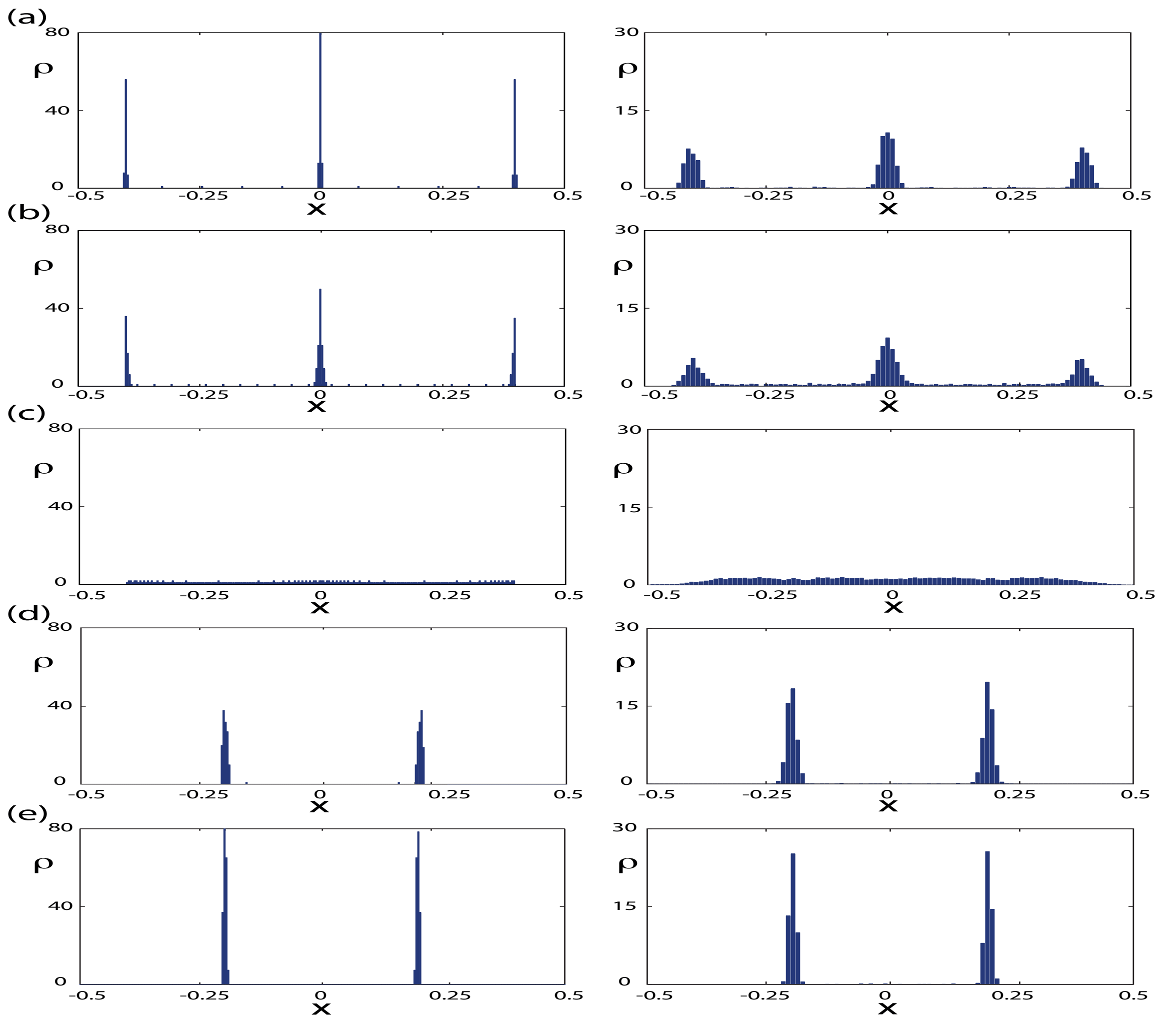
$$\mathrm{R}_i(k) = H\Big(r_i(k) + l_i(k) \Big),$$

$$\mathrm{L}_i(k) = -\Big[1 - H\Big(r_i(k) + l_i(k) \Big) \Big].$$

Doubly singular double-well

$W_{r,\lambda}(x)$ **mit** $r = 0.4$ **und** $\lambda = 0.5, 0.9, 1.0, 1.1, 2.0$ **(a)-(e)**

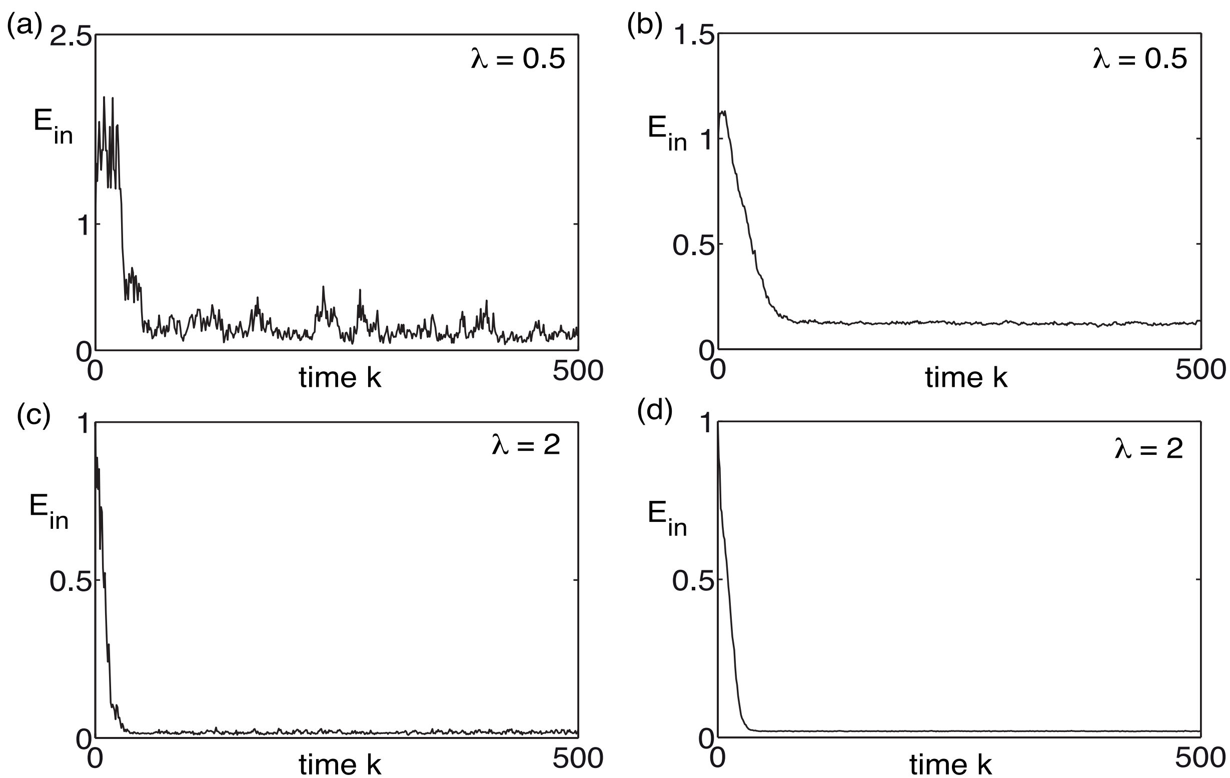
Aggregates on islands, spaced with r



Doubly singular double-well

Energie Evolution: single realisation and average

Scaled inverse energy function $E_{\rm in}(k) = \frac{E(0)}{E(k)}$ with $E(k) = \frac{1}{2}\Delta^2 \sum_i \sum_j \rho_i(k)\rho_j(k) W(\Delta i - \Delta j)$:



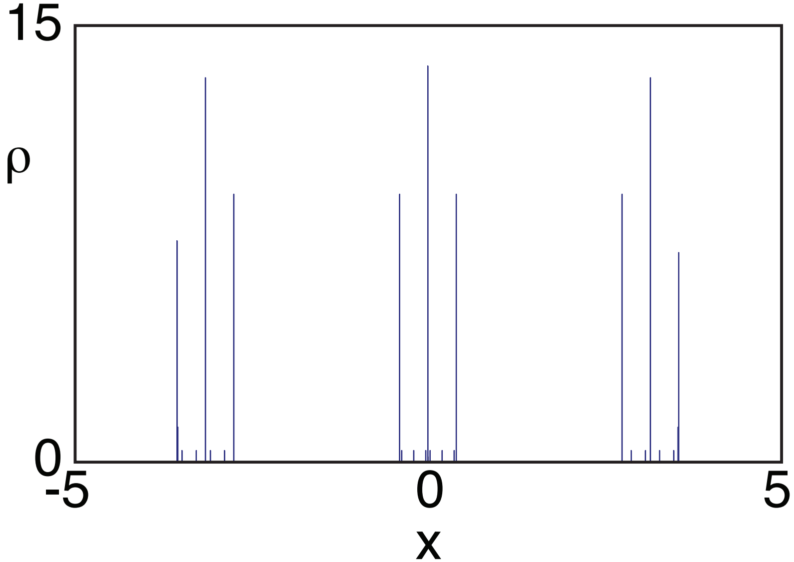
Doubly singular double-well

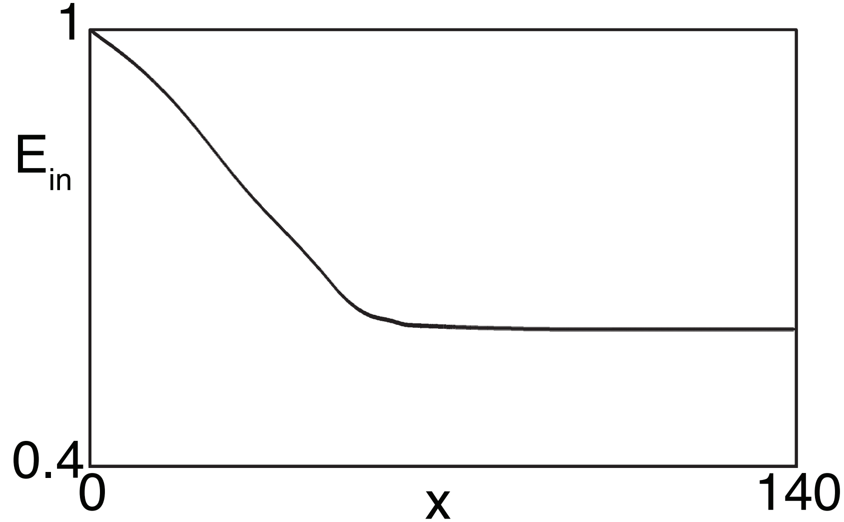
Large Initial Support and Cut-Off

$W_{r,\lambda,c}$ for $r = 0.4, \lambda = 0.5, c = 1.2$.

Uniformly distributed initial mass with support $[-5, 5]$.

Continuum Model:



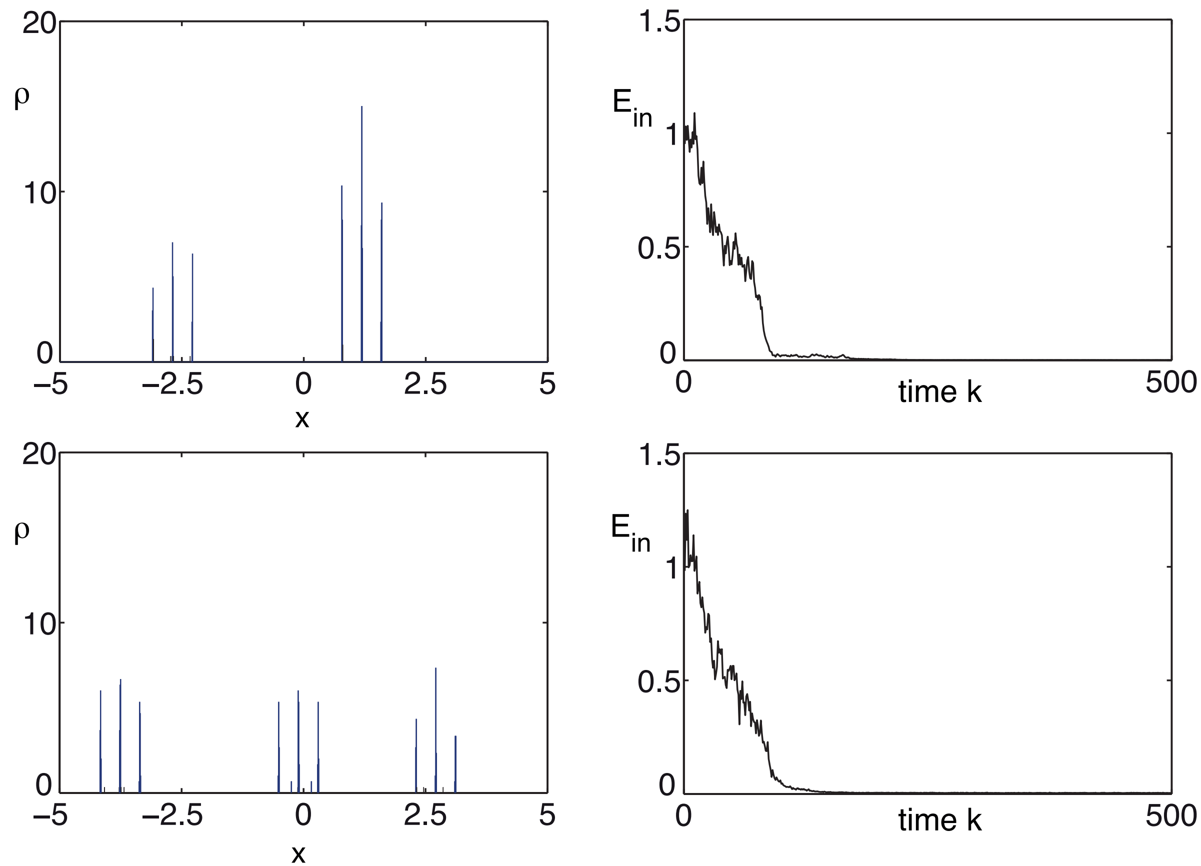


Doubly singular double-well

Large Initial Support and Cut-Off

$W_{r,\lambda,c}$ for $r = 0.4, \lambda = 0.5, c = 1.2$. Initial support $[-5, 5]$.

Two Realisations of Stochastic Model:

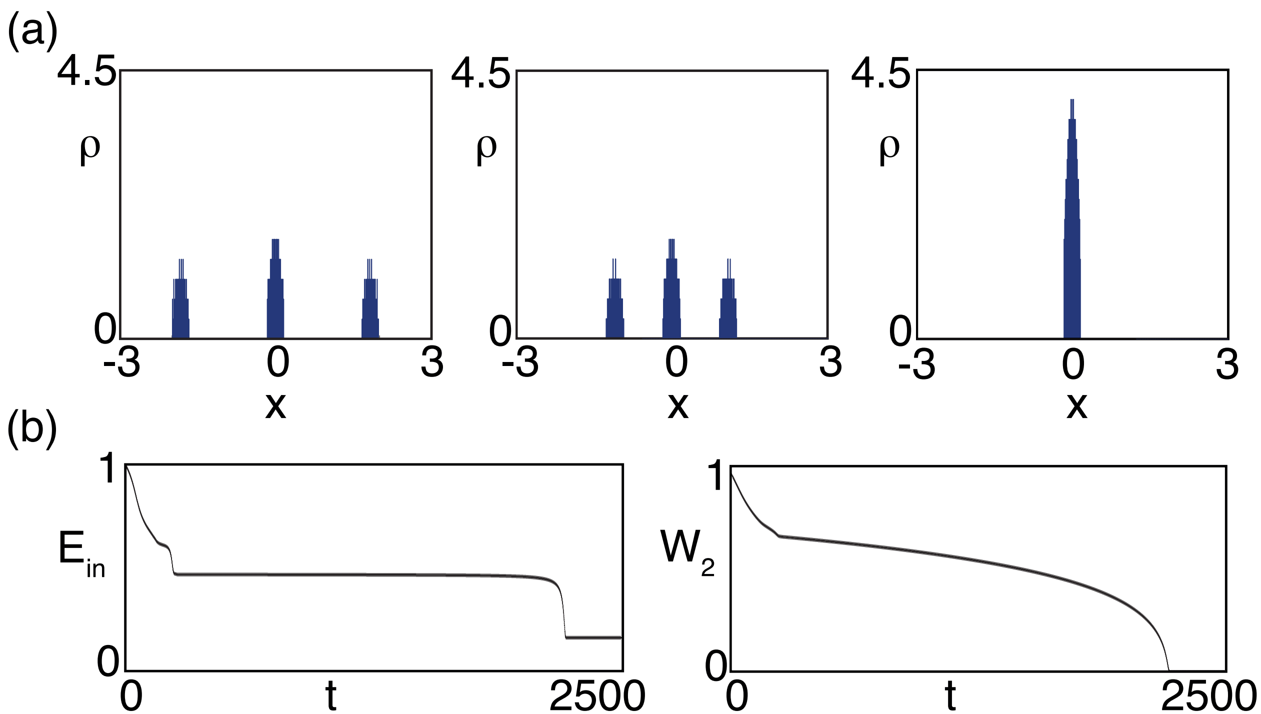


Morse Potential

Continuum model: Slow-Fast Time Evolution

W_{F,L_1,L_2} with $F = 0.5$, $L_1 = 0.25$ and $L_2 = 0.1$.

Uniform initial support is within $[-3, 3]$.

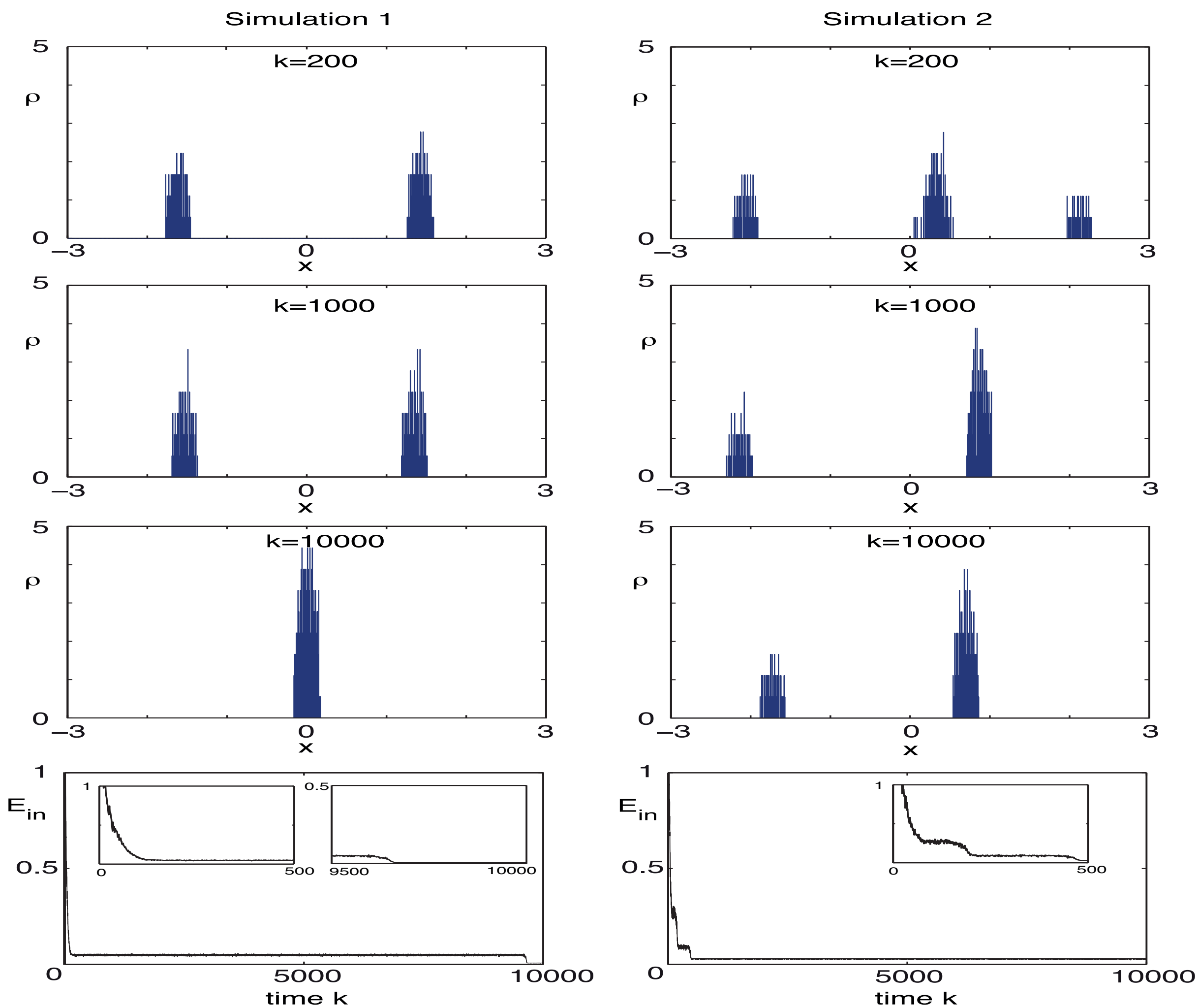


(a) Densities $\rho(x, t)$ at the three times $t = 520, 2170, 2509$.

(b) Time evolution of $\frac{E(0)}{E(k)}$ and the Wasserstein W_2 norm.

Morse Potential

Stochastic Model: Slow-Fast Time Evolution



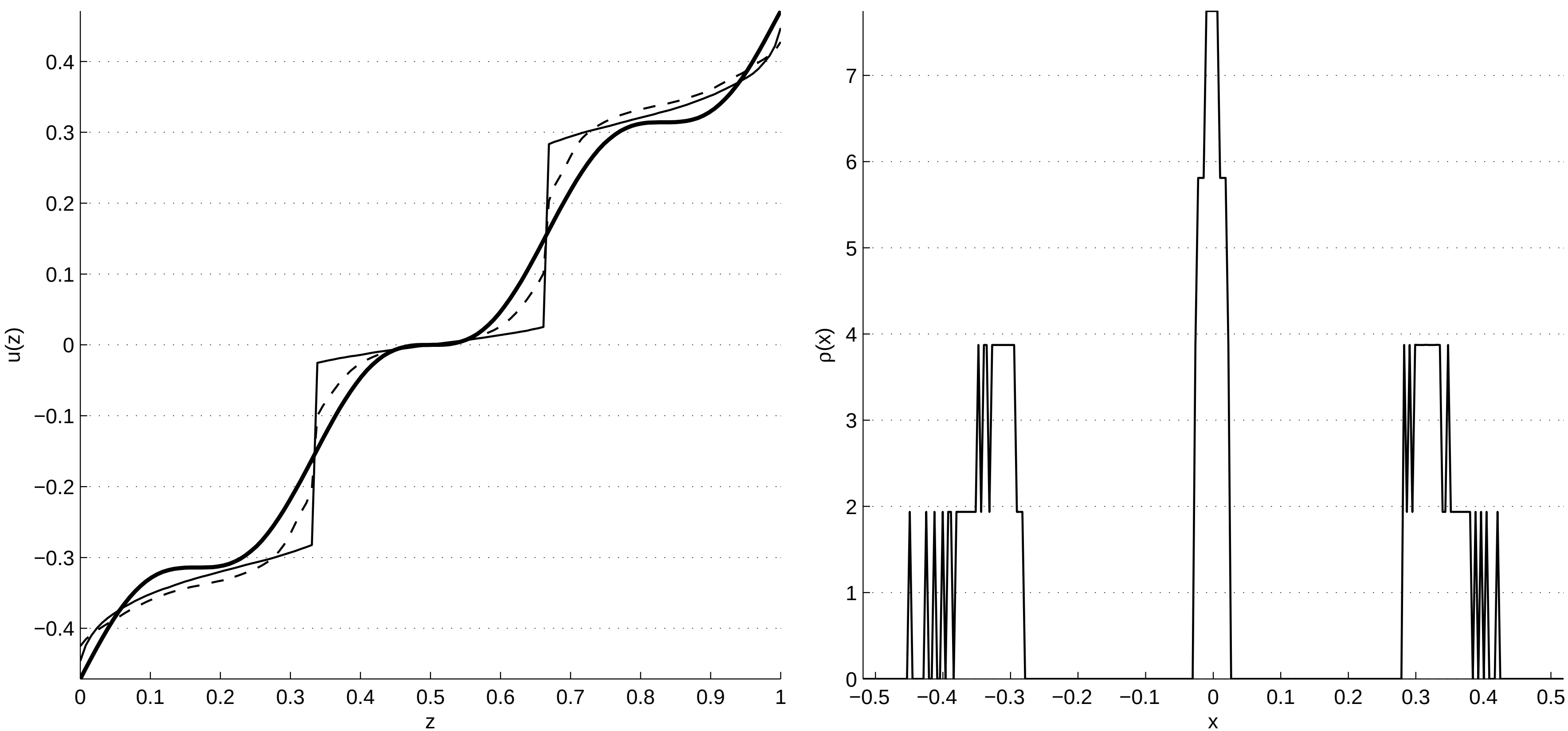
ρ at the three time steps $k = 200$, $k = 1000$, and $k = 10000$.

Non-local Stochastic Models

Non-uniqueness of aggregates

Double-well potential, Gaussian random walk “diffusion”

initial data with three smoothed aggregates

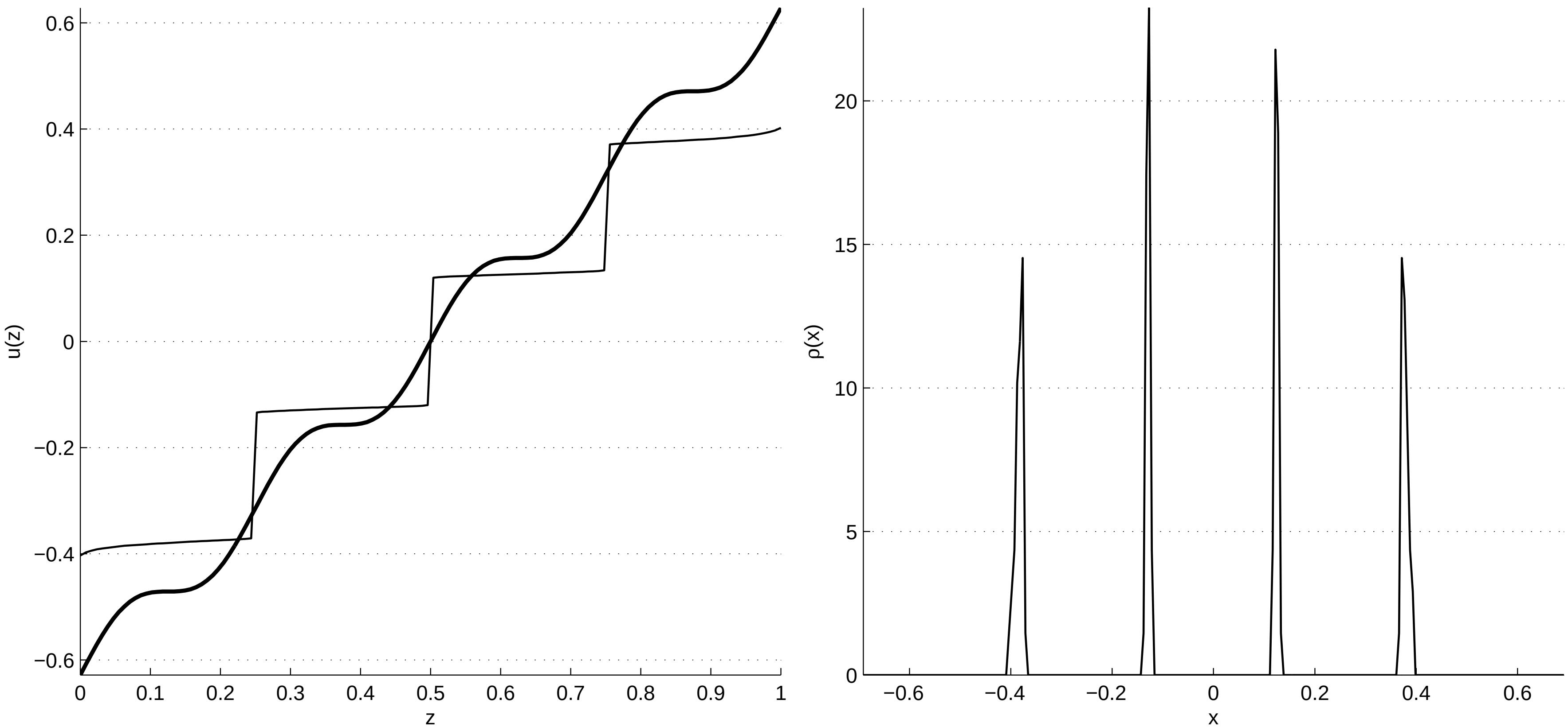


Non-local Stochastic Models

Non-uniqueness of aggregates

Same double-well potential, same random walk “diffusion“

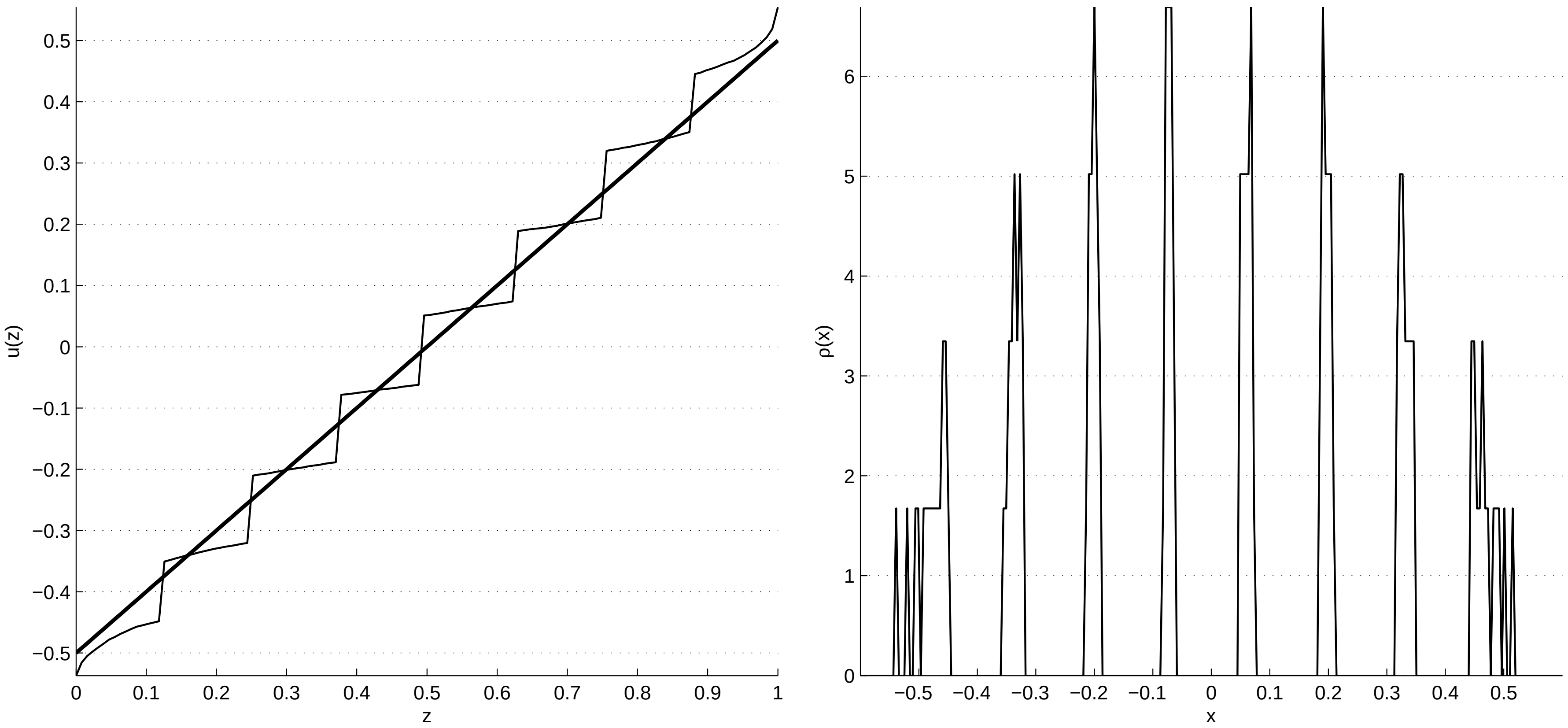
initial data with four smoothed aggregates



Non-local Stochastic Models

Increasing variance of random walk

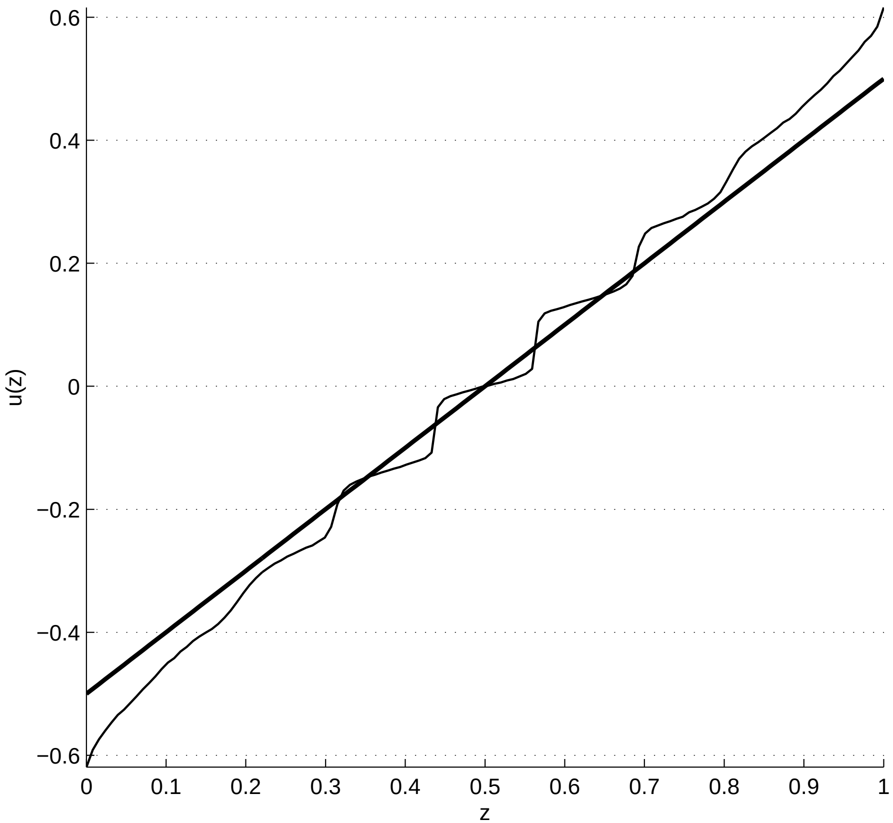
Low variance: 8 aggregates

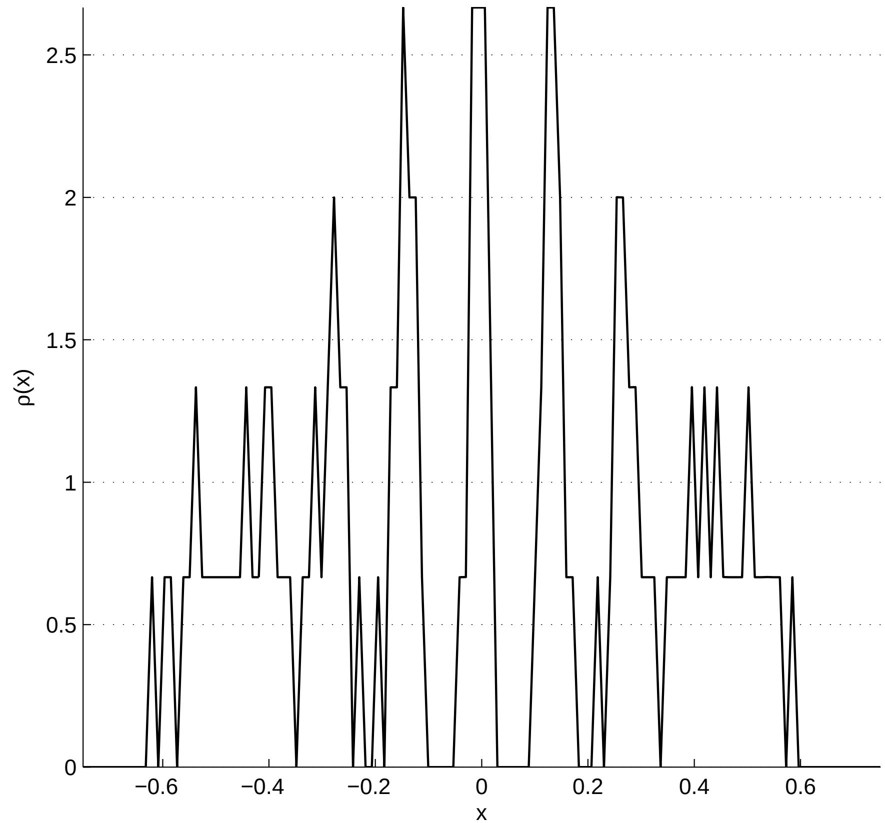


Non-local Stochastic Models

Increasing variance of random walk

Medium variance: about 7 aggregates

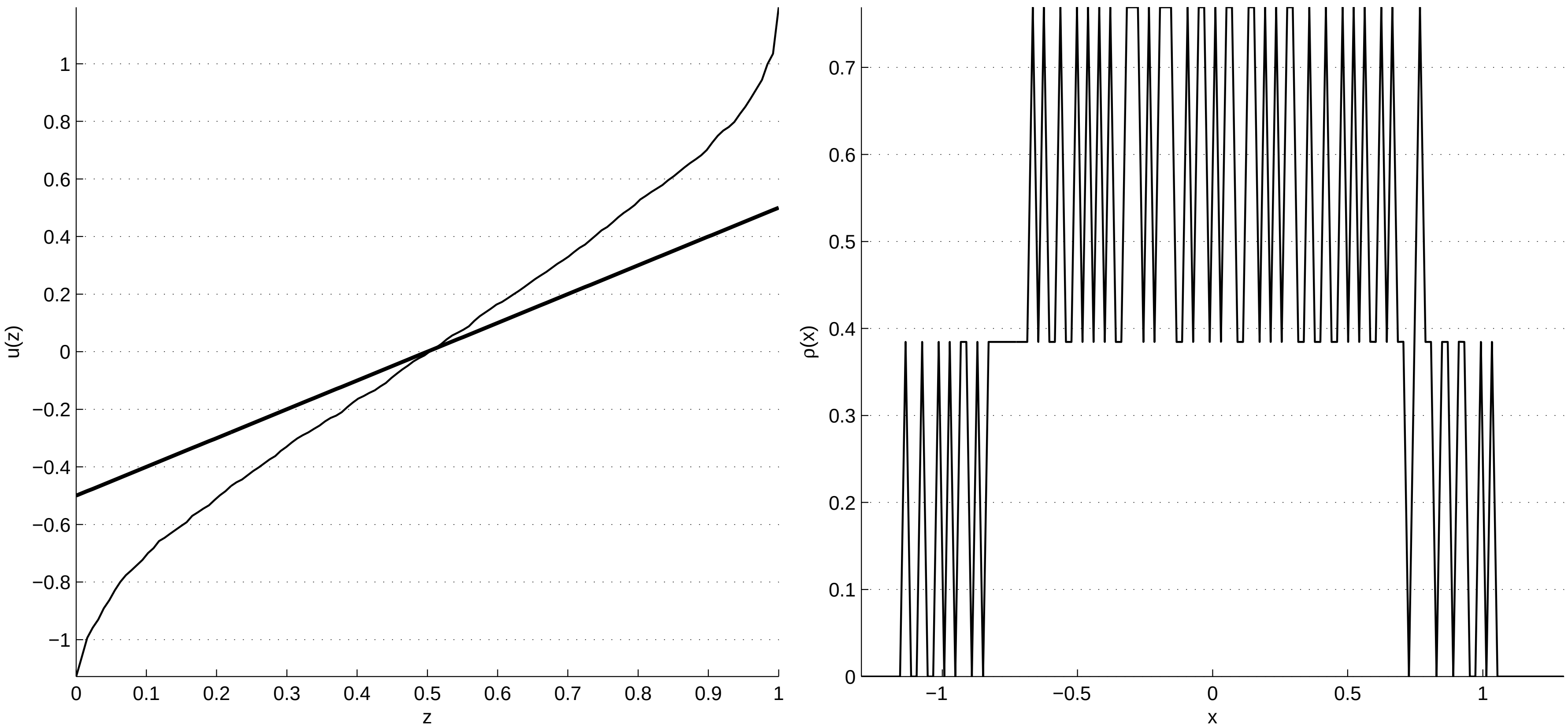




Non-local Stochastic Models

Increasing variance of random walk

High variance: 1 aggregate



Non-local Stochastic Models

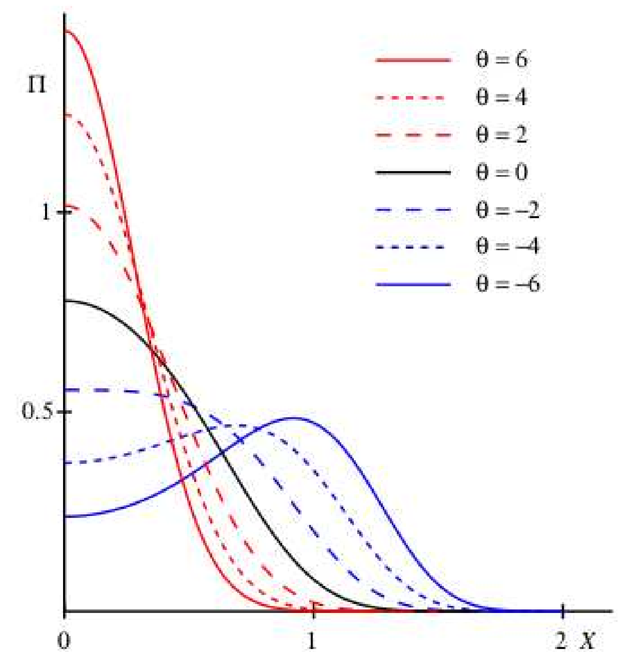
Stationary States with Diffusion

Steady State Equation: $D\rho' = -C\rho W' * \rho$.

Example: $W(x) = \beta x^2 + \delta x^4$

$$\rho(x) = \rho(\mu_1) e^{-\frac{C}{D}[\delta(x-\mu_1)^4 + (6\mu_2^{(c)}\delta+\beta)(x-\mu_1)^2]}$$

where $\mu_2^{(c)} = \int_{\mathbb{R}} (x-\mu_1)^2 \rho(X)\, dx$.



Bimodality criterium: $-\beta = 6\frac{\Gamma(3/4)}{\Gamma(1/4)}\sqrt{\frac{D\delta}{C}}$

Non-local Stochastic Models

Stationary States with Nonlinear Diffusion

Steady State Equation: $D\rho' = -C\rho W' * \rho.$

What with: $W(x) = x^2 - |x|_\varepsilon$?

Nonlocal ODE:

$$h'' = k - \frac{T}{\varepsilon} \int_{x-\varepsilon}^{x+\varepsilon} e^{h(y)}\, dy$$

has non-small periodic oscillation,

but not the localised limit problem:

$$h'' = k - Te^h$$

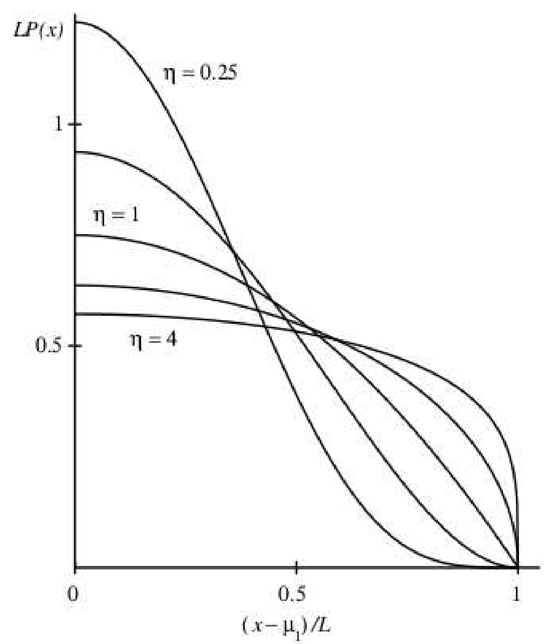
Non-local Stochastic Models

Stationary States with Nonlinear Diffusion

Steady State Equation: $D\rho^\eta \rho' = -C\rho W' * \rho.$

Example: $W(x) = \beta x^2$ (or $W(x) = \alpha|x| + \beta x^2$)

Profile of Stationary State



Non-local interaction equations

Conclusions

- smooth double-well potentials feature multiple, non-unique Dirac-type stationary pattern
- complicated relation between W and stationary pattern
- singular repulsion of interaction potential at 0 has smoothing effect on fewer stationary pattern
- doubly-singular interaction potential offer predictable aggregates on islands.
- good agreement of continuum and stochastic model

THANK YOU!