

Aggregation-pattern due to repulsive-aggregating interaction potentials

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inspired by: Marco Di Francesco, Christian Schmeiser

supported by: KAUST

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 “smooth” interaction potential

V : external (confining) potential

- inelastic material $\rightarrow W \sim |x|^{1+\varepsilon}$, aggregation
- collective behaviour, swarming/flocking $\rightarrow W \sim e^{\pm|x|}, e^{\pm x^2}$
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

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

1D: consider $u(z)$ **pseudo-inverse**^a of the distribution function

$$u(z) = \inf \left\{ x \in \mathbb{R}; \int_{-\infty}^x \rho dx > z \right\}, \text{ for } z \in [0, 1]$$

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

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

Non-local repulsion-aggregation

$V = 0 \Rightarrow$ 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 $\int_0^1 u_{in}(z) dz$:

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

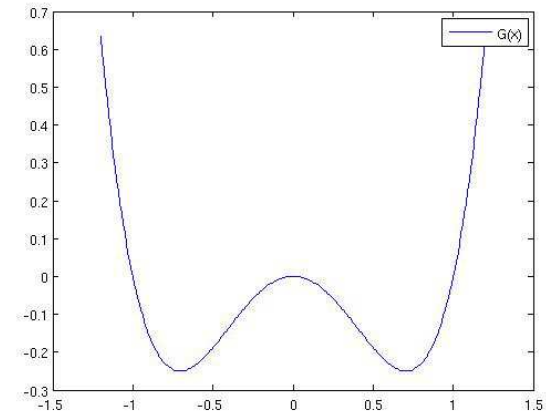
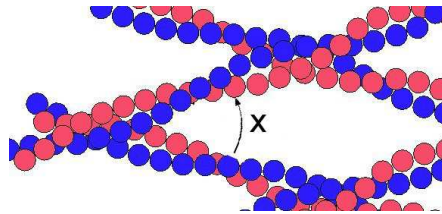
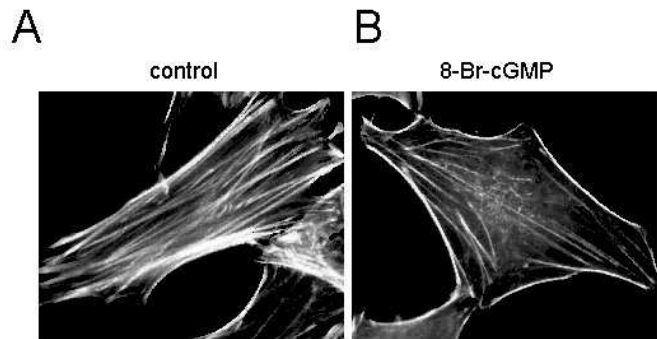
Normalisation

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

Non-local repulsion-aggregation

A double-well repulsion-aggregation potential

Actin filaments with or without cross-linking proteins^a



W double-well potential, $V = 0$:

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

Two Diracs stationary states

trivial stationary state $\bar{\rho} = \delta_0$, $\Leftrightarrow \bar{u}(z) = 0$, **unstable**

Family of monotone increasing two-valued stationary states

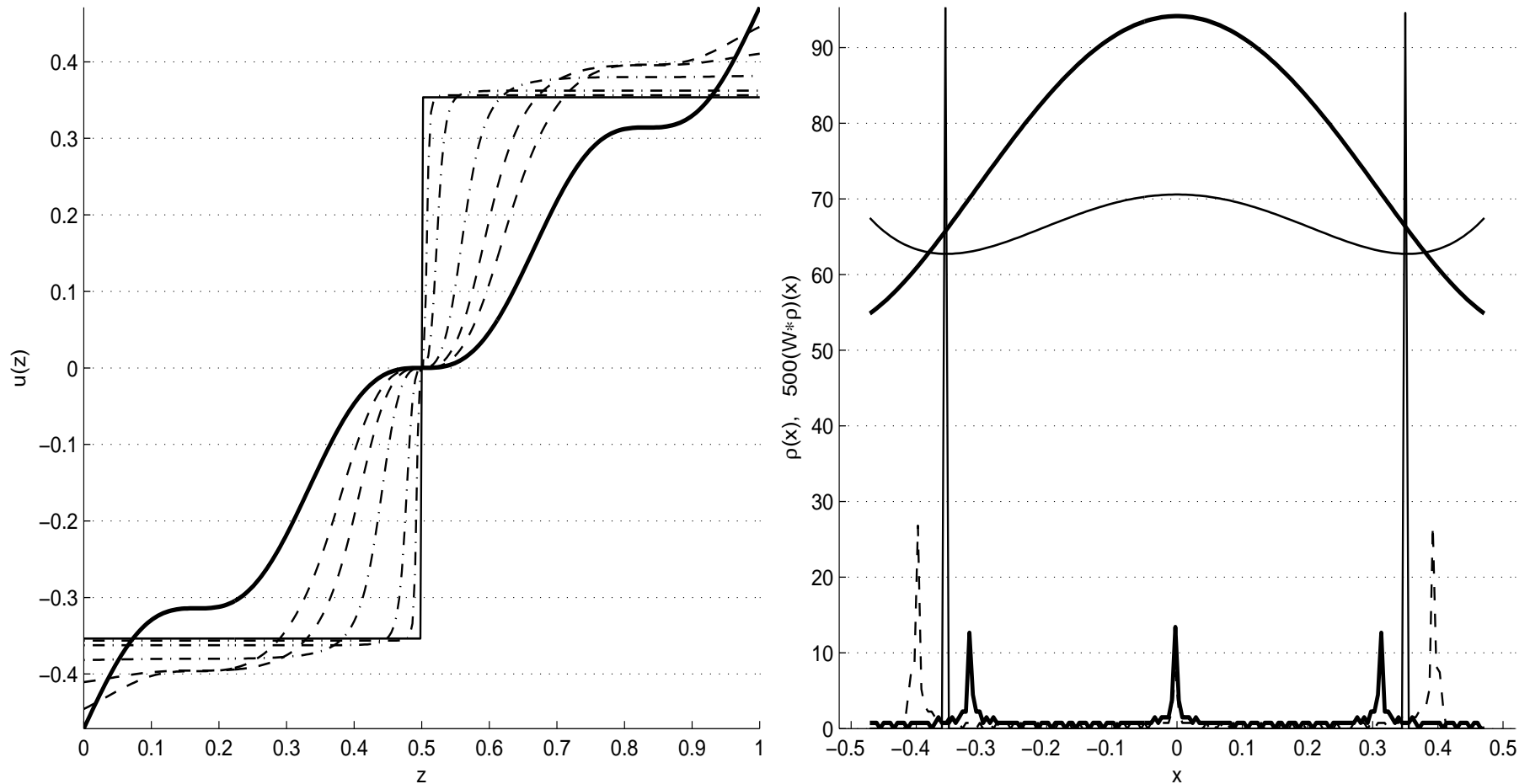
$$\bar{\rho}(x, z_0) = z_0 \delta_{-2(1-z_0)x_0} + (1 - z_0) \delta_{2z_0x_0}$$

$$\bar{u}(z, z_0) = \begin{cases} -2(1 - z_0)x_0 & z < z_0, \\ 2z_0x_0 & z > z_0. \end{cases}$$

mass distribution parameter $z_0 \in (0, 1)$

Non-local repulsion-aggregation

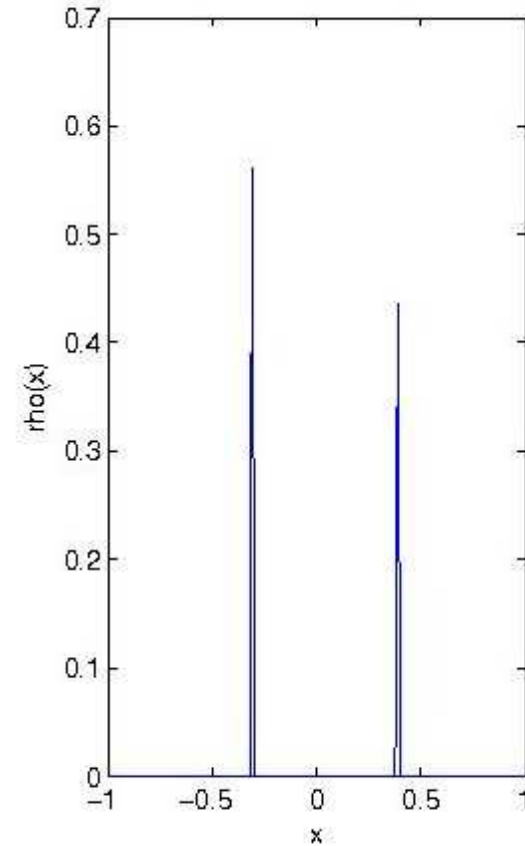
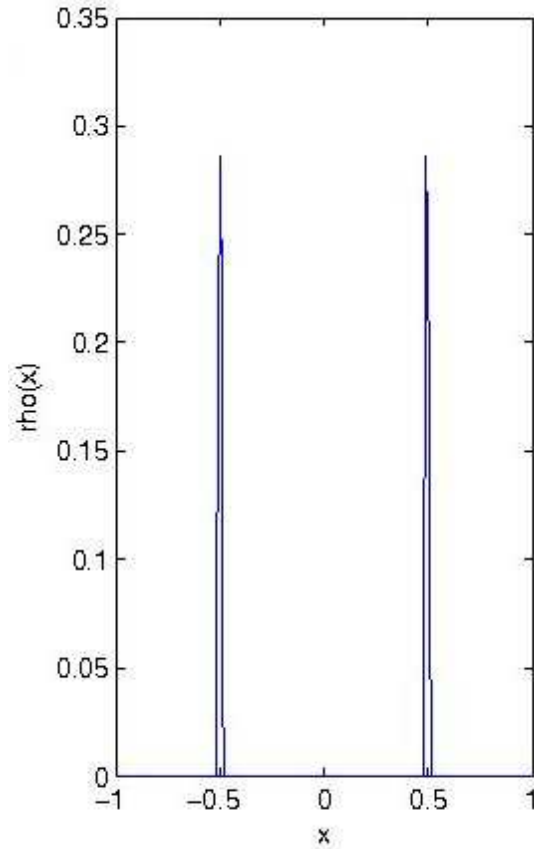
Numerical convergence to two-valued stationary states



mass conserving scheme for $\partial_t u(z) = \int_0^1 W'(u(\zeta) - u(z)) d\zeta$

Non-local repulsion-aggregation

Non-uniqueness of two-valued stationary state



but also

Nevertheless, both should be stable.

Non-local repulsion-aggregation

Linearised nonlocal operator

Consider mass preserving perturbations $v(z)$: $\int_0^1 v(z) dz = 0$.

$$F'(\bar{u}(z_0))(v(z)) = \begin{cases} \lambda_1 v(z) - (\alpha + \beta) \int_0^{z_0} v(z) dz & z < z_0, \\ \lambda_2 v(z) + (\alpha + \beta) \int_0^{z_0} v(z) dz & z > z_0. \end{cases}$$

with

$$\lambda_1 := z_0\beta - (1 - z_0)\alpha, \quad \lambda_2 := (1 - z_0)\beta - z_0\alpha,$$

and λ_1 and λ_2 are convex combinations of β and $-\alpha$.

Non-local repulsion-aggregation

Linear stability: Ansatz $v(z) = e^{\lambda t} \varphi(z)$

Eigenproblem $\lambda \varphi = F'(\bar{u}(z_0))(\varphi)$ with $\int_0^1 \varphi(z) dz = 0$

$$\begin{cases} (\lambda_1 - \lambda) \varphi(z) = +(\alpha + \beta) \int_0^{z_0} \varphi(z) dz & z < z_0, \\ (\lambda_2 - \lambda) \varphi(z) = -(\alpha + \beta) \int_0^{z_0} \varphi(z) dz & z > z_0. \end{cases}$$

$\lambda_1 \neq \lambda \neq \lambda_2$: Then, φ is piecewise constant and

$$\lambda = -\alpha < 0, \quad v(z) = \begin{cases} -\frac{1-z_0}{z_0} v_r & z < z_0, \\ v_r & z > z_0. \end{cases}$$

Aggregation yields stability w.r.t. (mass preserving) “shifts”.

Non-local repulsion-aggregation

Linear stability: Ansatz $v(z) = e^{\lambda t} \varphi(z)$

Eigenproblem $\lambda \varphi = F'(\bar{u}(z_0))(\varphi)$ with $\int_0^1 \varphi(z) dz = 0$

$$\begin{cases} (\lambda_1 - \lambda) \varphi(z) = +(\alpha + \beta) \int_0^{z_0} \varphi(z) dz & z < z_0, \\ (\lambda_2 - \lambda) \varphi(z) = -(\alpha + \beta) \int_0^{z_0} \varphi(z) dz & z > z_0. \end{cases}$$

$\lambda_1 = \lambda = \lambda_2, z_0 = \frac{1}{2}$: Then,

$$\lambda = \frac{\beta - \alpha}{2}, \quad v(z) = \begin{cases} v_l(z) : \int_0^{1/2} v_l dz = 0 & z < \frac{1}{2}, \\ v_r(z) : \int_{1/2}^1 v_r dz = 0 & z > \frac{1}{2}. \end{cases}$$

If aggregation controls repulsion, then
stability w.r.t. (mass preserving) “**reallocations**”.

Non-local repulsion-aggregation

Linear stability: Ansatz $v(z) = e^{\lambda t} \varphi(z)$

Eigenproblem $\lambda \varphi = F'(\bar{u}(z_0))(\varphi)$ with $\int_0^1 \varphi(z) dz = 0$

$$\begin{cases} (\lambda_1 - \lambda) \varphi(z) = +(\alpha + \beta) \int_0^{z_0} \varphi(z) dz & z < z_0, \\ (\lambda_2 - \lambda) \varphi(z) = -(\alpha + \beta) \int_0^{z_0} \varphi(z) dz & z > z_0. \end{cases}$$

similar $\lambda_1 = \lambda$ or $\lambda_2 = \lambda$, $z_0 \neq \frac{1}{2}$ (symmetry $z_0 \rightarrow (1 - z_0)$)

Summary: Given $\beta < \alpha$, then there exists an open interval of parameters z_0 with linearly stable stationary states $\bar{u}(z_0)$:

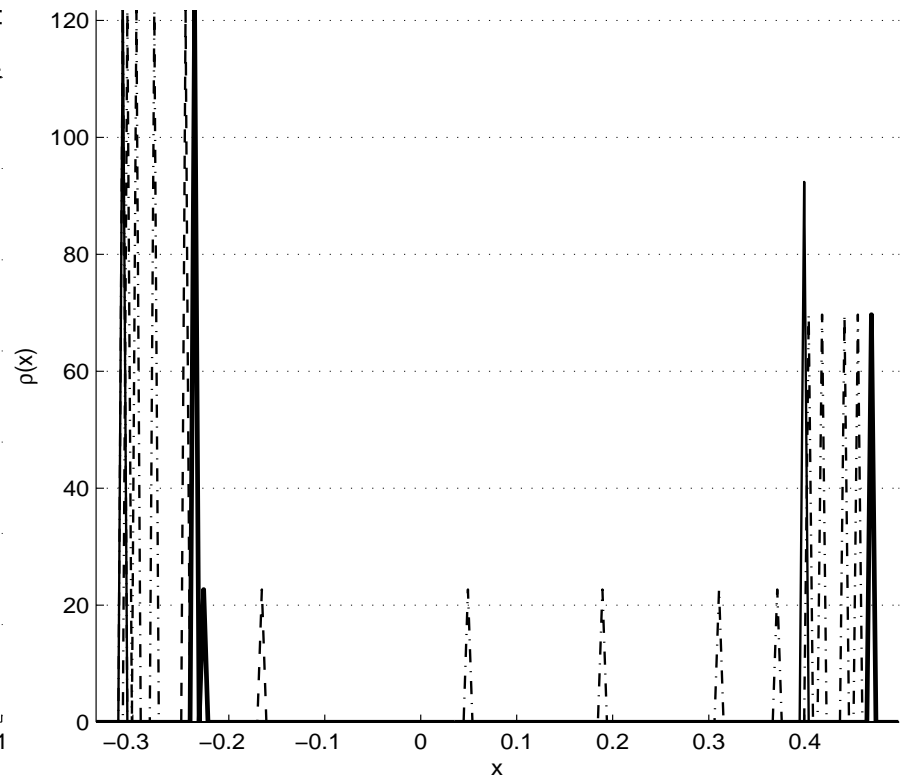
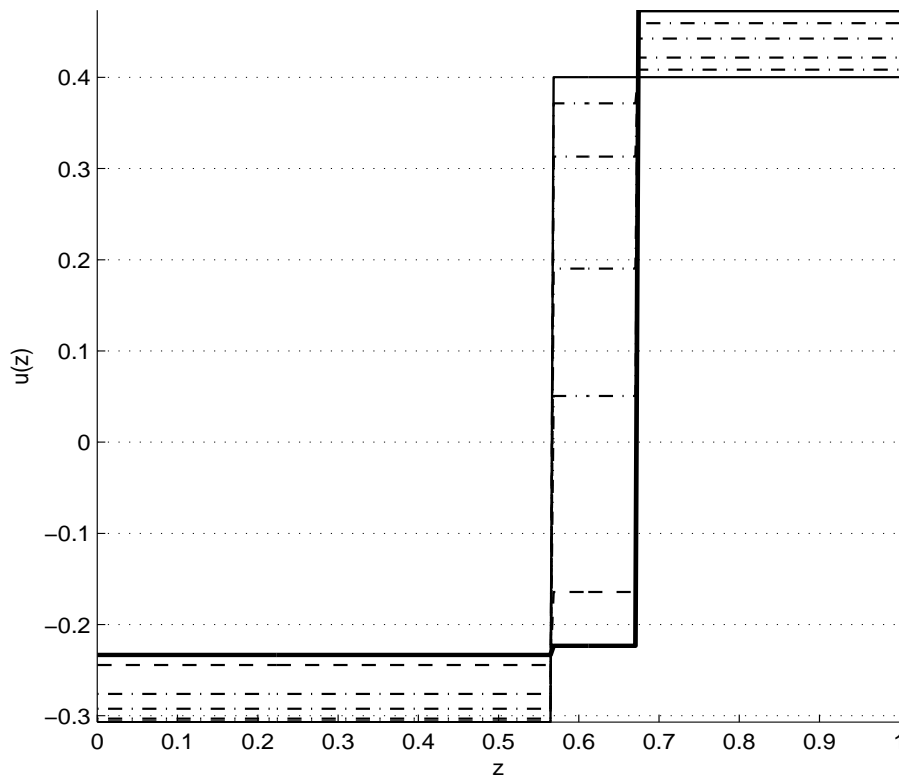
$$\max_{i=1,2} \{\lambda_i(z_0)\} < 0 \quad \forall z_0 \in (1 - z_0^*, z_0^*), \quad z_0^* := \frac{\alpha}{\alpha + \beta} > \frac{1}{2}.$$

Non-local repulsion-aggregation

Bifurcation analysis in $\varepsilon := \lambda_1 \ll 1$

Ansatz: $u(z) = \bar{u}(z, z_0 + \varepsilon a) + \varepsilon v(z), \quad \int_0^1 v(z) dz = 0$

\Rightarrow A too heavy Dirac **splits** (somehow) into two small Diracs.



Non-local interaction equation

General 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 $\bar{u} = \sum_{i=1}^n u_i \mathbb{1}_{I_i}$ with $|I_i| = \rho_i$ is stationary state iff

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

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

Three Dirac stationary states for W double-well, $V = 0$

A positive, normalised vector of masses

$$(\rho_1, \rho_2, \rho_3) = \frac{(-W'(u_3 - u_2), W'(u_3 - u_1), -W'(u_2 - u_1))}{-W'(u_3 - u_2) + W'(u_3 - u_1) - W'(u_2 - u_1)}$$

solves

$$\begin{pmatrix} -W'(u_3 - u_2) \\ W'(u_3 - u_1) \\ -W'(u_2 - u_1) \end{pmatrix} \times \begin{pmatrix} \rho_1 \\ \rho_2 \\ \rho_3 \end{pmatrix} = 0,$$

for the double-well if and only if choose (u_i) such that

$0 < u_2 - u_1, u_3 - u_2 < x_1$ and $u_3 - u_1 > x_1$.

Similar for **any odd number** of Diracs.

Local stability analysis

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

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

has a positive spectrum

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

Local stability analysis

Local 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.

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

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

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

Stability in higher dimensions via atomisation [CDFLS]

Towards singular repulsion

An explicit example

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

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

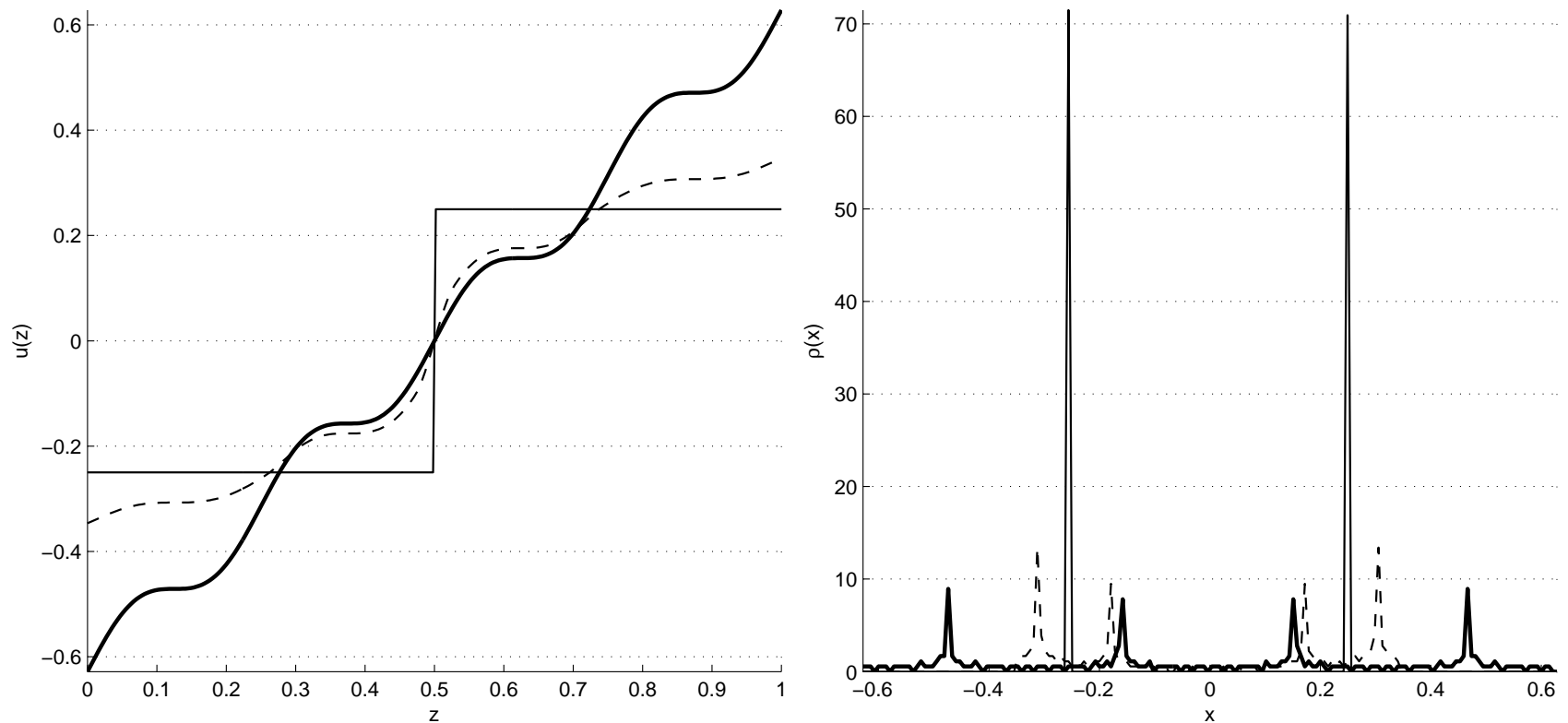
where we assume

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

Towards singular repulsion

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

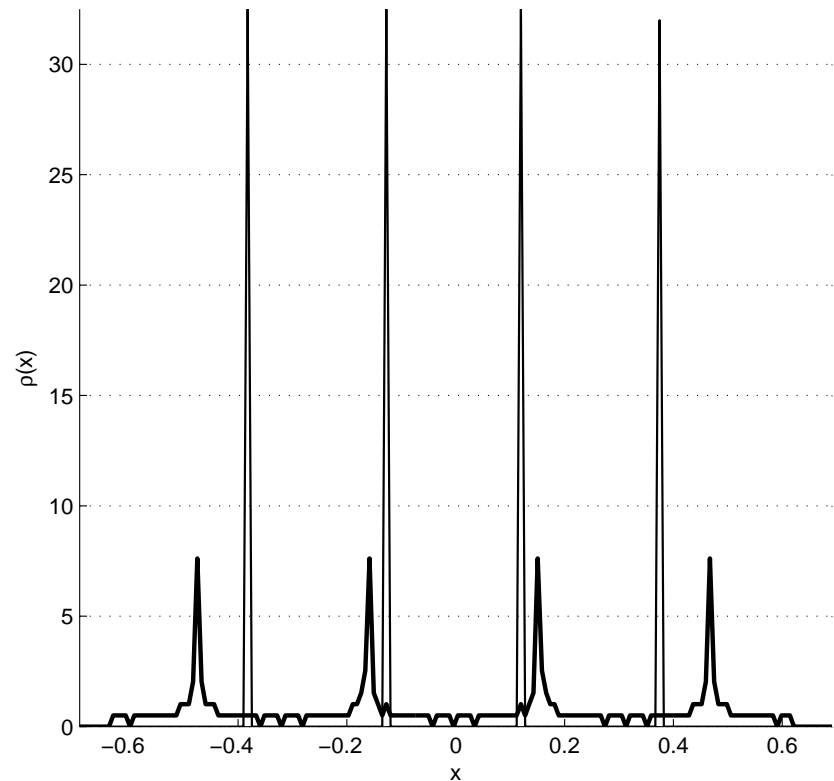
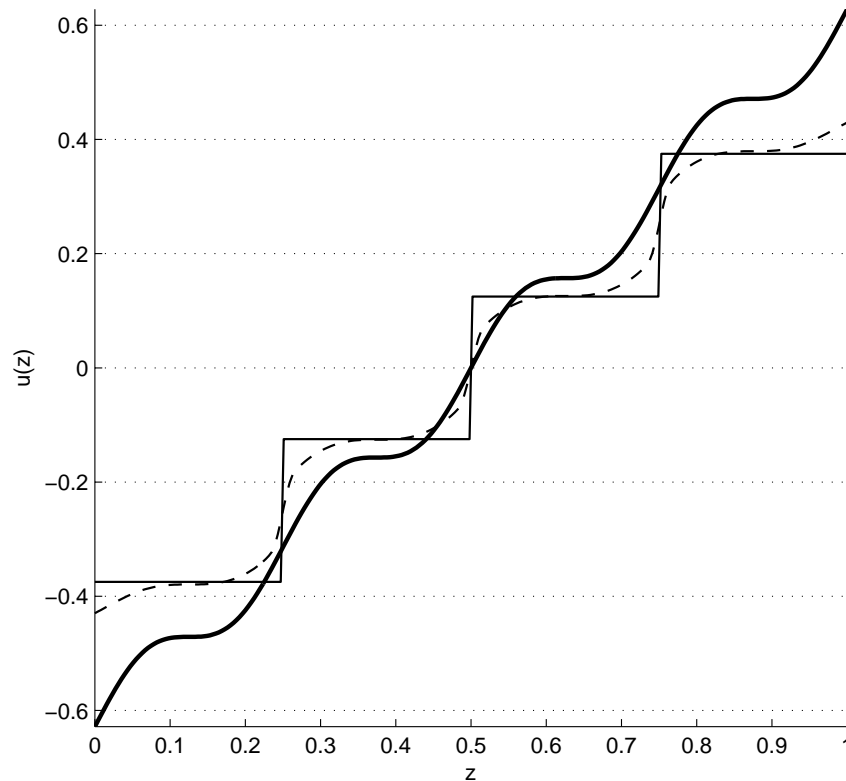
Weak repulsion: Four initial humps converge to two Diracs



Towards singular repulsion

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

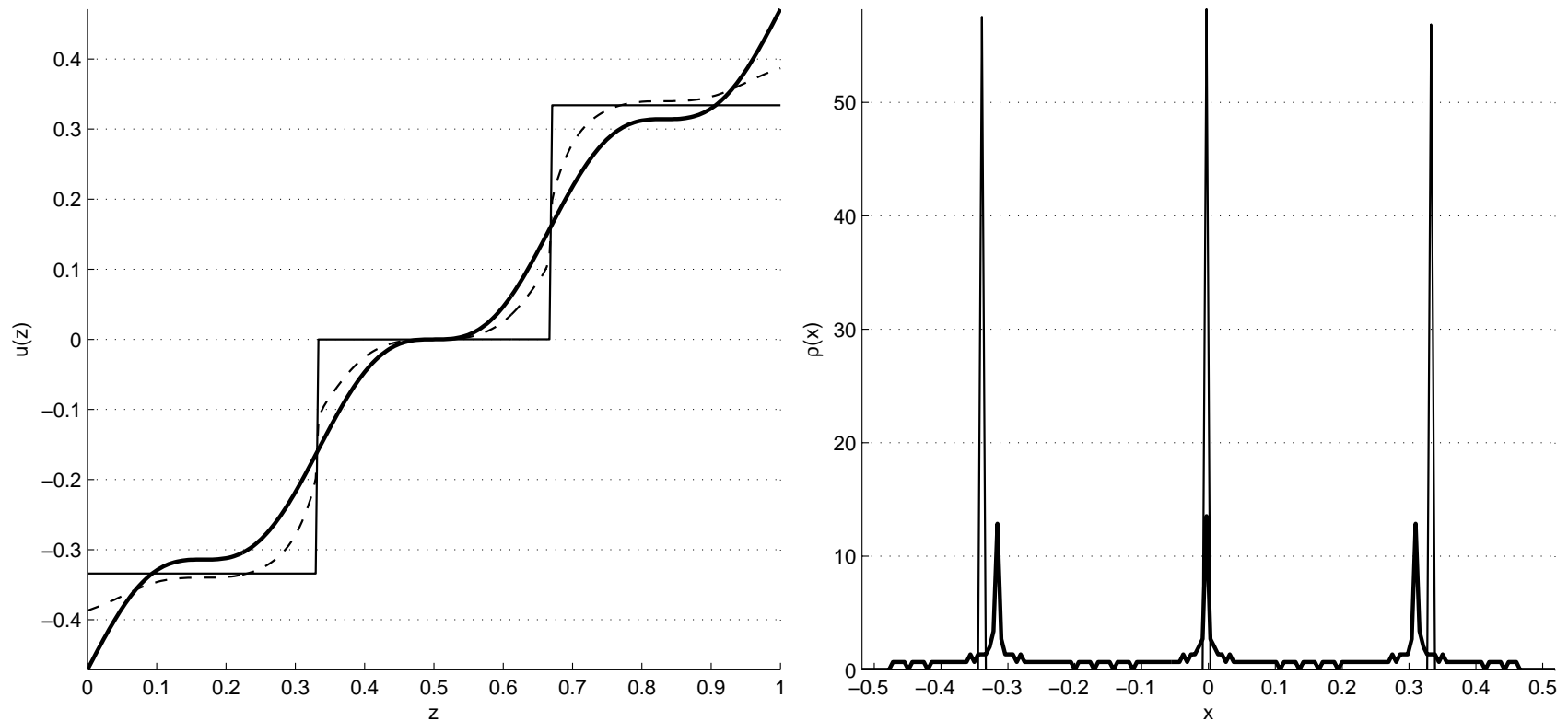
More repulsion: Four initial humps converge to four Diracs



Towards singular repulsion

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

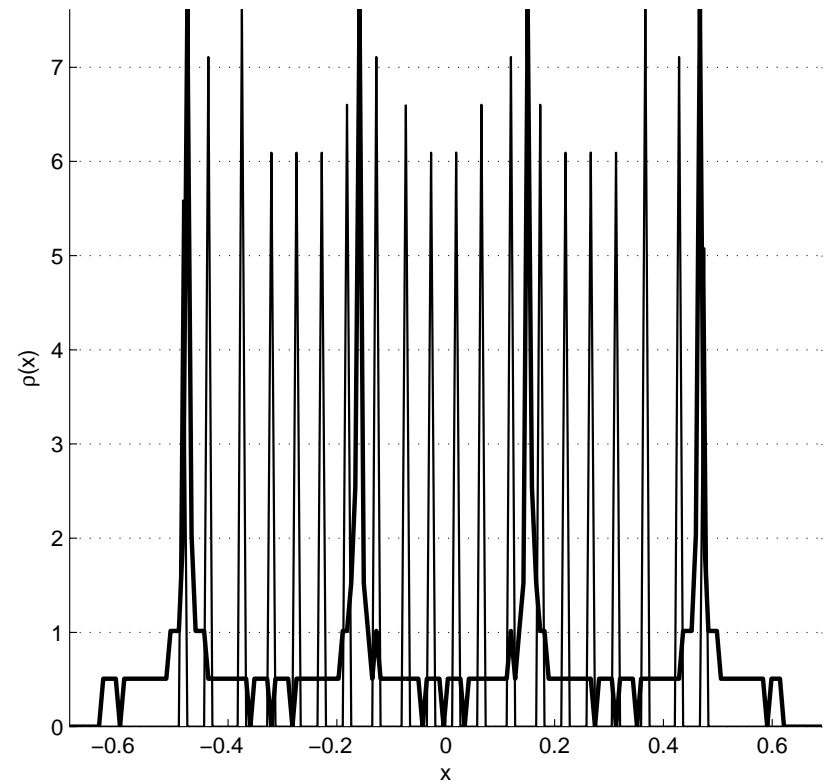
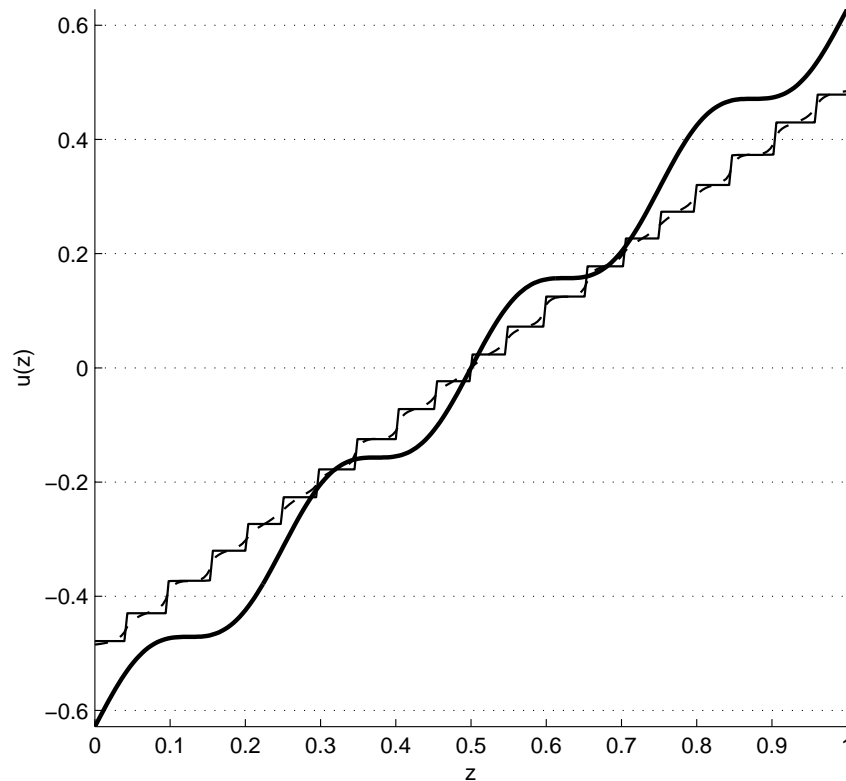
More repulsion: Three initial humps converge to three Diracs



Towards singular repulsion

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

Strong repulsion: Convergence to multiple Diracs



Singular interaction potential

An explicit example

formal: local repulsion \rightarrow Dirac \implies 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 $\text{supp}(\rho)$:

$$\begin{aligned} 0 &= W' * \rho = \int_{\mathbb{R}} 2(x - y) d\rho(y) - \int_{\mathbb{R}} \text{sign}(x - y) d\rho(y) \\ &= 2x - \int_{-\infty}^x d\rho(y) + \int_x^{-\infty} d\rho(y) = 2x + 1 - 2 \int_{-\infty}^x d\rho(y) \end{aligned}$$

Singular repulsion

Arbitrary many stable Diracs: an explicit example

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

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

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

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

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

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, $\varphi \in C$

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

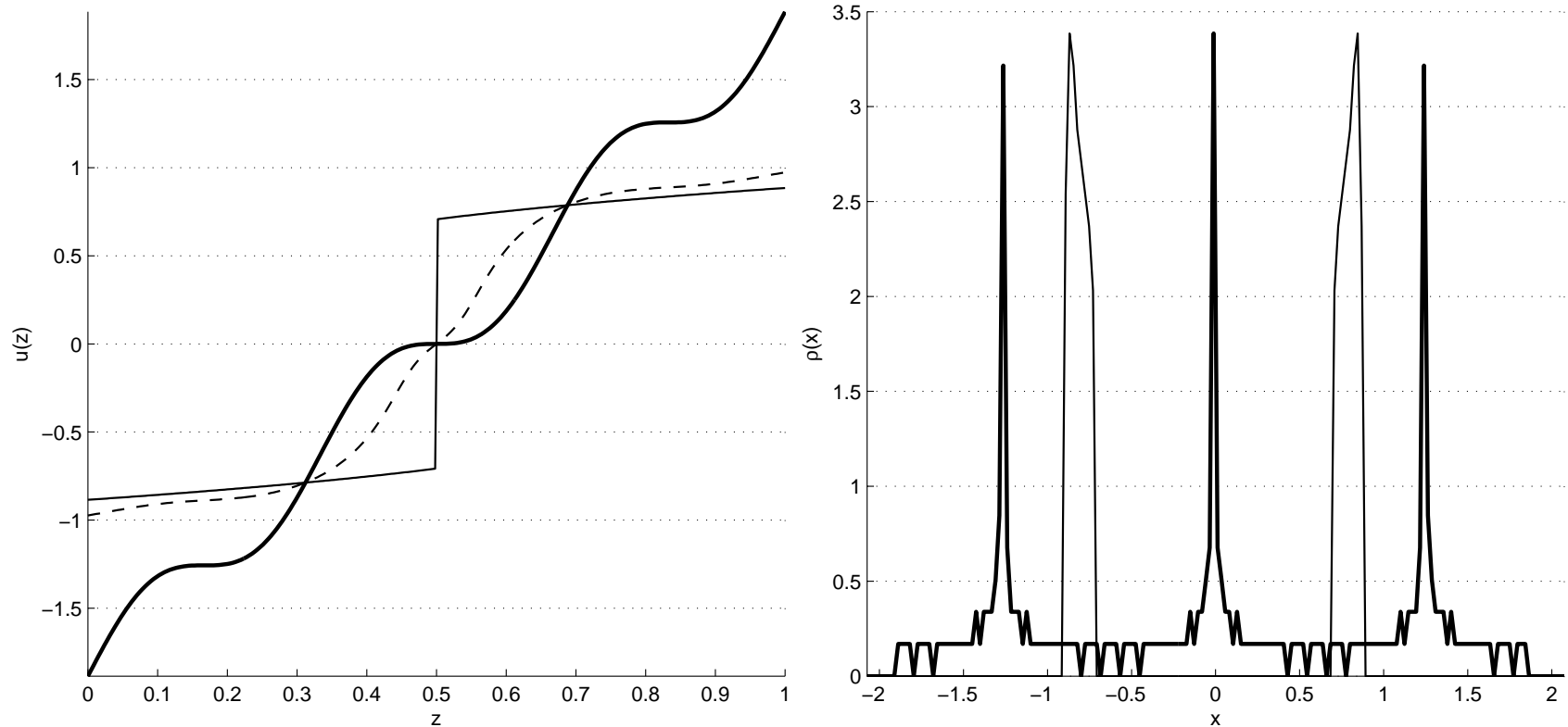
$$\begin{aligned}\int_{\mathbb{R}} \varphi(x) d\bar{\rho}(x) &= \sum_{i=1}^n \varphi(u_i) \rho_i = \sum_{i=1}^n \int_{u_i - \frac{\rho_i}{2}}^{u_i + \frac{\rho_i}{2}} \varphi(u_i) dx \\ &= \int_{u_1 - \frac{\rho_1}{2}}^{u_n + \frac{\rho_n}{2}} \sum_{i=1}^n \varphi(u_i) \mathbb{I}_{[u_i - \frac{\rho_i}{2}, u_i + \frac{\rho_i}{2}]} dx \\ &\rightarrow \int_{-\frac{1}{2}}^{\frac{1}{2}} \varphi(x) dx = \int_{\mathbb{R}} \mathbb{I}_{[-\frac{1}{2}, \frac{1}{2}]} \varphi(x) dx,\end{aligned}$$

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

Singular repulsion

Numerics: $W(x) = -|x|$ and $V(x) = x^4 - x^2$

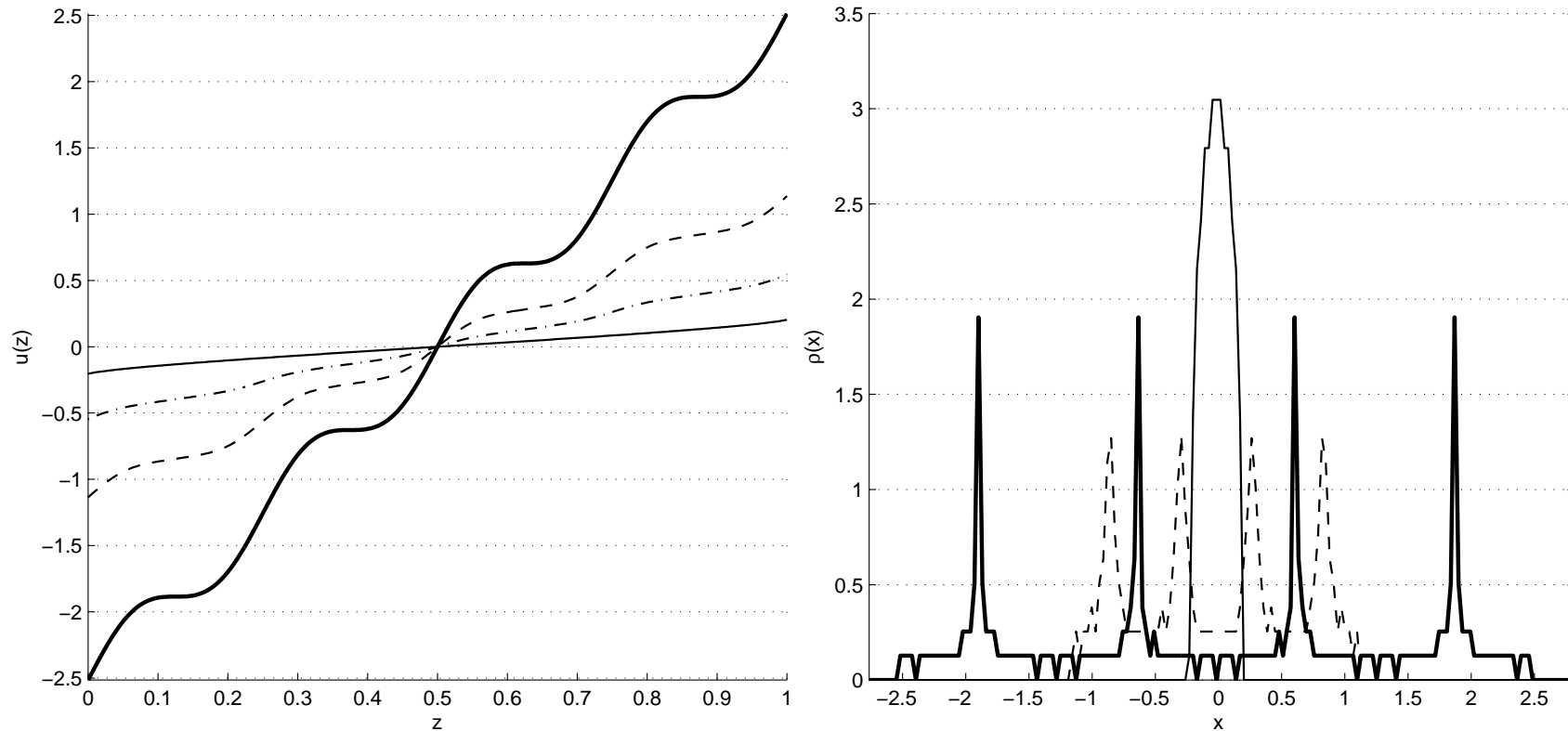
Double-well confinement \Rightarrow separate continuous parts



Singular repulsion

Numerics: $W(x) = x^2 - |x|^\alpha$ with $\alpha = 0.05$

Strong repulsion: Four initial humps converge to a lump

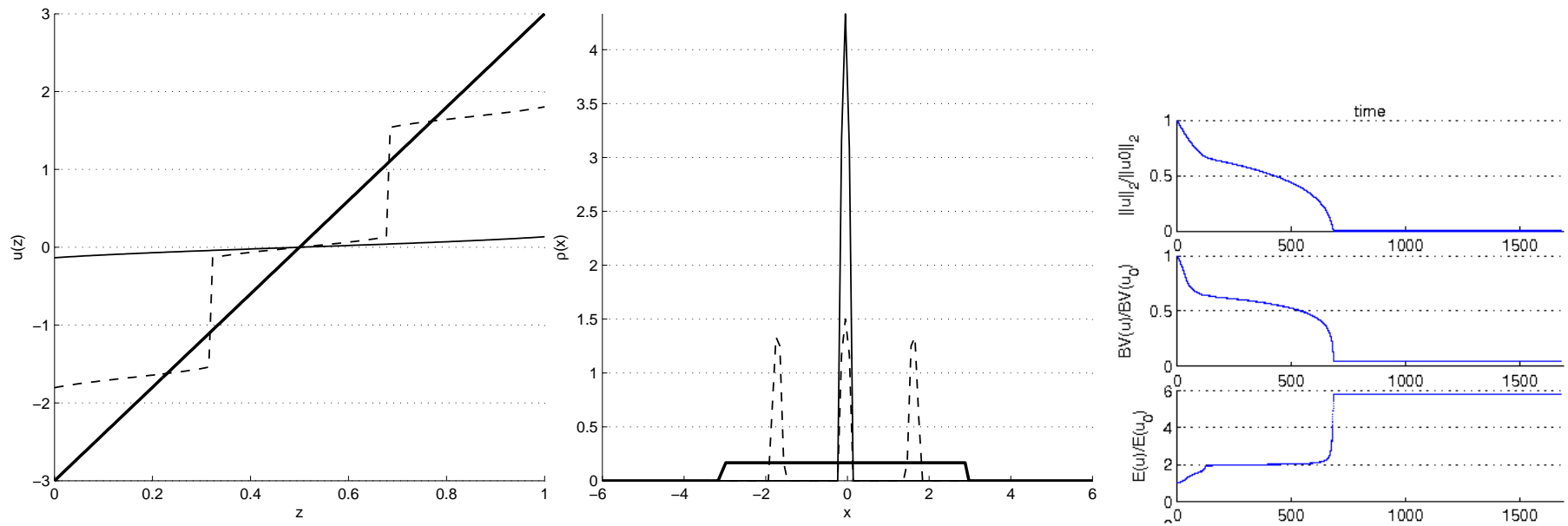


Morse potential

$$W_{F,L_1,L_2}(x) = -FL_1e^{-\frac{|x|}{L_1}} + L_2e^{-\frac{|x|}{L_2}} \text{ with } L_2 > L_1, 0 < F < 1$$

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

Single aggregate as (numerically) stable stationary state^a



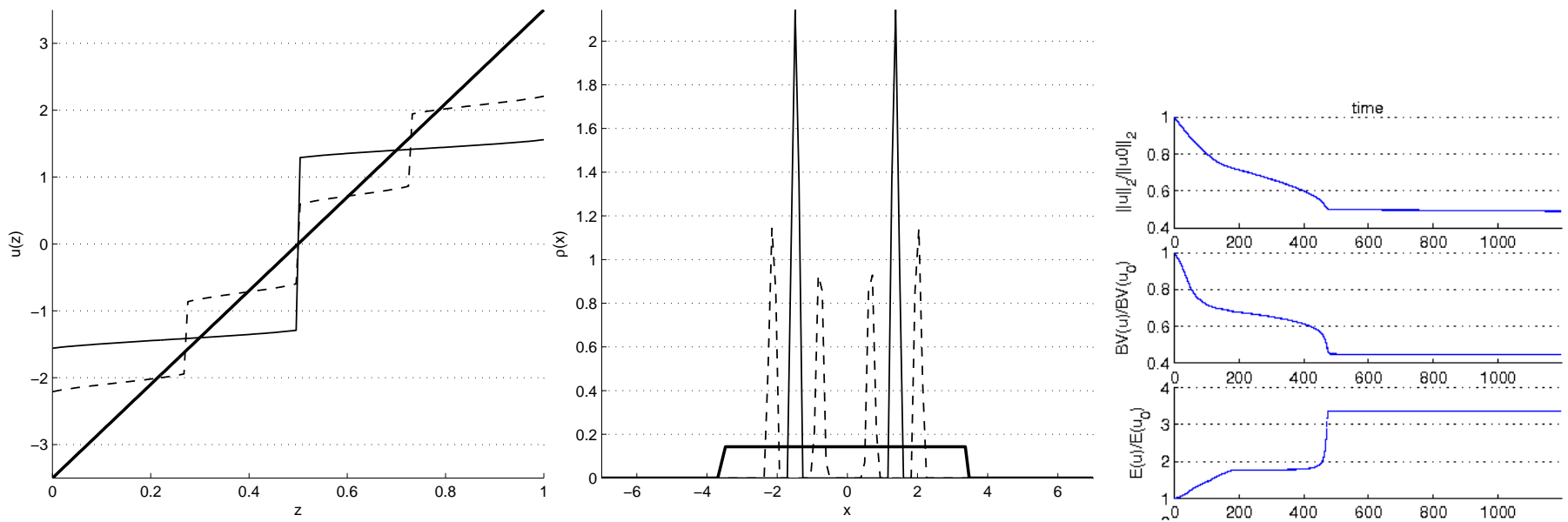
^aImplicit Newton-iteration scheme for $\partial_t u(z) = \int_0^1 W'(u(\zeta) - u(z)) d\zeta$

Morse potential

$$W_{F,L_1,L_2}(x) = -FL_1e^{-\frac{|x|}{L_1}} + L_2e^{-\frac{|x|}{L_2}} \text{ with } L_2 > L_1, 0 < F < 1$$

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

Two aggregates as (numerically) stable stationary state

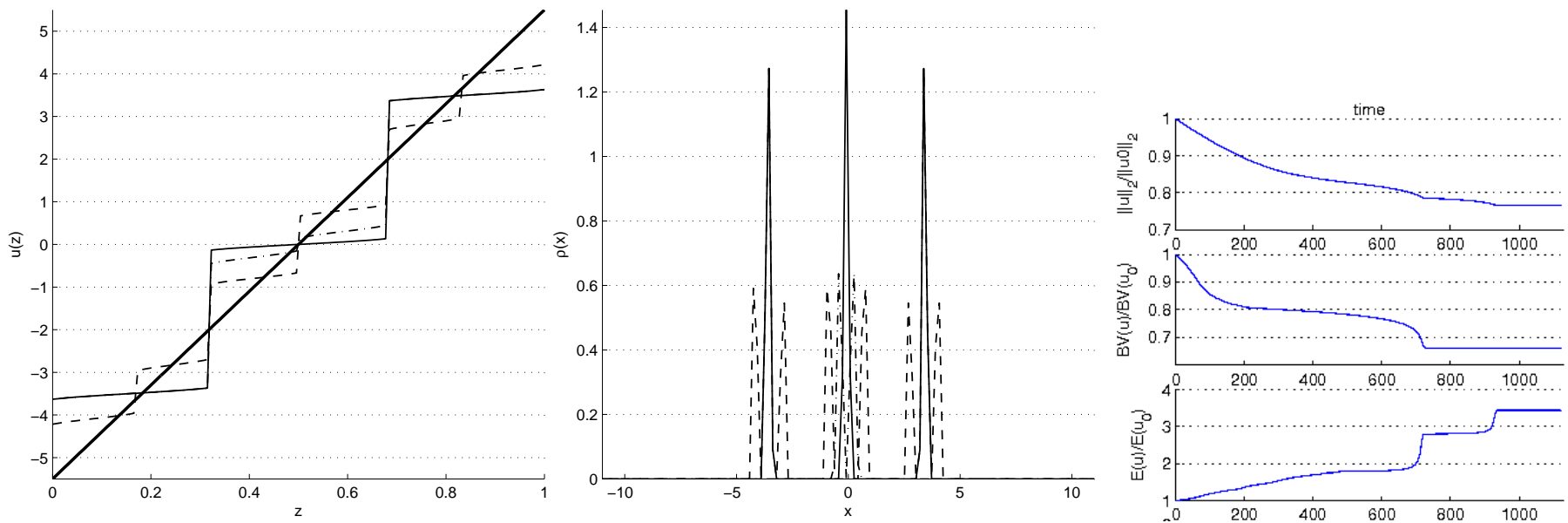


Morse potential

$$W_{F,L_1,L_2}(x) = -FL_1e^{-\frac{|x|}{L_1}} + L_2e^{-\frac{|x|}{L_2}} \text{ with } L_2 > L_1, 0 < F < 1$$

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

Three aggregates as (numerically) stable stationary state



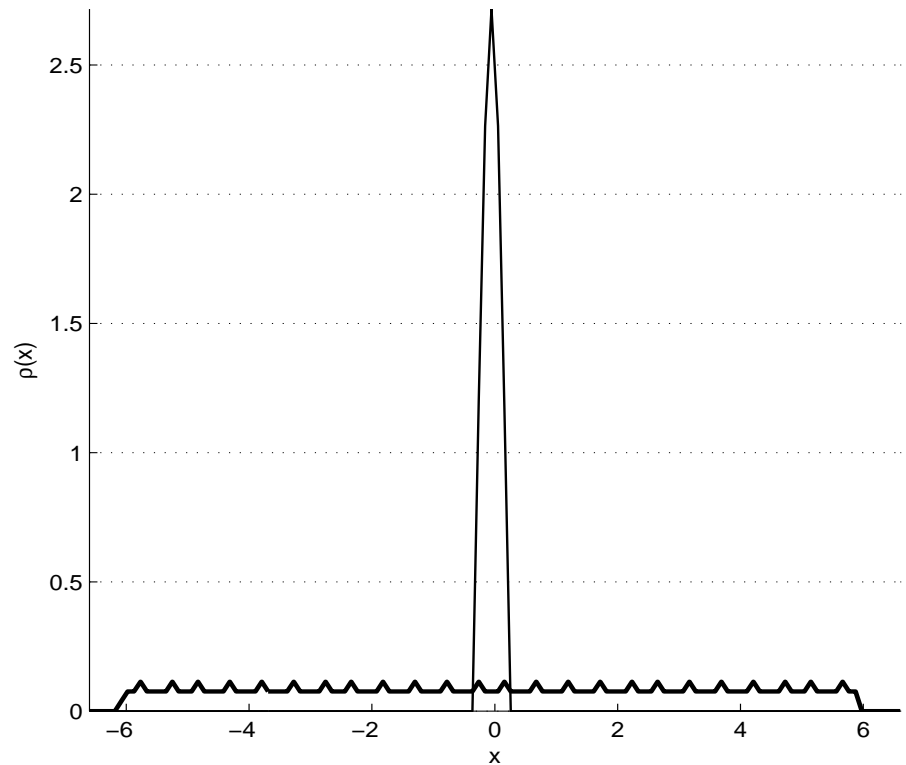
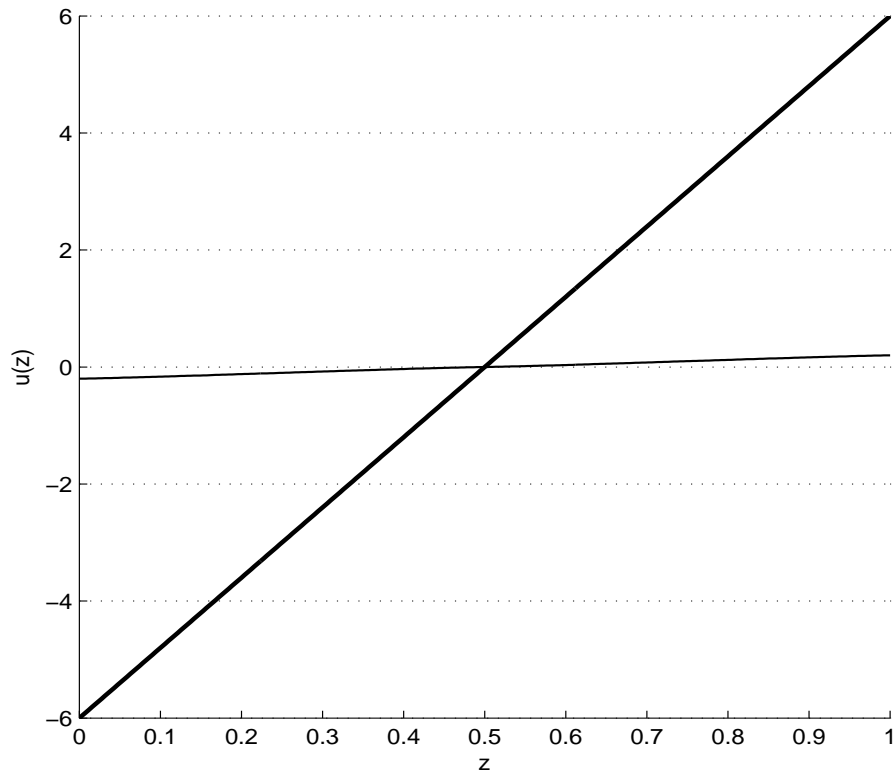
Slow-Fast dynamics similar to Keller-Segel^a

^a[Dolak, Schmeiser, 2005]

Doubly singular double-well

Numerics: $W_r(x) = -|x| \mathbb{I}_{|x| < r} + (|x| - 2r) \mathbb{I}_{|x| > r}$

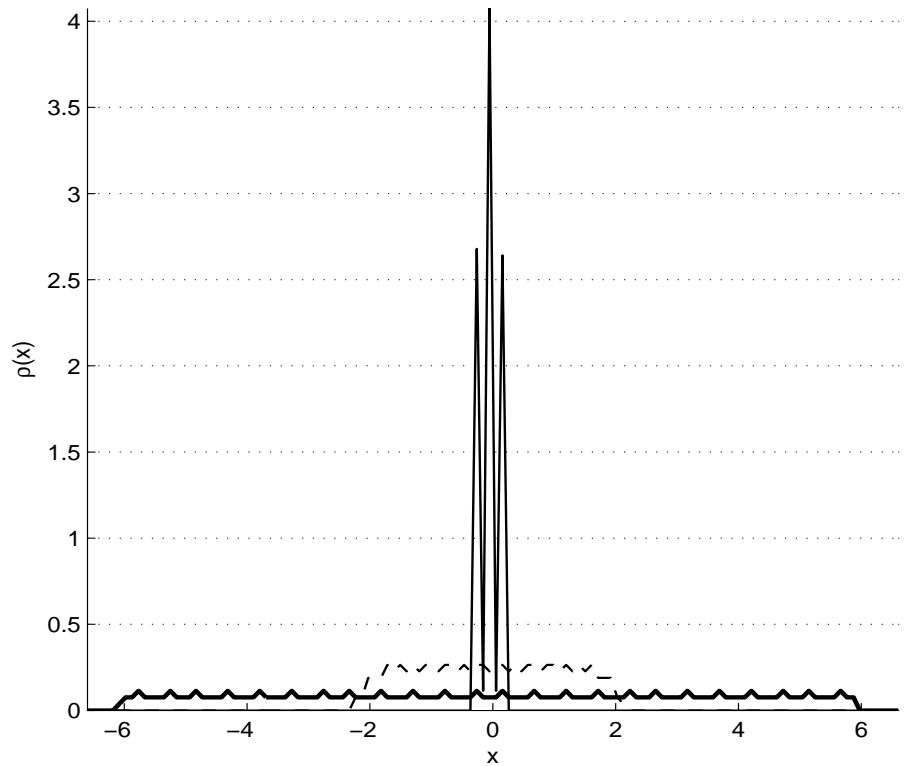
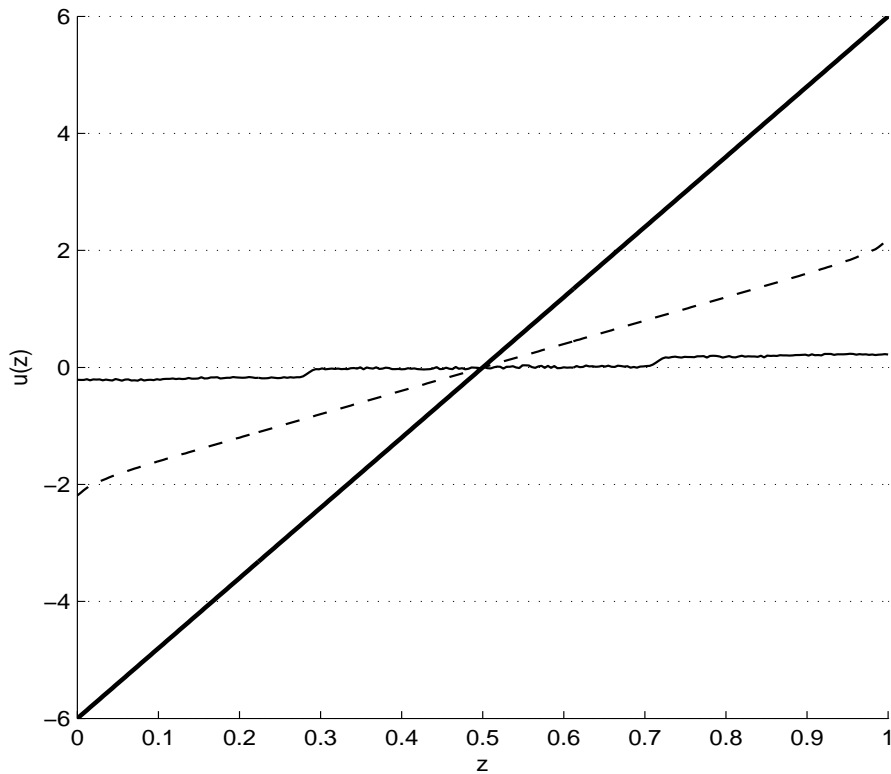
range of repulsion $r = 0.2$



Doubly singular double-well

Numerics: $W_{r,\lambda}(x) = -|x| \mathbb{I}_{|x|<r} + (\lambda|x| - r(\lambda + 1)) \mathbb{I}_{|x|>r}$

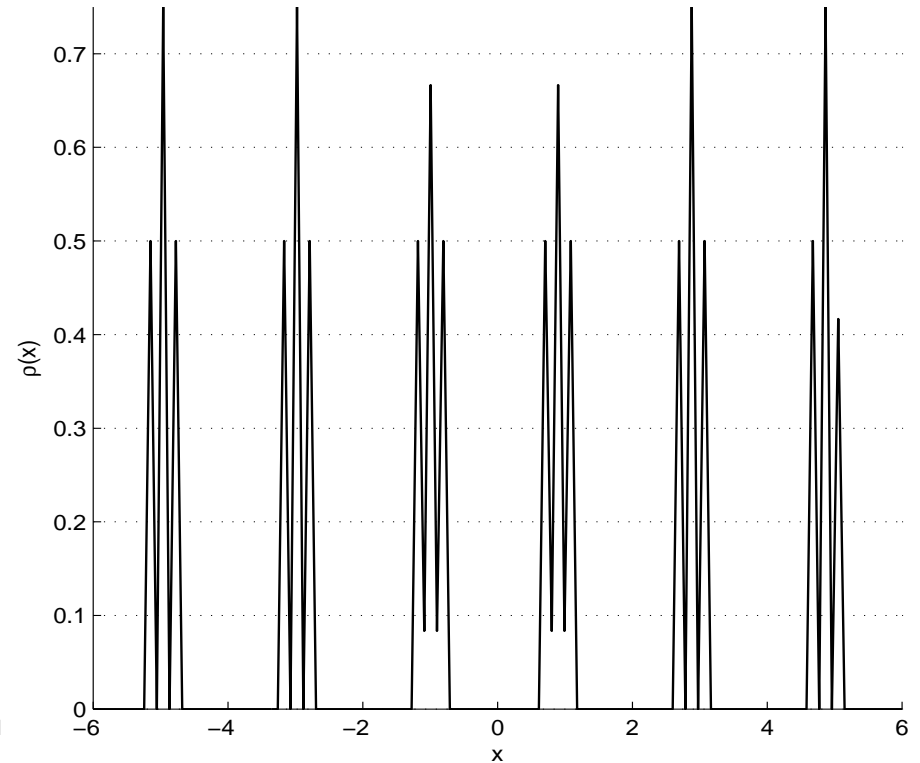
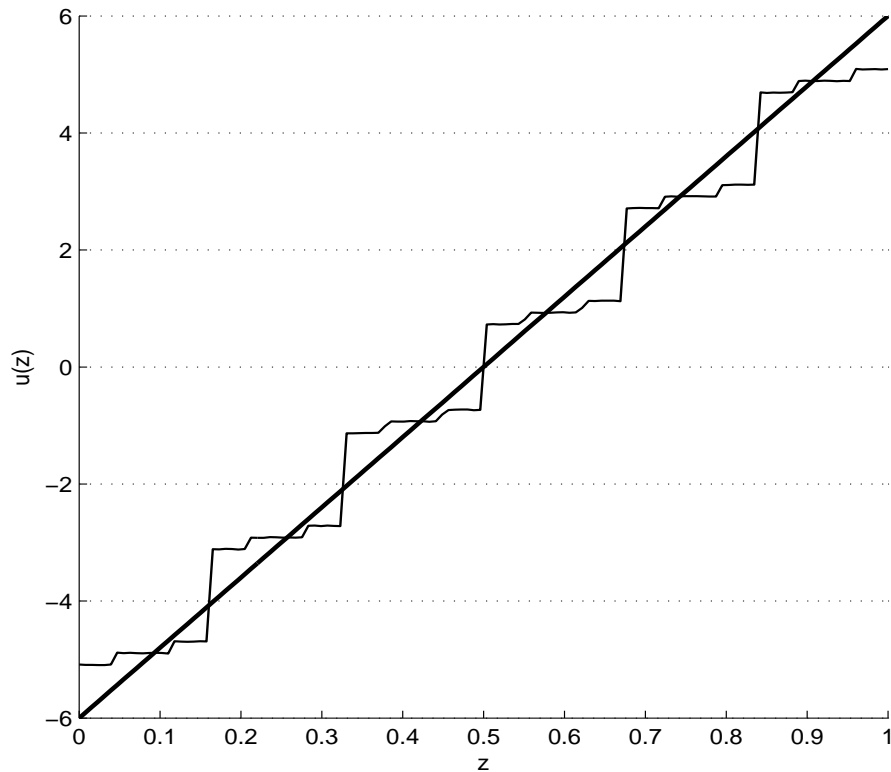
$r = 0.2$, dominating repulsion $\lambda = 0.5$



Doubly singular double-well

Numerics: $W_{r,c,\lambda}(x) = -|x| \mathbb{I}_{|x| < r} + (\lambda|x| - r(\lambda + 1)) \mathbb{I}_{r < |x| < c}$

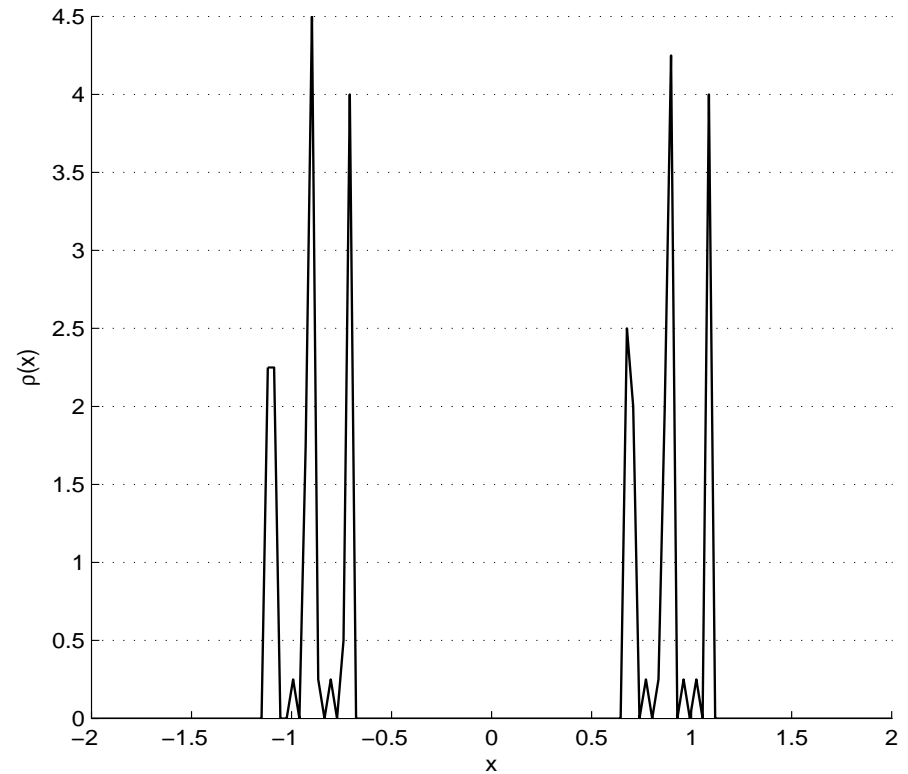
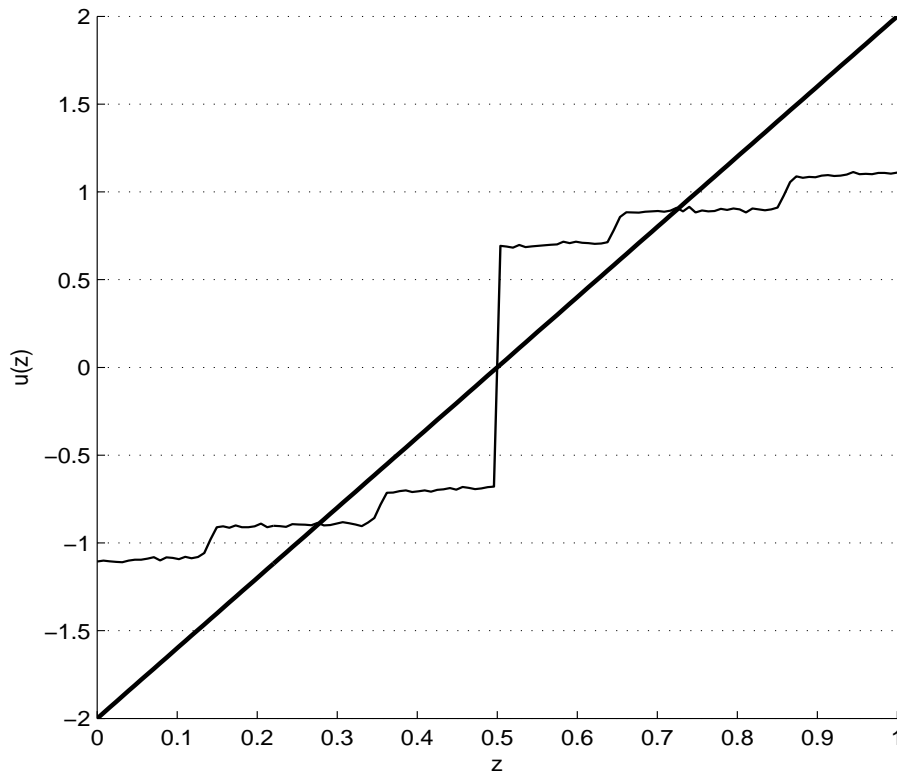
Cut-off at $c = 0.8$, $r = 0.2$, dominating repulsion $\lambda = 0.5$



Doubly singular double-well

Numerics: $W_{r,c,\lambda}(x) = -|x| \mathbb{I}_{|x|<r} + (\lambda|x| - r(\lambda + 1)) \mathbb{I}_{|x|>r}$

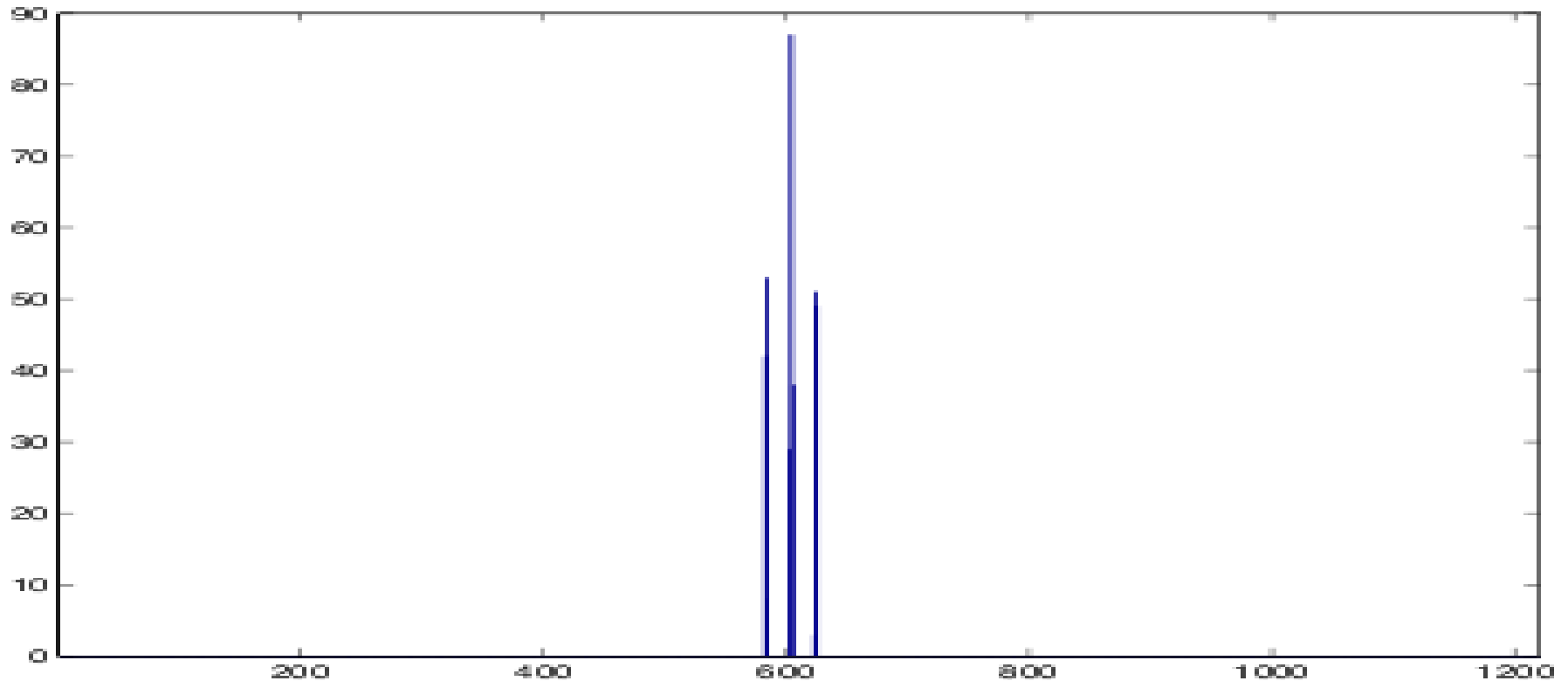
Three times smaller initial support, $r = 0.2$, $c = 0.8$, $\lambda = 0.5$



Doubly singular double-well

Numerics: $W_{r,\lambda}(i) = -|i| \mathbb{I}_{|i| < r} + (\lambda|i| - r(\lambda + 1)) \mathbb{I}_{|i| > r}$

lattice walk of randomly chosen agents $r = 20, \lambda = 0.5^a$

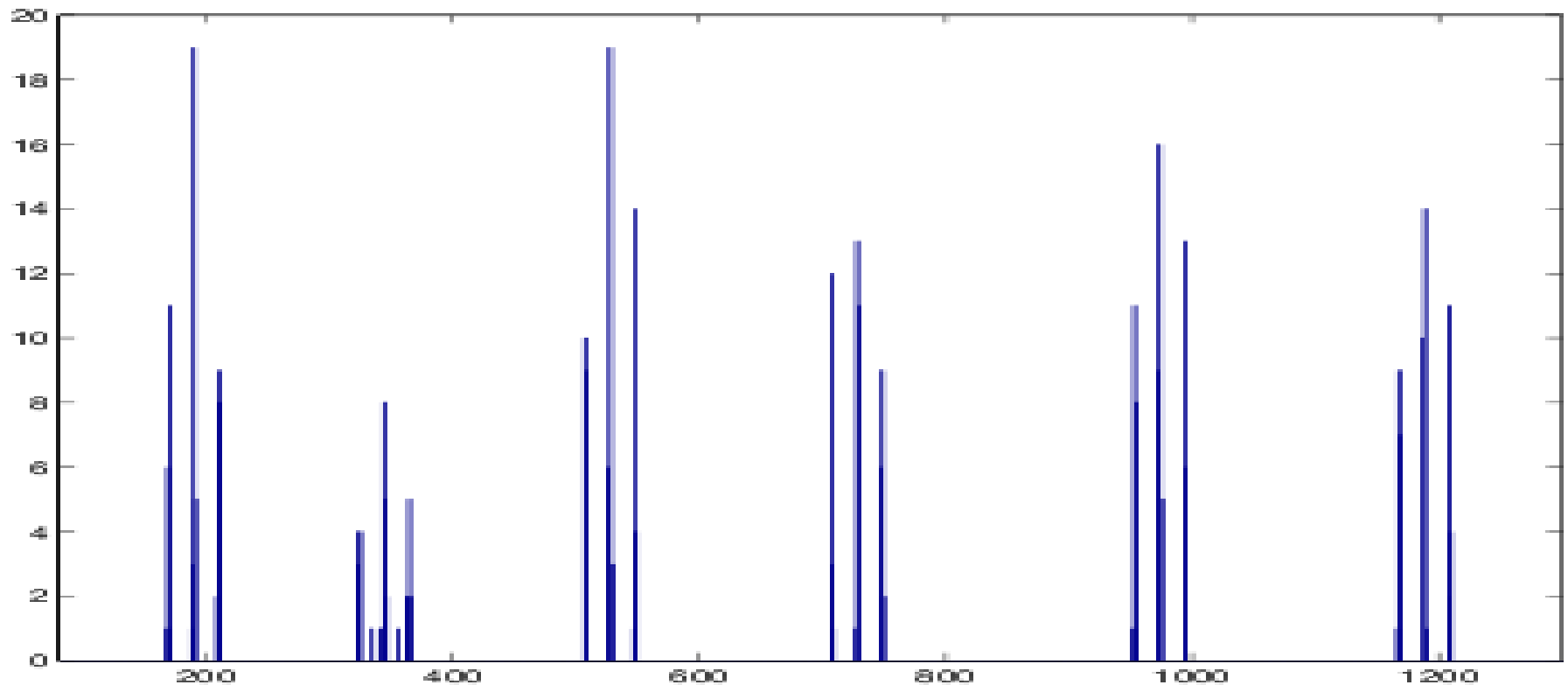


^awith E. Hackett-Jones, B. Hughes, K. Landman: University of Melbourne

Doubly singular double-well

Numerics: $W_{r,c,\lambda}(i) = -|i| \mathbb{I}_{|i| < r} + (\lambda|i| - r(\lambda + 1)) \mathbb{I}_{r < |i| < c}$

Cut-off at $c = 80$, $r = 20$, dominating repulsion $\lambda = 0.5^a$

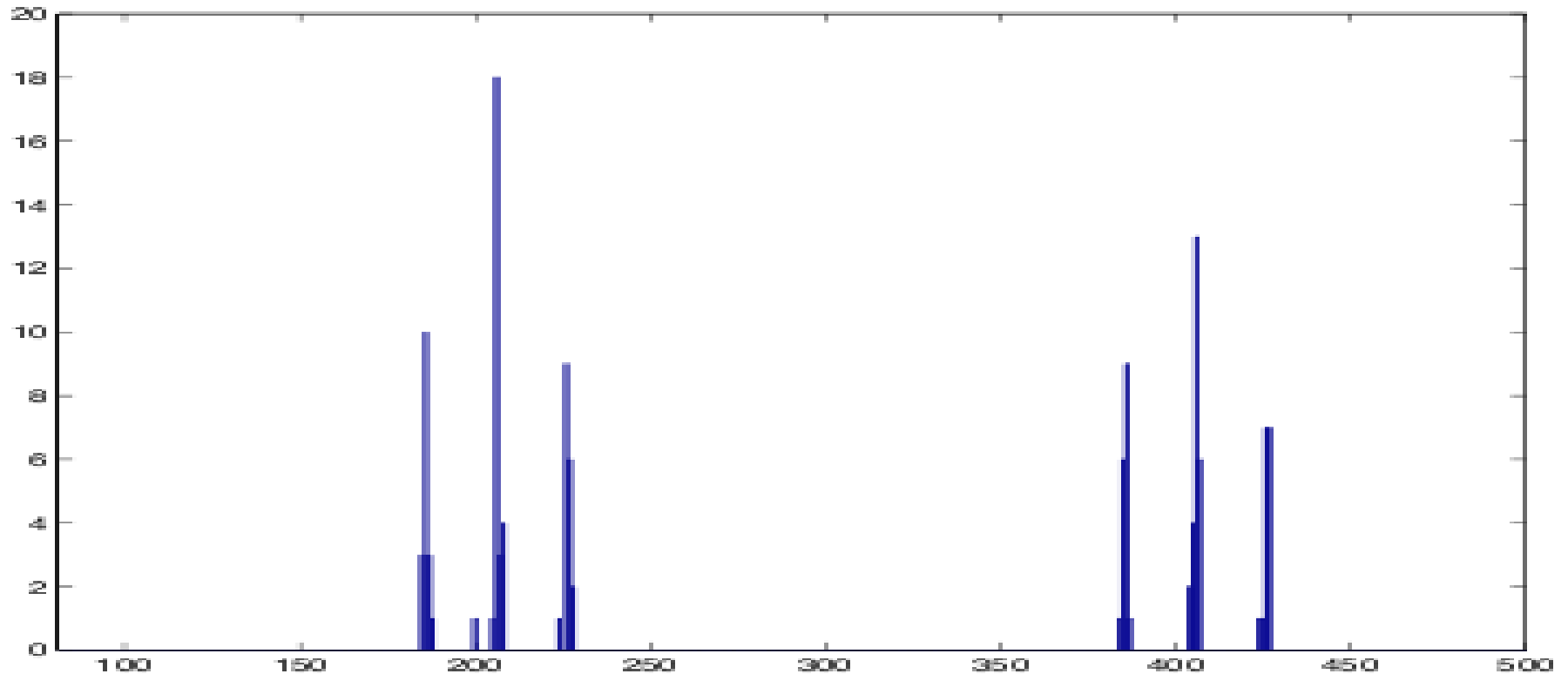


^awith E. Hackett-Jones, B. Hughes, K. Landman: University of Melbourne

Doubly singular double-well

Numerics: $W_{r,c,\lambda}(i) = -|i| \mathbb{I}_{|i|<r} + (\lambda|i| - r(\lambda + 1)) \mathbb{I}_{|i|>r}$

Three times smaller initial support, $r = 20$, $c = 80$, $\lambda = 0.5^a$



^awith E. Hackett-Jones, B. Hughes, K. Landman: University of Melbourne

Stability for singular attraction

Local non-linear stability for singular attractive potentials

$$\tilde{W}(x) := W(x) - W'(0^+) |x| \in C^{2,\alpha}(\mathbb{R}), \quad V \in C^{2,\alpha}(\mathbb{R})$$

singular attractive: $W'(0^+) > 0$,

stationary state $\bar{u}(z) = \sum_{i=1}^n u_i \mathbb{1}_{I_i}$, linear stable w.r.t. **shifts**:

$$M_{ij} := \begin{cases} \rho_i W''(u_j - u_i), & \text{if } i \neq j, \\ -\sum_{k \neq i} \rho_k W''(u_k - u_i) - V''(u_i), & \text{if } i = j. \end{cases}$$

has a strictly positive spectrum

iff $V = 0$ the on the hyperspace $\{(w_i)_{i=1,\dots,n} : \sum_{i=1}^n w_i = 0\}$.

Then, $\|u_{in} - \bar{u}\|_\infty \leq \varepsilon \Rightarrow \|u(t, \cdot) - \bar{u}\|_\infty \leq C(1 + t^{n-1}) e^{-\nu t}$.

Stability for singular repulsion

Local non-linear stability for singular repulsive potentials

$W(x) - W'(0^+)|x| \in C^{2,\alpha}(\mathbb{R})$, $V \in C^{2,\alpha}(\mathbb{R})$, $\rho_{in} \in W^{2,\infty}(\mathbb{R})$

singular repulsive: $W'(0^+) < 0$

stationary state $\bar{u}(z) = \sum_{i=1}^n u_i \mathbb{1}_{I_i}$,

- $V'' > C > 0$ and $W|_{(0,\infty)}$ is convex,
- or $V = 0$ and $W''|_{(0,\infty)} > C > 0$.

Then, there exists a unique (up to a shift in x if $V = 0$)

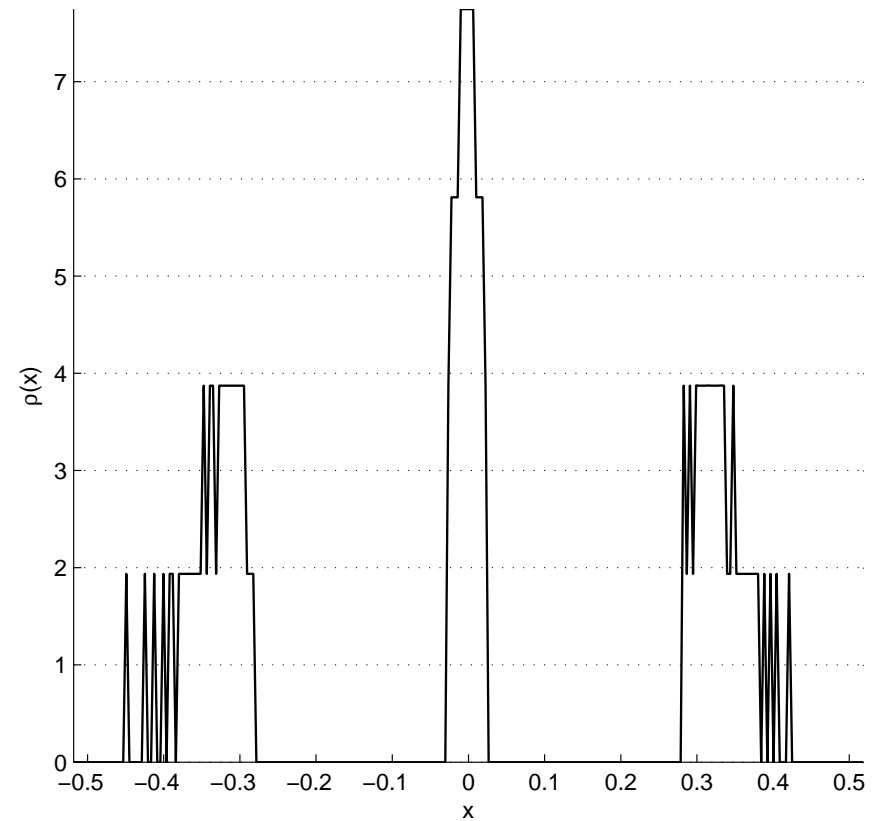
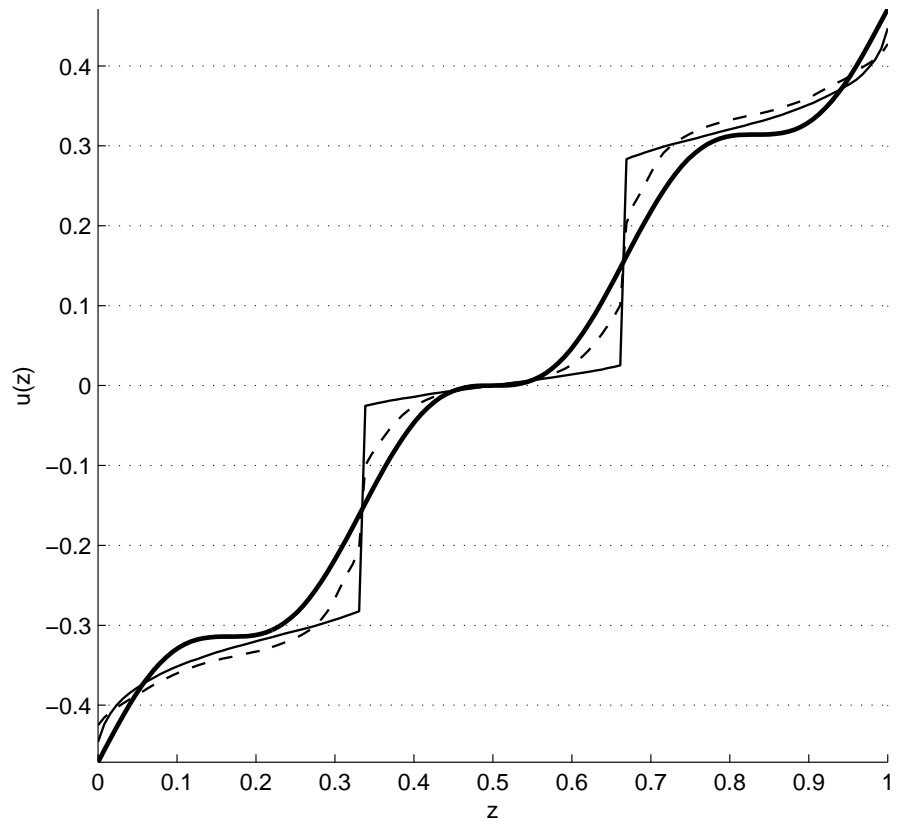
stationary state $\bar{\rho} \in L^1 \cap L^\infty(\mathbb{R})$

$$W_\infty(\rho(t, \cdot), \bar{\rho}) = \|u(t, \cdot) - \bar{u}\|_\infty \rightarrow 0.$$

Non-local Stochastic Models

Non-uniqueness of aggregates

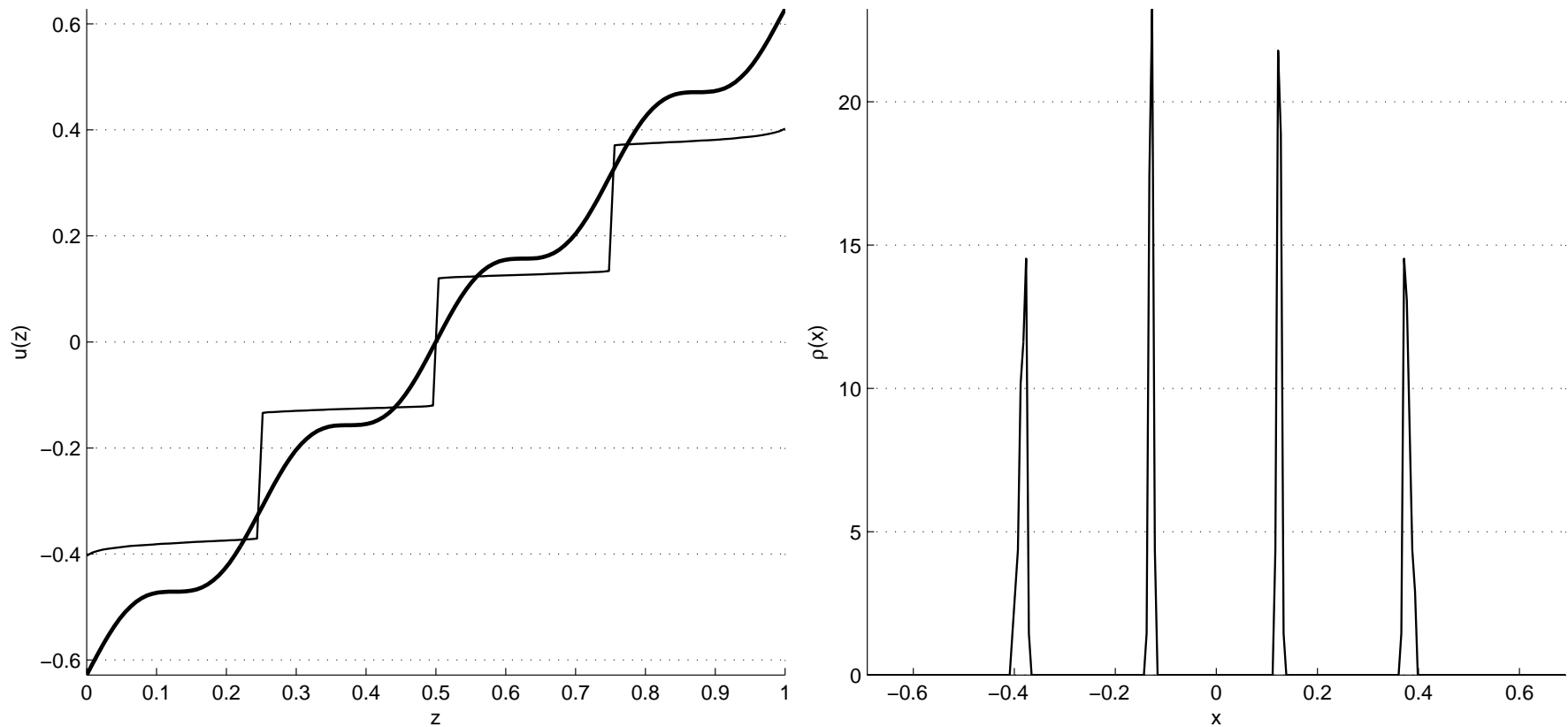
Double-well potential, Gaussian random walk “diffusion”
initial data with three smoothed aggregates



Non-local Stochastic Models

Non-uniqueness of aggregates

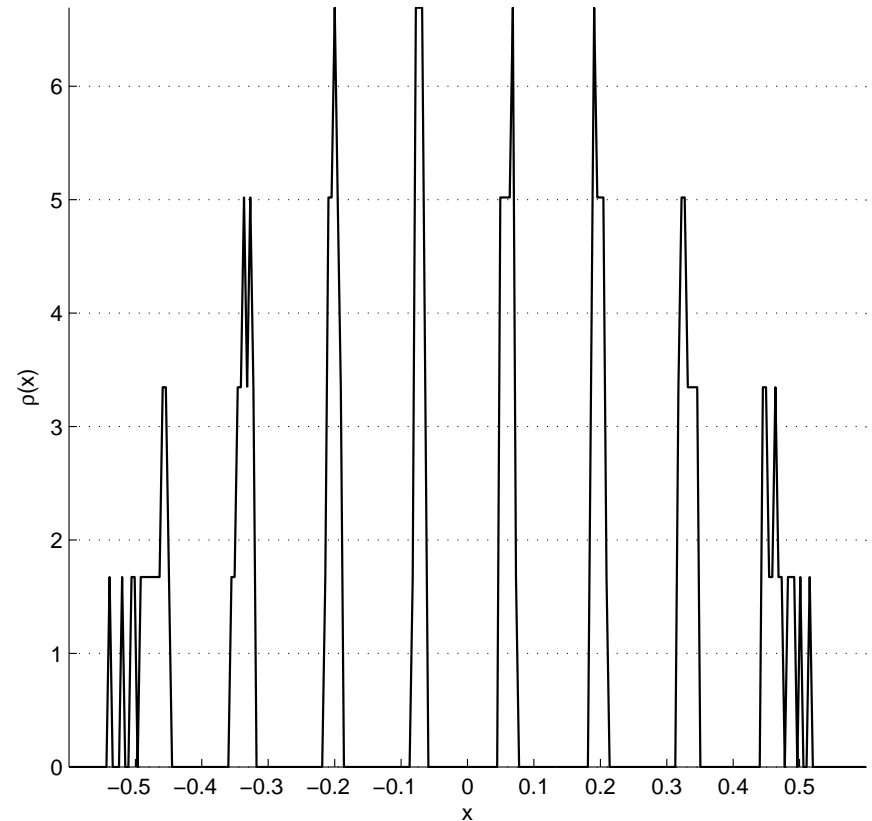
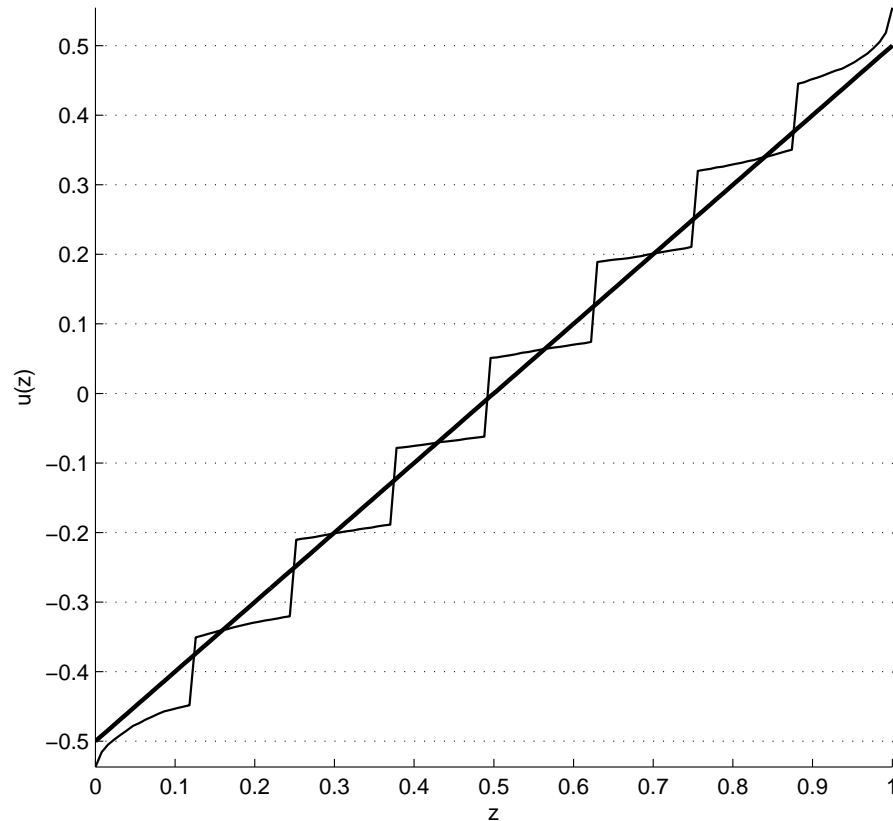
Same double-well potential, same random walk “diffusion”
initial data with four smoothed aggregates



Non-local Stochastic Models

Increasing variance of random walk

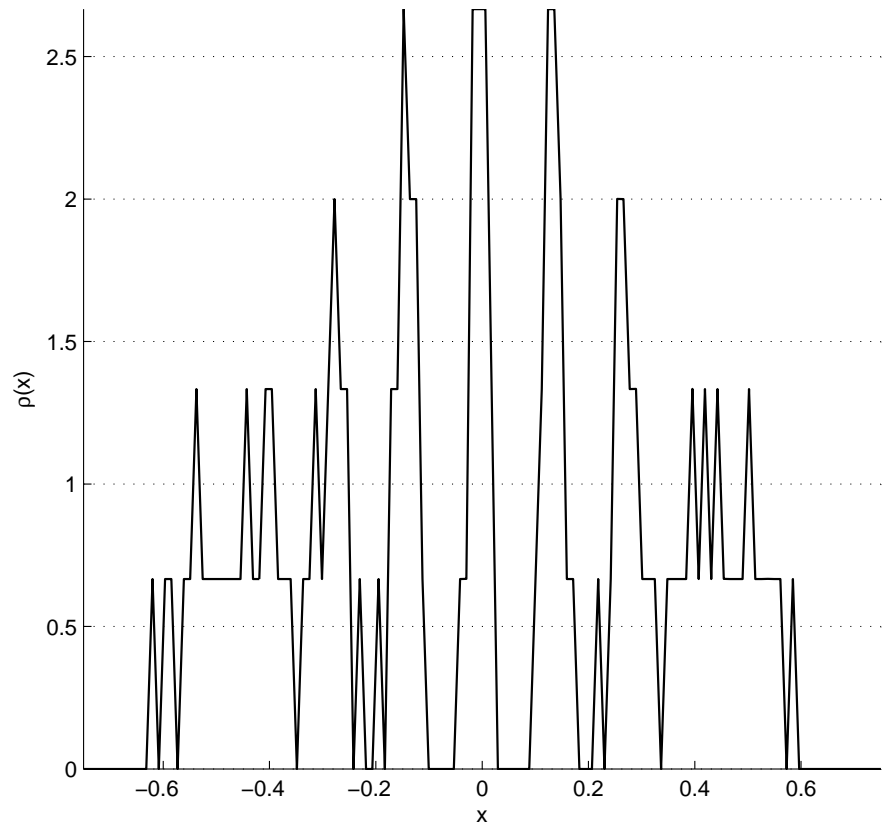
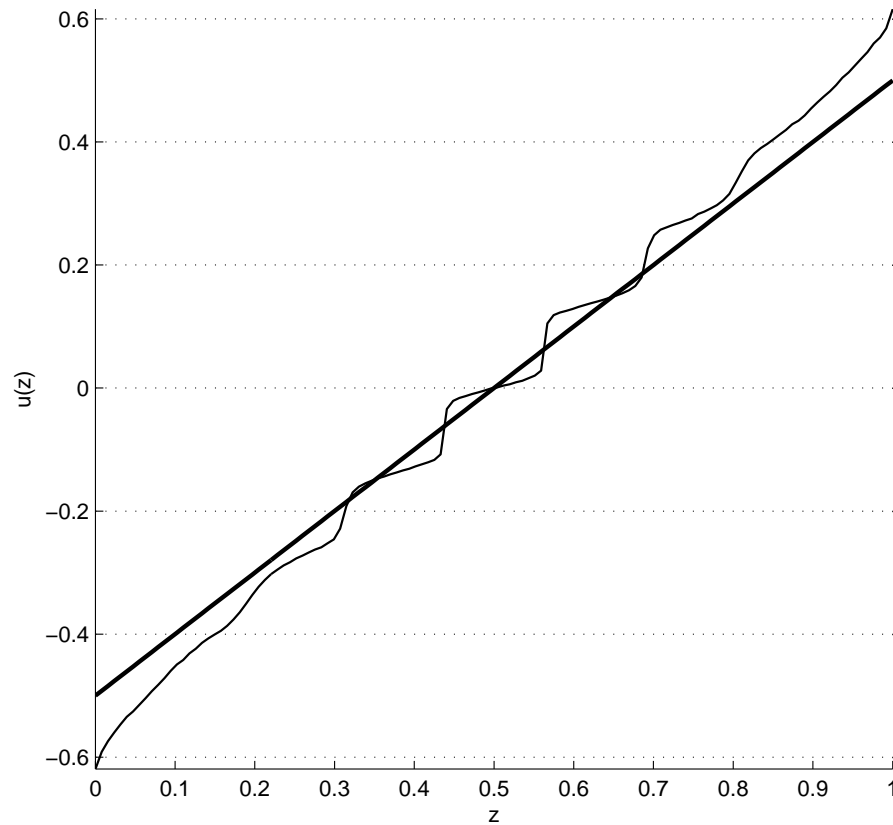
Low variance: 8 aggregates



Non-local Stochastic Models

Increasing variance of random walk

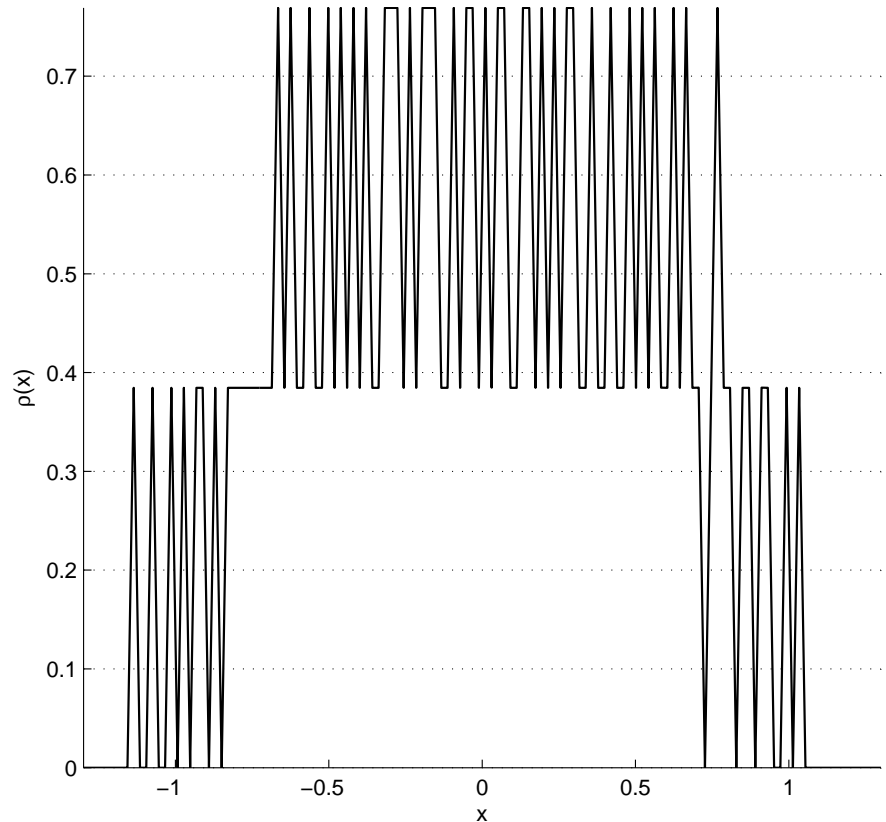
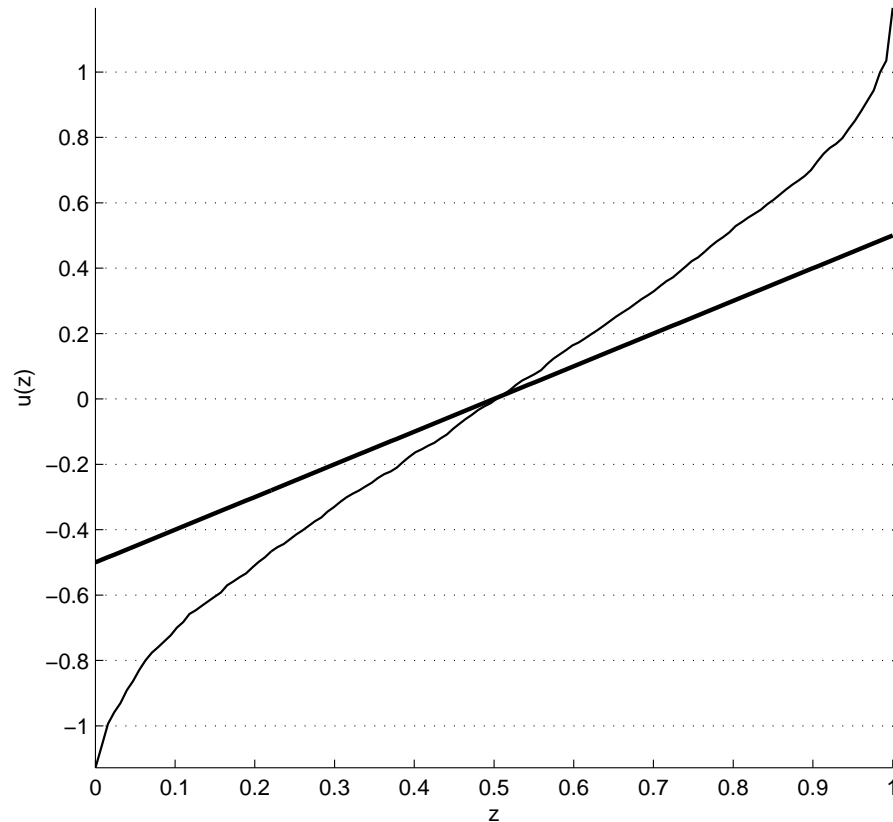
Medium variance: **about 7 aggregates**



Non-local Stochastic Models

Increasing variance of random walk

High variance: 1 aggregate



Non-local interaction equations

Conclusions

- double-well does NOT imply that only two Dirac steady state are stable
- singular repulsion of interaction potential at 0 has smoothing effect

K.F., G. Raoul, Stable stationary states of non-local interaction equation, to appear in M3AS.

K.F., G. Raoul, Stability of stationary states of non-local equations with singular interaction potentials, to appear in MCM

Non-local Stochastic Models

THANK YOU!