Breakdown of the mean-field description of interacting particle systems

Phase transitions, metastability and coarsening

Minicourse – Particle Systems and PDEs XIV – Toulouse

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joint with José Carrillo, Nicolai Gerber, Rishabh Gvalani, Martin Hairer, Greg Pavliotis, Anna Shalova

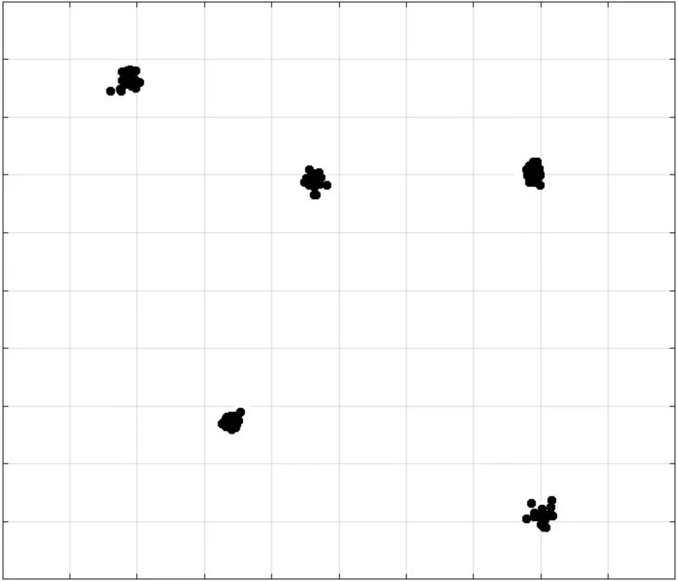
Institute for Applied Analysis

Toulouse 2026

Motivation

Consider

- *weakly* interacting *diffusions* on a periodic domain
- with *locally attractive interaction potential*



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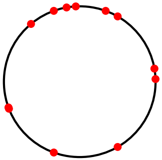
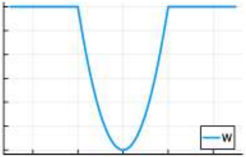


Particles on 1-dim torus



Interaction potential

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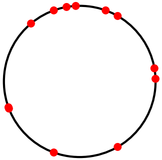

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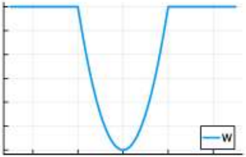

Interaction potential

On one-dimensional torus $\mathbb{T} \cong \mathbb{R}/\mathbb{Z} \cong [0,1]$, consider

interaction strength

$$\mathrm{d}X_t^i = -\frac{\gamma}{N}\sum_{j=1}^{N} \nabla w\left(\frac{X_t^i - X_t^j}{\ell}\right)dt + \sqrt{2}\,\mathrm{d}B_t^i, \qquad \text{for } i = 1,\dots,N$$

interaction range

- the *interaction potential* $w : \mathbb{R} \to \mathbb{R}$ is given by $w(x) = \begin{cases} \frac{1}{2}(x^2-1) & \text{if } |x| \le 1 \\ 0 & \text{if } |x| > 1, \end{cases}$
- $B_t^1, \dots, B_t^N$ are independent standard Brownian motions in $\mathbb{R}$.

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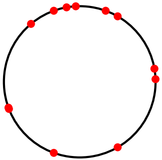

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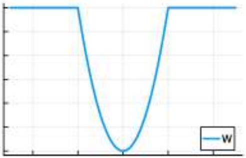

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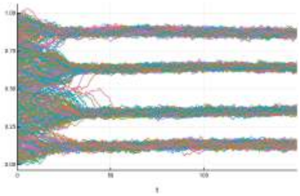

Clustering

On one-dimensional torus $\mathbb{T} \cong \mathbb{R}/\mathbb{Z} \cong [0,1]$, consider

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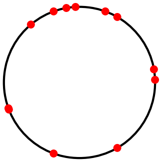

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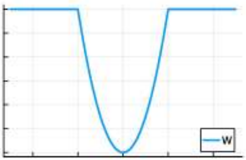

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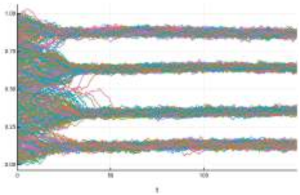

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- The *interaction potential* $w : \mathbb{R} \to (-\infty, 0]$ satisfies:
  - w is *even* and *non-decreasing* on $[0, \infty)$.
  - $\operatorname{supp} w = [-s_w, s_w]$ for some $s_w > 0$;
  - w is C^2 on its support, $w''(0) > 0$, depth $\Delta_w = -w(0)$;

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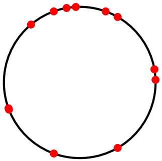

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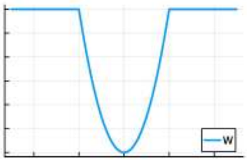

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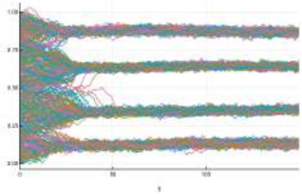

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Our regime: strong ($\gamma \gg 1$) and localized ($\ell \ll 1$) interaction

What is the (expected) behaviour as $N \to \infty$?

As $N \to \infty$, the microscopic model

$$\mathrm{d}X_t^i = -(\nabla W_{\gamma,\ell} * \mu_t^N)(X_t^i)\,\mathrm{d}t + \sqrt{2}\,\mathrm{d}B_t^i\,, \qquad \mu_t^N := \frac{1}{N}\sum_{j=1}^N \delta_{X_t^j}, \qquad W_{\gamma,\ell}(x) = \gamma\ell w\Big(\frac{x}{\ell}\Big)$$

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becomes the *mean-field* McKean-Vlasov *SDE*

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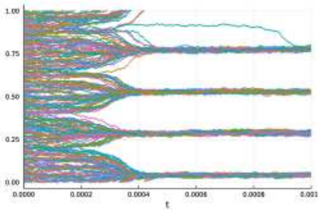
with *free energy dissipation:*

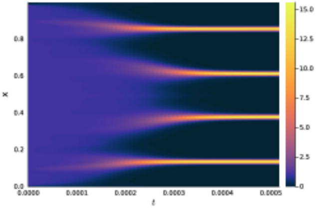
$$\frac{\mathrm{d}}{\mathrm{d}t}\mathcal{F}_{\gamma,\ell}(\rho_t) = -\int_{[0,1]} \big|\nabla(\log\rho_t + W_{\gamma,\ell} * \rho_t)\big|^2 \rho_t\,\mathrm{d}x \le 0.$$

Outline of effects for $\gamma \gg 1$ and $\ell \ll 1$

Effect I: Initial clustering

- Heuristics by (Garnier, Papanicolaou, and Yang 2017)





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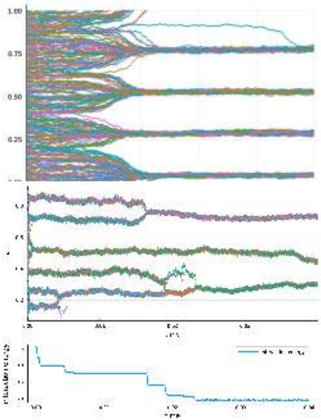
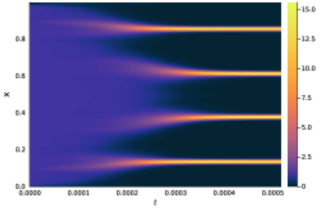
- Cluster centers behave like *coalescing heavy Brownian motions*
- Timescale of order N





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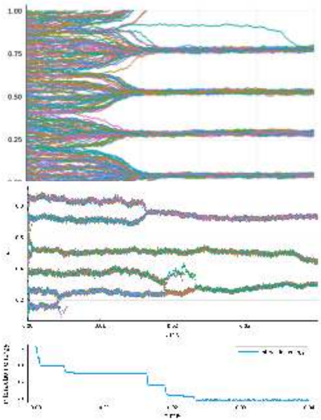

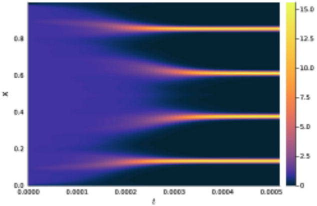

not present in the PDE, clusters cannot move

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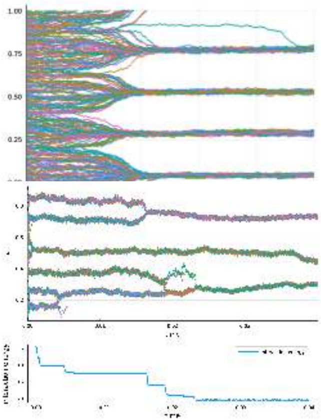

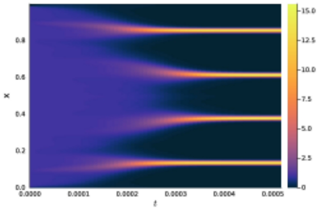

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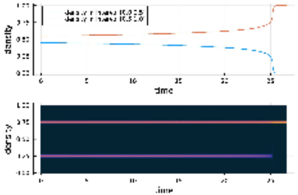

Effect III: Mass exchange

- Timescale $e^{\gamma \ell \Delta_w m}$ for clusters of mass $m \in (0,1)$
- Dynamic metastability (Otto and Reznikoff 2007)

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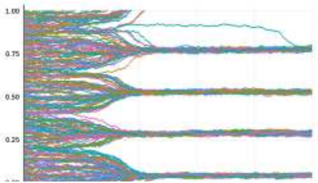

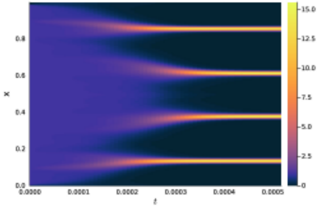

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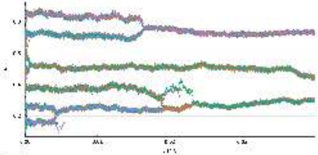

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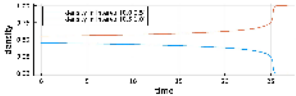
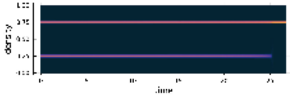
also present, but needs a lot of particles to be visible





Effect IV: Microscopic reversibility

dissolution of cluster [GS '21]

not possible

Stochastically perturbed gradient flow

The empirical measure μ_t^N satisfies the *Dean–Kawasaki* equation (Kawasaki 1973; Dean 1996)
see (V. Konarovskyi, Lehmann, and Renesse 2019; Cornalba and Fischer 2023; Wehlitz et al. 2025) and references therein

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(E3) **Slow (deterministic) gradient flow:** $\mathcal{F}_{\gamma,\ell}$ has a slow manifold (small Lipschitz constant)

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(E2) **Coalescence of clusters** driven by multiplicative noise

(E3) **Slow (deterministic) gradient flow:** $\mathcal{F}_{\gamma,\ell}$ has a slow manifold (small Lipschitz constant)

(E4) **Microscopic reversibility:** the process (μ_t^N) is ergodic with Gibbs measure "$e^{-N\mathcal{F}_{\gamma,\ell}(\mu)}$".

Outline

Minimizers of the mean-field free energy

What is the long-term behaviour of the *mean-field PDE*?

$$\partial_t \rho = \Delta \rho + \nabla \cdot \big((\nabla W_{\gamma,\ell} * \rho)\rho \big) \qquad \text{on } [0,1] \qquad \text{where } W_{\gamma,\ell}(x) = \gamma \ell w\Big(\frac{x}{\ell}\Big)$$

Free energy dissipation: $\frac{\mathrm{d}}{\mathrm{d}t}\mathcal{F}_{\gamma,\ell}(\rho_t) = -\int_{[0,1]} \big|\nabla(\log \rho_t + W_{\gamma,\ell} * \rho_t)\big|^2 \rho_t \, \mathrm{d}x \leq 0.$

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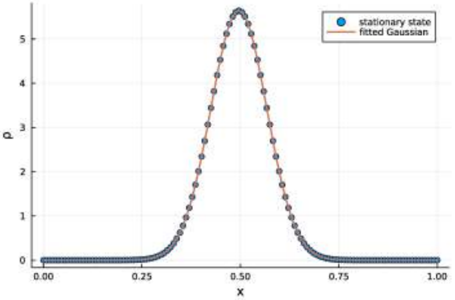
Numerically:

- If γ small: $\rho_t \to \rho_0 \equiv 1$ (*uniform state*) as $t \to \infty$.
- If γ large enough: Generically, ρ_t converges to a *single-cluster state* as $t \to \infty$, which is approximately a Gaussian of variance $\sigma^2 = \frac{\ell}{\gamma w''(0)}$.

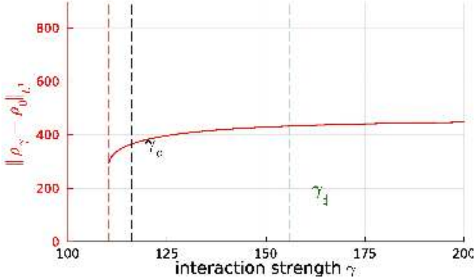


Existence of a discontinuous phase transition

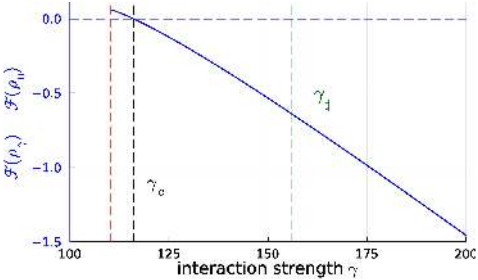
Proposition (Carrillo et al. 2020; Gvalani and Schlichting 2020)

Let $w\colon \mathbb{R} \to \mathbb{R}$ be even compact support and $\int_{\mathbb{R}} w(x)\,\mathrm{d}x < 0$.
Let $\ell \ll 1$. Then, the free energy $\mathcal{F}_{\gamma,\ell}$ has a discontinuous transition point $\gamma_c < \gamma_\sharp$:

- *For $\gamma < \gamma_c$, the uniform state ρ_0 is the unique minimizer of $\mathcal{F}_{\gamma,\ell}$.*
- *For $\gamma > \gamma_c$, there exists a minimizer ρ_γ of $\mathcal{F}_{\gamma,\ell}$ distinct from the uniform state ρ_0.*



L^1 distance of ρ_γ to uniform state $\rho_0 \equiv 1$



Free energy gap ρ_γ to uniform state $\rho_0 \equiv 1$

Structure of the global minimizers

Theorem (Gerber et al. 2025)

Let $S^1 = \{x \in \mathbb{R}^2 : |x| = 1\}$. *Assume that*

- $w : \mathbb{R} \to \mathbb{R}$ *continuous, even, symmetrically non-decreasing*
- $\operatorname{supp} w = [-s_w, s_w]$ *for some* $s_w > 0$;
- w *is* C^2 *on* $\operatorname{supp} w$ *and* $w''(0) > 0$.

Let ρ *be a global minimizer of the free energy.*
Then there exists a rotation $T : S^1 \to S^1$ *such that* $\rho = \rho^* \circ T$, *where* ρ^* *is the symmetric decreasing rearrangement of* ρ.

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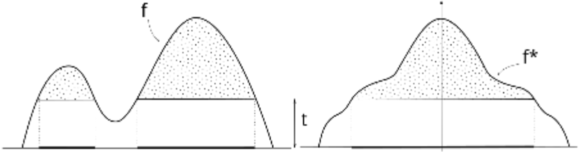
Symmetric decreasing rearrangement of $\rho : S^1 \to [0, \infty)$**:**



Proof

Free energy: $\mathcal{F}(\rho) = S(\rho) + I(\rho)$ where

- *entropy:* $S(\rho) := \int_{[0,1]} \rho(x) \log(\rho(x))\, \mathsf{d}x$
- *interaction energy:* $I(\rho) := \frac{1}{2} \iint_{[0,1]^2} \rho(x)\rho(y) W_{\gamma,\ell}(x-y)\, \mathsf{d}x\, \mathsf{d}y$

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The interaction energy can *only decrease* under rearrangement:

Theorem (Riesz rearrangement inequality [Baernstein-Taylor 1976])

Let $K : [0,\pi] \to [0,\infty)$ be a non-decreasing function. Then, for all measurable non-negative functions f, g on S^n it holds that

$$\int_{S^n \times S^n} f(x) g(y) K(d(x,y)) \,\mathrm{d}x \,\mathrm{d}y \geq \int_{S^n \times S^n} f^*(x) g^*(y) K(d(x,y)) \,\mathrm{d}x \,\mathrm{d}y.$$

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This gives $\mathcal{F}(\rho) \overset{\text{Riesz}}{\geq} \mathcal{F}(\rho^*) \overset{\rho \text{ minimizer}}{\geq} \mathcal{F}(\rho)$. $\Rightarrow$ $\mathcal{F}(\rho) = \mathcal{F}(\rho^*)$.

Equality case in the Riesz rearrangement inequality

Theorem (Strict Riesz rearrangement inequality, Beckner 1993)

Let $K : [0, \pi] \to [0, \infty)$ *be strictly increasing.*
Let $f, g : S^n \to [0, \infty)$ *be measurable non-constant functions such that*

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Lemma (Variant of strict Riesz rearrangement inequality)

Let $K : [0, \pi] \to [0, \infty)$ be non-decreasing and strictly increasing on $[0, \delta]$ for some $\delta > 0$.
Let $\rho : S^n \to [0, \infty)$ be an analytic function for which

$$\int_{S^n \times S^n} \rho(x)\rho(y)K(d(x,y))\,\mathrm{d}x\,\mathrm{d}y = \int_{S^n \times S^n} \rho^*(x)\rho^*(y)K(d(x,y))\,\mathrm{d}x\,\mathrm{d}y.$$

Then there exists a rotation $T : S^n \to S^n$ such that $\rho = \rho^* \circ T$.

Proof Part I: Polarizations

Main idea: Analyticity allows to 'globalize' local strictness

Variant of Beckner's polarization argument[1]:

[1] William Beckner (1993). "Sharp Sobolev inequalities on the sphere and the Moser–Trudinger inequality". In: *Annals of Mathematics* 138.1, pp. 213–242.

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- Let $M^0 = S^n \cap H$. Split S^1 into two open halfspheres M^+ and M^- such that $S^1 = M^+ \dot\cup M^0 \dot\cup M^-$ and $\overrightarrow{n} \in M^+$ where $M^0 = S^1 \cap H$.
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- Let $\sigma : S^1 \to S^1$ be the reflection with respect to H
- We define the polarization $\rho^\sigma : S^n \to [0, \infty)$ by

$$\rho^\sigma(x) := \begin{cases} \max\{\rho(x), \rho(\sigma x)\} & \text{if } x \in M^+ \\ \rho(x) & \text{if } x \in M^0 \\ \min\{\rho(x), \rho(\sigma x)\} & \text{if } x \in M^-. \end{cases}$$

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Proof Part II: Rewriting $I(\rho^\sigma) - I(\rho)$

Fix some reflection σ. Then we have by polarization (Burchard 2009, Lemma 2.6, Beckner 1993)

$$\begin{aligned} I(\rho) &:= \int_{S^n \times S^n} \rho(x)\rho(y)K(d(x,y))\,\mathrm{d}x\,\mathrm{d}y \\ &= \int_{M^+ \times M^+} \Big[\rho(x)\rho(y) + \rho(\sigma x)\rho(\sigma y)\Big] K(d(x,y))\,\mathrm{d}x\,\mathrm{d}y \\ &\quad + \int_{M^+ \times M^+} \Big[\rho(x)\rho(\sigma y) + \rho(\sigma x)\rho(y)\Big] K(d(x,\sigma y))\,\mathrm{d}x\,\mathrm{d}y \end{aligned}$$

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Replace $\rho \mapsto \rho^\sigma$ and use symmetry and cases $\rho(x) \lesseqgtr \rho(\sigma x)$ to find

$$\begin{aligned} &I(\rho^\sigma) - I(\rho) \\ &\quad = \int_{M^+ \times M^+} \max\Big\{\big(\rho(\sigma x) - \rho(x)\big)\big(\rho(y) - \rho(\sigma y)\big), 0\Big\}\Big\{K(d(x,\sigma y)) - K(d(x,y))\Big\}\,\mathrm{d}x\,\mathrm{d}y. \end{aligned}$$

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Since ρ is *global minimizer:* $I(\rho) = I(\rho^{\sigma})$.

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$$\big(\rho(x) - \rho(\sigma x)\big)\big(\rho(y) - \rho(\sigma y)\big) \geq 0 \quad \text{for all } x, y \in M^+ \quad \text{with } d(x,y) < \delta.$$

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Conclude using:

Lemma (Lemma 2.11, Burchard 2009)

If $\rho = \rho^\sigma$ or $\rho = \rho^\sigma \circ \sigma$ for all reflections σ, then there exists a rotation $T : S^1 \to S^1$ such that $\rho = \rho^* \circ T$.

Analyticity of minimizers

A probability density ρ is stationary if and only if it is a fixed point of the Kirkwood–Monroe map:

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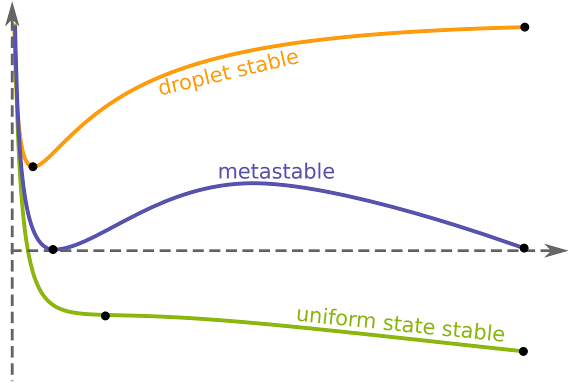
Theorem (Gerber et al. 2025)

Any ρ global minimizer of the free energy is spherical decreasing upto a rotation.

Phase transitions in the McKean–Vlasov model

[Carrillo-Gvalani-Pavliotis-S. '20]



Transition points and types of phase transitions

Free energy functional (Lyapunov property, gradient flow)

$$\mathcal{F}_\gamma(\varrho) = \int_{\mathbb{T}_L^d} \varrho \log \varrho \, \mathrm{d}x + \frac{\gamma}{2} \iint_{\mathbb{T}_L^d \times \mathbb{T}_L^d} W(x-y)\varrho(x)\varrho(y) \, \mathrm{d}x \, \mathrm{d}y \ .$$

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Definition: Let $\varrho_\infty \equiv L^{-d}$. γ_c is transition point, if:

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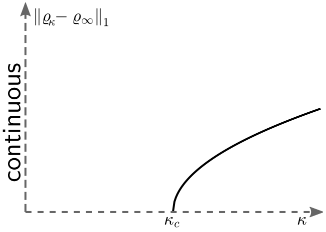

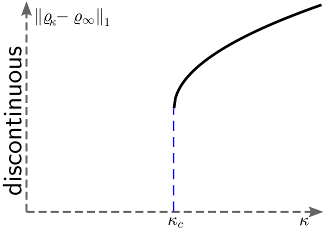

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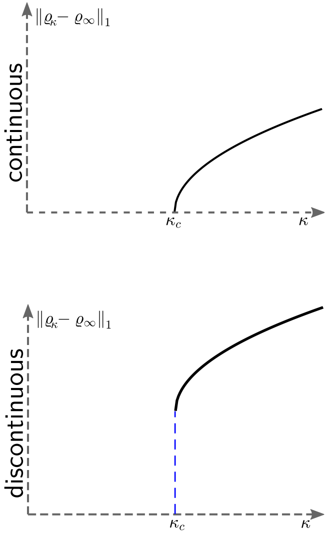
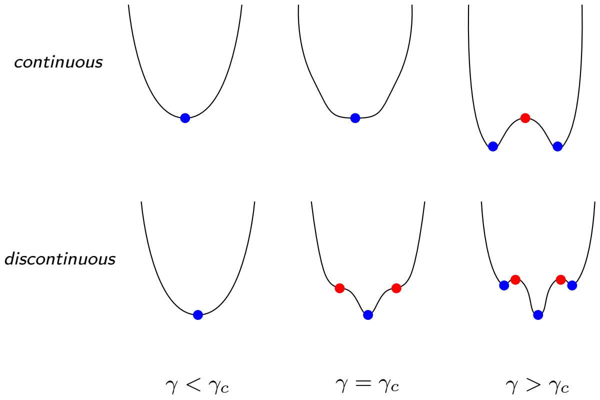
- For $\gamma > \gamma_c$ exists another global minimizer ϱ_γ

Results and Goals:

- Bifurcation analysis and local stability around $\varrho_\infty \equiv L^{-d}$
- Classification for continuous and discontinuous transitions
- Understanding of the free energy landscape
- Dynamical properties related to nucleation and coarsening



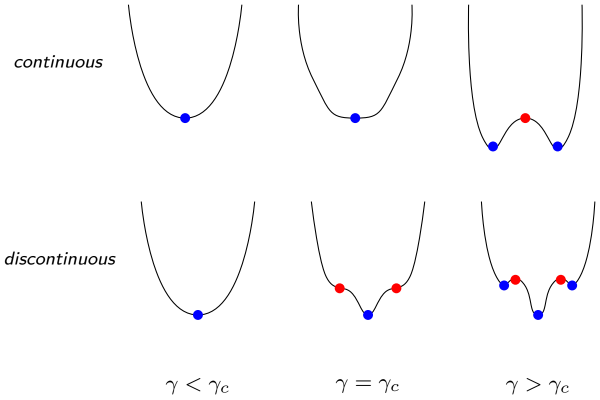
Continuous vs. discontinuous: a bifurcation-theoretic view



Continuous (pitchfork): the uniform state (•) *loses* local stability and bifurcates into new locally stable minima.

Discontinuous (saddle-node): the uniform state *keeps* local stability while new minima (•) appear, separated by saddles (•).

Continuous vs. discontinuous: a bifurcation-theoretic view



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In the absence of a phase transition ($W \in \mathbb{H}_s$) / away from γ_c

The unique minimizer enjoys a *uniform-in-time* log-Sobolev inequality and hence *uniform-in-time propagation of chaos*:
See Malrieu 2001; Guillin et al. 2022; Delgadino et al. 2023

Characterization of phase transition

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Theorem [Carrillo-Gvalani-Pavliotis-S. '20]

Let $\widetilde{W} : \mathbb{N}^d \to \mathbb{R}$ denote the (real) Fourier modes of W.

- If there is only one dominant unstable mode k^*: For $\alpha > 0$ small enough holds

$$\alpha \widetilde{W}(k^*) \leq \widetilde{W}(k) \qquad \text{for all } k \neq k^* : \widetilde{W}(k) < 0 \,,$$

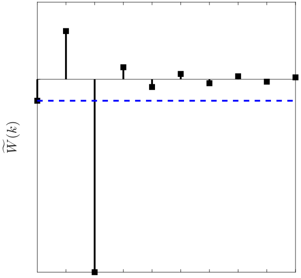
  then the transition point γ_c is continuous.

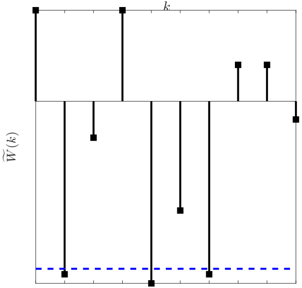
- If there exist (near)-dominant resonating modes k^a, k^b, k^c: That is for δ small enough exist

$$k^a, k^b, k^c \in \left\{ k' \in \mathbb{N}^d : \widetilde{W}(k') \leq \min_{k \in \mathbb{N}^d} \widetilde{W}(k) + \delta \right\} \quad \text{with } k^a = k^b + k^c,$$

  then the transition point γ_c is discontinuous.

$\Rightarrow$ local attractive potentials lead to discontinuous phase transitions





Basic properties of transition points

Summary of critical points:

- γ_c transition point (defined before)
- γ_* bifurcation point (Hessian of $\mathcal{F}$ becomes non-definite)
- $\gamma_\sharp$ point of linear stability, i.e., $\gamma_\sharp = -\frac{L^{\frac{d}{2}}}{\beta \min_k \widetilde{W}(k)/\Theta(k)}$.

  If $k_\sharp = \arg\min \widetilde{W}(k)$ is unique, then $\gamma_\sharp = \gamma_*$ is a bifurcation point (Crandall-Rabinowitz)

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Results from [Gates & Penrose 1970] and [Chayes & Panferov '10]

- $\mathscr{F}_\gamma$ has a transition point γ_c iff $W \notin \mathbb{H}_s$, that is $\widetilde{W}(k)$ negative for some k
- $\min \mathscr{F}_\gamma$ is non-increasing as a function of γ
- If for some γ' : ϱ_∞ is no longer the unique minimizer,
  then $\forall \gamma > \gamma'$: ϱ_∞ is no longer a unique minimizer
- If γ_c is continuous, then $\gamma_c = \gamma_\sharp$

Conclusion:

- To prove a discontinuous transition: Show ϱ_∞ is no longer global minimizer at $\gamma_\sharp$.
- To prove a continuous transition:
  If $\gamma_* = \gamma_\sharp$, sufficient to show that ϱ_∞ at $\gamma_\sharp$ is the unique global minimizer.

Argument for resonating dominant modes ($\delta = 0$)

Let $\varepsilon > 0$ be sufficiently small such that $\varrho = \varrho_\infty\left(1 + \varepsilon \sum_{k\in K^\delta} w_k\right) \in \mathcal{P}^+(\mathbb{T}^d)$.

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Entropy and energy of ansatz:

$$S(\varrho) = \left(S(\varrho_\infty) + \frac{|K^\delta|}{2} \varrho_\infty \varepsilon^2 - \frac{\varrho_\infty}{3} \int \varepsilon^3 \left(\sum_{k \in K^\delta} w_k \right)^3 + O(\varepsilon^4) \right)$$

$$\frac{\gamma_\sharp}{2} \mathcal{E}(\varrho, \varrho) = \frac{\gamma_\sharp}{2} \mathcal{E}(\varrho_\infty, \varrho_\infty) + \frac{\gamma_\sharp \varepsilon^2 |K^\delta| \varrho_\infty^2}{2} \min_{k \in \mathbb{N}^d} \frac{\widetilde{W}(k)}{\Theta(k)} L^{d/2}$$

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Combining both estimates, recalling $\gamma_\sharp = -\frac{L^{\frac{d}{2}}}{\min_k \widetilde{W}(k)/\Theta(k)}$, yields

$$\mathscr{F}_{\gamma_\sharp}(\varrho) - \mathscr{F}_{\gamma_\sharp}(\varrho_\infty) \le -\frac{\varepsilon^3 \varrho_\infty}{3} \int \left(\sum_{k \in K^\delta} w_k\right)^3 + O(\varepsilon^4).$$

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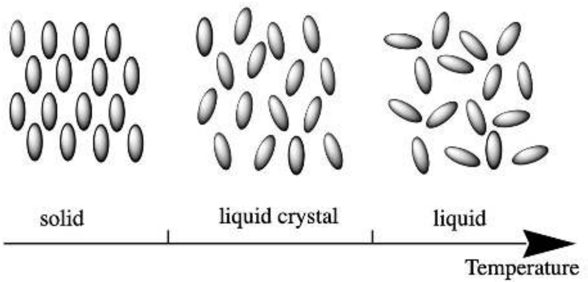
The resonance condition $k^a = k^b + k^c$ ensures that

$$\int \Big(\sum_{k \in K^{\delta *}} w_k\Big)^3 > 0\ .$$

Phase transitions on high dimensional spheres

[Shalova-S., Adv. Nonlinear Anal. 2025][2]



https://advlabs.aapt.org/wiki/Physics_of_Liquid_Crystals

[2] Anna Shalova and André Schlichting (2025). “Solutions of stationary McKean–Vlasov equation on a high-dimensional sphere and other Riemannian manifolds”. In: *Advances in Nonlinear Analysis* 14.1.

Generalization to spheres

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What changes if $\mathbb{T}_L^d$ is replaced by compact Riemannian manifold $\mathcal{M}^d$?

General case: $\mathcal{M}^d$

- thermodynamic formulation of stationary points is coordinate free:

  Stationary McKean-Vlasov equation: $\gamma^{-1}\Delta\rho + \nabla \cdot (\rho \nabla W * \rho) = 0$

  Zero of Gibbs Map $F : \mathcal{P}_{ac}(\mathcal{M}) \times \mathbb{R}_+ \to \mathcal{P}_{ac}(\mathcal{M})$: $F(\rho, \gamma) = \rho - \frac{1}{Z(\gamma,\rho)} e^{-\gamma W * \rho}$

  Critical point for free energy functional $\mathcal{F} : \mathcal{P}_{ac}^+(\mathcal{M}) \to \mathbb{R}$ with

  $$\mathcal{F}(\mu) := \gamma^{-1} \int \log \mu \, \mathrm{d}\mu + \frac{1}{2} \int_{\mathcal{M}\times\mathcal{M}} W(x,y) d\mu(x) d\mu(y)$$

- Ricci curvature enters condition on convexity and uniqueness of stationary points [Sturm '05][3]

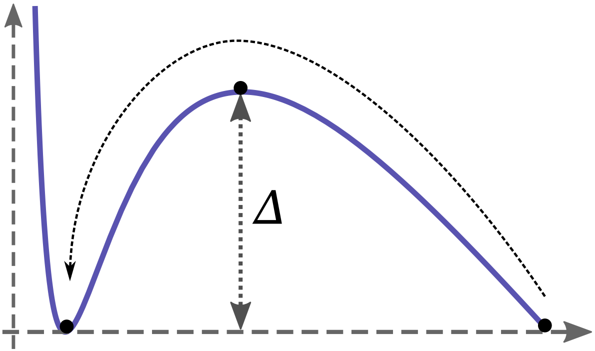
Model case: $\mathbb{S}^{n-1}$

- Use spherical harmonics ONS
- translational symmetry on $\mathbb{T}^d$ replaced by spherical symmetry on $\mathbb{S}^{n-1}$ (zonal spherical harmonics)
- local bifurcation analysis via Crandall-Rabinowitz
- Spherical harmonics can self-resonate making discontinuous with one negative mode possible

[3] Karl-Theodor Sturm (2005). "Convex functionals of probability measures and nonlinear diffusions on manifolds". In: *Journal de mathématiques pures et appliquées* 84.2, pp. 149–168.

A mountain pass theorem in the presence of discontinuous phase transitions

[Gvalani-S. '20]



Noise-induced transitions in $\mathbb{R}^d$

Start form deterministic gradient flow in $\mathbb{R}^d$

$$\dot{x}(t) = -\nabla F(x) \quad \text{with} \quad x(0) = x_0 \in \mathbb{R}^d$$

- F has two global minima $m_1, m_2 \in \mathbb{R}^d$.

Describe the particle transition from m_1 to m_2 under the influence of noise.

Modelproblem: Add Brownian motion

$$dX_t = -\nabla F(X_t)\,\mathrm{d}t + \sqrt{2\sigma} dB_t\,,$$

Question: Given $X(0) = m_1$, what is the probability that in some finite time $T > 0$, we have that $X(T) = m_2$ in the regime $\sigma \ll 1$?

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Theorem (Freidlin–Wentzell)

The family of processes $\{X_t^\sigma\} \in C([0,T];\mathbb{R}^2)$ satisfy a LDP with good rate function $I : C([0,T];\mathbb{R}^d) \to \mathbb{R} \cup \{+\infty\}$

$$I(x(\cdot)) = \frac{1}{4}\int_0^T |\dot{x}(t) + \nabla F(x(t))|^2\,\mathrm{d}t.$$

and it holds

$$\mathbb{P}(X_t^\sigma \in \Gamma) \approx \exp\Big(-\sigma^{-1} \inf_{x\in\Gamma} I(x(\cdot))\Big) \qquad \sigma \ll 1,$$

for any $\Gamma \subset C([0,T];\mathbb{R}^d)$.

Noise-induced transitions in $\mathbb{R}^d$

For $x \in \Gamma = \{f \in C^1([0,T];\mathbb{R}^d) : x(0) = m_1, x(T) = m_2\}$ let $T^* = \arg\max_{t\in[0,T]}(F(x(t)) - F(x(0)))$:

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$$= \frac{1}{4}\int_0^{T^*} |\dot{x}(t) - \nabla F(x(t))|^2 \,\mathrm{d}t + \int_0^{T^*} \dot{x}(t)\cdot\nabla F(x(t))\,\mathrm{d}t + \frac{1}{4}\int_{T^*}^{T} |\dot{x}(t) + \nabla F(x(t))|^2 \,\mathrm{d}t$$

Noise-induced transitions in $\mathbb{R}^d$

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$$\begin{aligned} I(x(\cdot)) &= \frac{1}{4}\int_0^T |\dot{x}(t) + \nabla F(x(t))|^2 \, \mathrm{d}t \\ &= \frac{1}{4}\int_0^{T^*} |\dot{x}(t) - \nabla F(x(t))|^2 \, \mathrm{d}t + \int_0^{T^*} \dot{x}(t) \cdot \nabla F(x(t)) \, \mathrm{d}t + \frac{1}{4}\int_{T^*}^T |\dot{x}(t) + \nabla F(x(t))|^2 \, \mathrm{d}t \\ &\geq F(x(T^*)) - F(x(0)) \geq \inf_{x(\cdot)\in\Gamma} (F(x(T^*)) - F(x(0))) =: c - F(x(0)) \, , \end{aligned}$$

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Classical mountain pass theorem.
c a *critical value* of F, that is $\exists s \in \mathbb{R}^d : \nabla F(s) = 0, F(s) = c$.

Noise-induced transitions in $\mathbb{R}^d$

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Freidlin-Wentzell:

$$
\Rightarrow \qquad \mathrm{P}(X_t^\sigma \in \Gamma) \lesssim \exp(-\sigma^{-1}\Delta F) \qquad \text{where} \quad \Delta F = F(s) - F(m_1).
$$

LDP for McKean-Vlasov interaction particle system

- Apply argument to the McKean–Vlasov N-particle system for $N \gg 1$

$$\mathrm{d}X_t^i = -\frac{\gamma}{N} \sum_{j=1, j\neq i}^{N} \nabla W(X^i - X^j)dt + \sqrt{2}\,\mathrm{d}B_t^i, \qquad i = 1, \dots, N$$

- [Dawson-Gärtner 1987] proved LDP with rate function for $\mu \in \mathrm{AC}^2([0,T], \mathcal{P}_2(\mathbb{T}_L^d))$ given by

$$I_\gamma(\mu(\cdot)) := \frac{1}{4}\int_0^T \|\partial_t \mu_t - \nabla\cdot(\mu_t \nabla(\log\mu_t + \gamma W \star \mu_t))\|_{-1,\mu_t}^2 \,\mathrm{d}t$$

- McKean-Vlasov is GF w.r.t. W_2: Associated quasipotential to LDP is $\mathcal{F}_\gamma$!

$$\mathbb{P}(\text{transition: } \varrho_\infty \to \varrho_\gamma) \simeq \exp\Big(-N \inf\{I_\gamma(\mu(\cdot)) : \mu(0) = \varrho_\infty, \mu(T) = \varrho_\gamma\}\Big)$$

$$\le \exp\left(-N \inf_{\mu}\left\{\sup_{T^*\in[0,T]} (\mathcal{F}_\gamma(\mu(T^*)) - \mathcal{F}_\gamma(\mu(0))) : \mu(0) = \varrho_\infty, \mu(T) = \varrho_\gamma\right\}\right).$$

Dawson-Gärtner 1987, Riemannian structure

$$|\nabla_t f|_t^2 = \sum_{i,j=1}^{d} a^{ij}(\cdot, t) \frac{\partial f}{\partial x^i} \frac{\partial f}{\partial x^j}.$$

(Of course, if $a(\cdot, t)$ is not sufficiently smooth, then there is not really a Riemannian structure associated with $a(\cdot, t)$. But the above formulae still makes sense in this case.)

For each $\mu \in \mathcal{M}$ and $t \in [0, T]$ we introduce a normed linear space

$$T_{\mu,t} = \{\vartheta \in \mathcal{D}' : \|\vartheta\|_{\mu,t} < \infty\},$$

where the norm $\| \ \|_{\mu,t}$ is defined by

$$\|\vartheta\|_{\mu,t}^2 = \frac{1}{2} \sup_{f \in \mathcal{D}_{\mu,t}} \frac{|\langle \vartheta, f \rangle|^2}{\langle \mu, |\nabla_t f|_t^2 \rangle}, \qquad \vartheta \in \mathcal{D}'. \tag{4.7}$$

Here $\mathcal{D}_{\mu,t} = \{f \in \mathcal{D} : \langle \mu, |\nabla_t f|_t^2 \rangle \neq 0\}$. For each $\vartheta \in \mathcal{D}'$,

$$\|\vartheta\|_{\mu,t}^2 = \sup_{f \in \mathcal{D}} [\langle \vartheta, f \rangle - \tfrac{1}{2} \langle \mu, |\nabla_t f|_t^2 \rangle]. \tag{4.8}$$

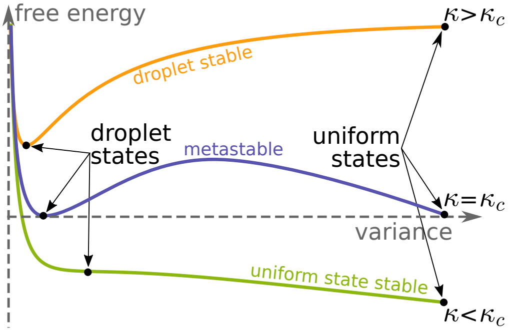
Indeed, replacing the function f in (4.8) by $c \cdot f$ and taking the supremum at first over all $c \in \mathbb{R}$ and then over $f \in \mathcal{D}_{\mu,t}$, we see that the expressions on the right of (4.7) and (4.8) coincide.

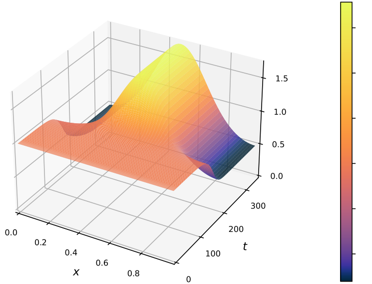
For each $\nu \in \mathcal{M}$ we introduce a functional $S_\nu : \mathcal{C} \to [0, \infty]$ by setting

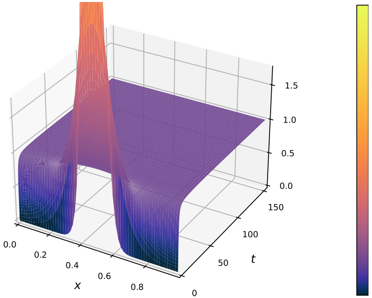
$$S_\nu(\mu(\cdot)) = \int_0^T \|\dot{\mu}(t) - \mathcal{L}_t^* \mu(t)\|_{\mu(t),t}^2 \, dt, \tag{4.9}$$

Discontinuous phase transitions and metastability

- N-particle system is metastable at discontinuous phase transit
- By [Dawson-Gärtner 1989] need to understand free energy $\mathcal{F}_\gamma$







- Missing ingredient: mountain pass theorem for $\mathcal{F}_\gamma$
  Difficulties:
  - $(\mathcal{P}(\mathbb{T}_L^d), W_2)$ only metric space
  - $\mathcal{F}_\gamma$ only lower semicontinuous

A mountain pass theorem

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Theorem [Gvalani-S. '20]

If $\mathcal{F}_\gamma$ has two distinct minimizers $\varrho_\infty \equiv 1/L^d$ and $\varrho_\gamma \in \mathcal{P}(\mathbb{T}^d_L)$, then there exists $\varrho^* \in \mathcal{P}(\mathbb{T}^d_L)$ distinct from ϱ_∞ and ϱ_γ such that $|\partial\mathcal{F}_\gamma|(\varrho^*) = 0$.

Moreover: $\mathcal{F}_\gamma(\varrho^*) = c$ with $c = \inf_{\gamma\in\Gamma} \max_{t\in[0,T]} \mathcal{F}(\gamma(t))$,

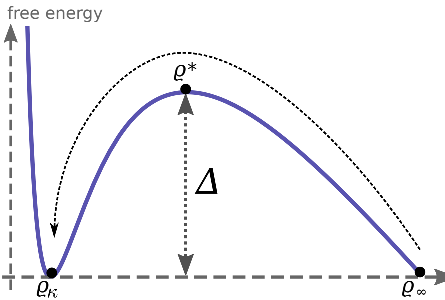
where $\Gamma = \{C([0,T];\mathcal{P}(\mathbb{T}^d_L)) : \gamma(0) = \varrho_\infty, \gamma(T) = \varrho_\gamma\}$.

Corollary (Arrhenius law)

The empirical McKean-Vlasov process $\varrho^{(N)}$ satisfies

$$\mathbb{P}\left[\varrho^N(T) \in \overline{B}^{W_2}_\varepsilon(\varrho_\gamma), \varrho^{(N)}(0) = \varrho^{(N)}_0\right] \lesssim e^{-N\Delta}$$

for N sufficiently large with $\mathbb{E}(W_2(\varrho^{(N)}_0, \varrho_\infty)) \to 0$ and $\Delta := \mathcal{F}_\gamma(\varrho^*) - \mathcal{F}_\gamma(\varrho_\infty)$ with ϱ^* the mountain pass point.



Starting the PDE from perturbations of $\rho_0 \equiv 1$

Heuristics by Garnier, Papanicolaou, and Yang 2017[4]:
Linearize the *mean-field PDE*

$$\partial_t \rho = \Delta \rho + \nabla \cdot \big((\nabla W_{\gamma,\ell} * \rho)\rho\big) \qquad \text{on } [0,1], \qquad W_{\gamma,\ell}(x) = \gamma\ell$$

around *uniform steady state* $\rho_0 \equiv 1$:

$$\rho \approx \rho_0 + \rho_1(t,x) \qquad \Rightarrow \qquad \partial_t \rho_1(t,x) = \partial_x^2 \rho_1(t,x) + \int_0^1 \partial_x \rho_1(t,x-y) \nabla W_{\gamma,\ell}(y)\, \mathrm{d}y$$

[4] Josselin Garnier, George Papanicolaou, and Tzu Wei Yang (2017). "Consensus Convergence with Stochastic Effects". In: *Vietnam Journal of Mathematics* 45.1-2. arXiv: 1508.07313v2, pp. 51–75.

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around *uniform steady state* $\rho_0 \equiv 1$:

$$\rho \approx \rho_0 + \rho_1(t,x) \qquad \Rightarrow \qquad \partial_t \rho_1(t,x) = \partial_x^2 \rho_1(t,x) + \int_0^1 \partial_x \rho_1(t, x-y) \nabla W_{\gamma,\ell}(y) \, \mathrm{d}y$$

Fourier modes $\hat{\rho}_1(t,k) := \int_0^1 \rho_1(t,x) e^{-ikx} \, \mathrm{d}x$ where $k \in 2\pi\mathbb{Z}$ satisfy

$$\partial_t \hat{\rho}_1(t,k) = \left[-k^2 + i \rho_0 k \int e^{-iky} \nabla W_{\gamma,\ell}(y) \, \mathrm{d}y \right] \hat{\rho}_1(t,k)$$

Fourier modes will grow as

$$|\widehat{\rho_1}(t,k)| = |\widehat{\rho_1}(0,k)| e^{\psi(k) t} \qquad \text{where} \qquad \psi(k) = -k^2 \left(1 + \int_0^1 \cos(ky) W_{\gamma,\ell}(y) \, \mathrm{d}y \right)$$

[4] Josselin Garnier, George Papanicolaou, and Tzu Wei Yang (2017). "Consensus Convergence with Stochastic Effects". In: *Vietnam Journal of Mathematics* 45.1-2. arXiv: 1508.07313v2, pp. 51–75.

Linear stability analysis

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  - *Initial clustering* with number of clusters $\approx \frac{k_{\max}}{2\pi}$

Coalescence following [GPY '17]

- Again assume $0 < \ell \ll 1$ and $\gamma \gg 1$.
- Recall SDE

$$\mathrm{d}X_t^i = -\frac{\gamma}{N}\sum_{j=1}^{N}\nabla w\left(\frac{X_t^i - X_t^j}{\ell}\right)dt + \sqrt{2}\,\mathrm{d}B_t^i,$$

- Consider a cluster of particles $I \subset \{1, \dots, N\}$ with center $X_t^{(I)} = \frac{1}{|I|}\sum_{i\in I} X_t^i$ and mass $m(I) = \frac{|I|}{N}$.

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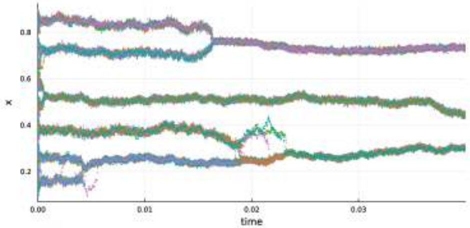
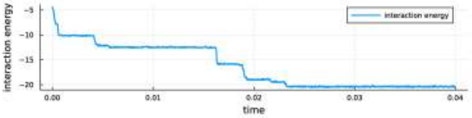
- Then, the cluster center evolves according to

$$\mathrm{d}X_t^{(I)} = \sqrt{\frac{2}{Nm(I)}}\,\mathrm{d}W_t,$$

until the cluster meets another cluster.





Within a cluster, particles relax like *Ornstein–Uhlenbeck* processes

$$\mathrm{d}X_t^i = -\frac{\gamma w''(0)}{\ell N}\sum_{k\in I}\left(X_t^i - X_t^k\right)\mathrm{d}t + \sqrt{2}\,\mathrm{d}B_t^i.$$

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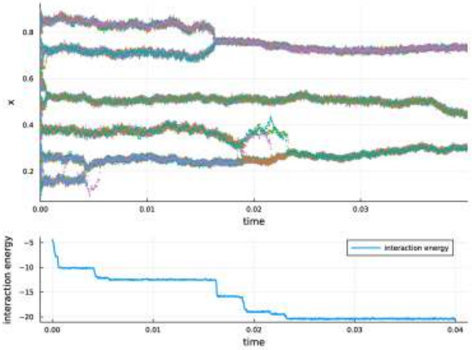

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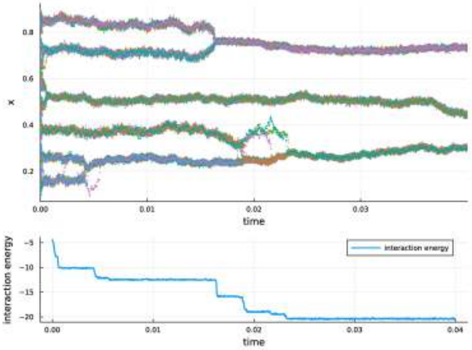

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- Clusters have size of σ, where $\sigma^2 = \frac{\ell}{\gamma w''(0) m(I)}$.
- When two clusters meet, they merge and their masses are added.

$\Rightarrow$ *coalescing heavy Brownian motions* on timescale $t_{\text{coalesence}} \asymp N$.

Mass exchange via Eyring–Kramers' law

- Assume $\gamma\ell \gg 1$, $\ell \ll 1$.
- Assume in the microscopic model that the particles are arranged in K clusters of masses $m^{(1)}, \dots, m^{(K)}$ and centers $X^{(1)}, \dots, X^{(K)}$.

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$$\mu_t^N \approx \sum_{k=1}^{K(t)} m^{(k)} \frac{1}{\sqrt{2\pi\sigma_k^2}} \exp\left(-\frac{1}{2\sigma_k^2}\left(\bullet - X_t^{(k)}\right)^2\right), \quad \text{where } \sigma_k^2 := \frac{\ell}{\gamma w''(0) m^{(k)}}$$

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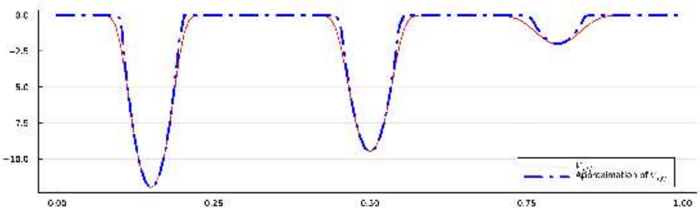
- Particles X_t^i move in *effective potential* $\mathrm{d}X_t^i = -V_{\mathrm{eff}}'(X_t^i)\,\mathrm{d}t + \sqrt{2}\,\mathrm{d}B_t^i$, where $V_{\mathrm{eff}} = W_{\gamma,\ell} * \mu_t^N$, $W_{\gamma,\ell}(\bullet) = \gamma\ell w(\bullet/\ell)$

Mass exchange via Eyring–Kramers' law II



- Effective potential V_{eff} has valleys of depth $\gamma\ell\Delta_w m^{(j)} + \frac{1}{2}$ around each cluster center $X^{(j)}$
- *Eyring–Kramers' law:* The expected time for a particle to leave cluster j and join another cluster is of order $e^{\gamma\ell\Delta_w m^{(j)}}$

$\Rightarrow$ *When* $\gamma \gg 1$, masses $m^{(1)}, \ldots, m^{(K)}$ of the clusters satisfy approximately

$$\frac{\mathrm{d}}{\mathrm{d}t} m^{(j)} = \alpha_{j-1} e^{-\gamma\ell\Delta_w m^{(j-1)}} m^{(j-1)} + \beta_{j+1} e^{-\gamma\ell\Delta_w m^{(j+1)}} m^{(j+1)} - (\alpha_j + \beta_j) e^{-\gamma\ell\Delta_w m^{(j)}} m^{(j)} .$$

The joint model for coalescence and mass exchange

A more refined approximation yields the model (still assuming $0 < \ell \ll 1$ and $\gamma \gg 1$):

$$\mathrm{d}X_t^{(j)} = \frac{\sqrt{2}}{\sqrt{Nm^{(j)}}}\,\mathrm{d}W_t^{(j)} t_{\text{coalesence}} \asymp N,$$

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$$t_{\text{metastab}} \asymp e^{\gamma\ell\Delta_w m^{(j)}},$$

for $j = 1, \dots, K$. Here,

$$\alpha_j = \frac{1}{X^{(j+1)} - X^{(j)} - 2s_w\ell}\sqrt{\frac{e\gamma w''(0)}{2\pi\ell}}\sqrt{m^{(j)}},$$

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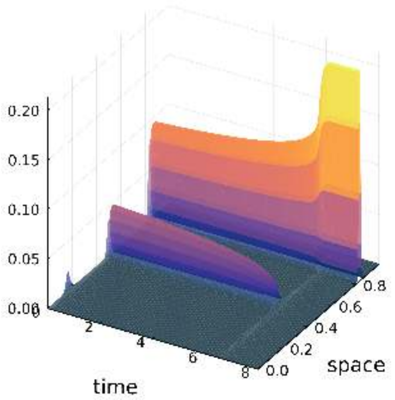
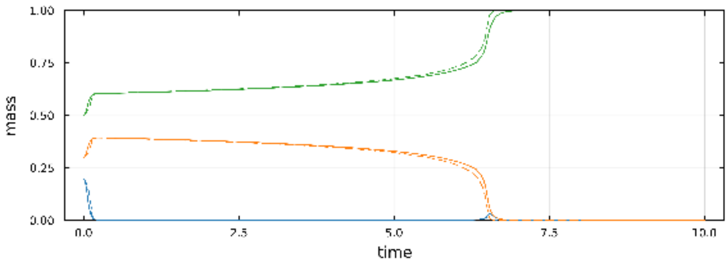
where $\operatorname{supp} w = [-s_w, s_w]$ and $\Delta_w = -\inf w$. The model is subject to *boundary conditions* due to

- clusters can merge $|X_t^{(j)} - X_t^{(k)}| \leq \ell s_w$
- cluster dissolution $m^{(j)}(t) < m_c$.

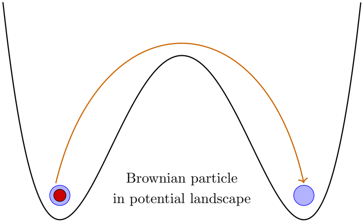
Numerics: Comparison of ODE with PDE





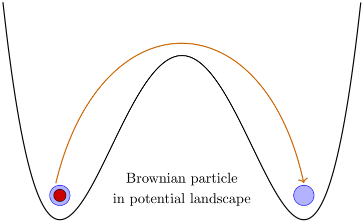
Comparison of the masses from the *PDE simulation* (solid) with the *mass ODE* (dashed lines)
$\gamma = 1000, \ell = 0.05.$

Dynamical metastability



Noise-induced metastability

Dynamical metastability



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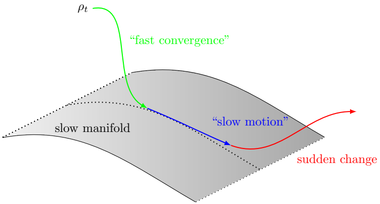

Dynamical metastability
(Otto and Reznikoff 2007)

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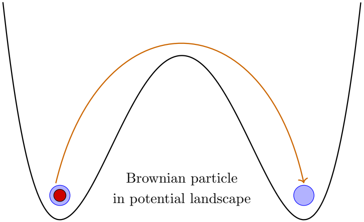

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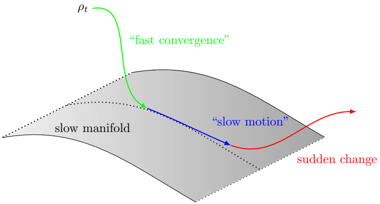

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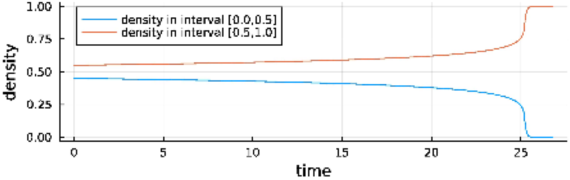
Dynamical metastability (PDE) for $\gamma\ell \gg 1$

- Leakage times are of order $e^{\gamma\ell\Delta_w m}$
- Mass exchange between two clusters of masses $m^{(1)}$ and $m^{(2)}$ is exponentially small in $\gamma\ell$



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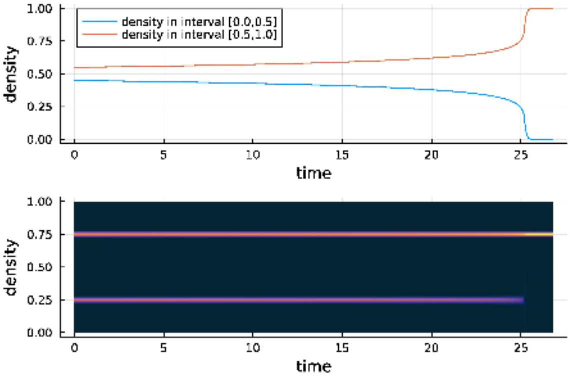


Slow manifold of **clustered states**
(tentative definition)

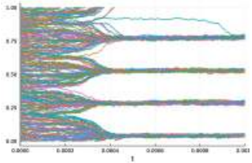
$$\bigcup_{n=1}^{N_c} \left\{ \sum_{k=1}^{n} m^{(k)} \delta_{X^{(k)}} : \sum_{k=1}^{n} m^{(k)} = 1, m^{(k)} \geq m_c, |X^{(k)} - X^{(j)}| \geq 2\ell s_w \right\}.$$

Conclusion

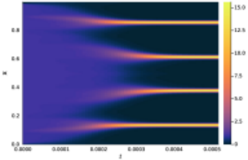
Effect I: Initial clustering

If sampled from iid uniform:
$t_{\text{cluster}} \asymp \log N$

Microscopic model



Mean-field PDE



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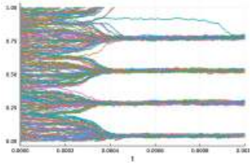

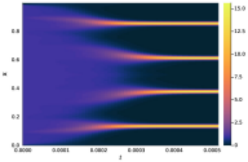

Effect II: Coalescence of clusters
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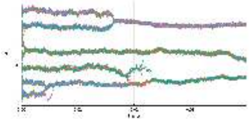

not present in the PDE, clusters cannot move

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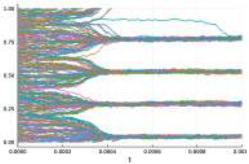
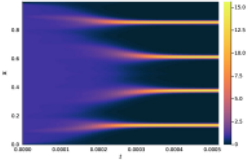
Microscopic model

Mean-field PDE





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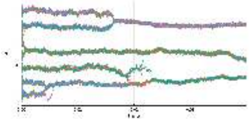

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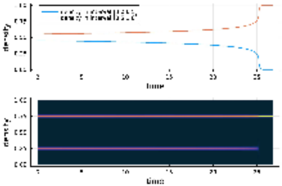

Effect III: Mass exchange

$t_{\text{metastab}} \asymp e^{\gamma \ell \Delta_w m}$ for clusters of mass m

also present, but needs a lot of particles to be visible

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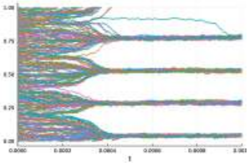

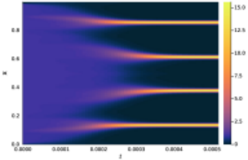

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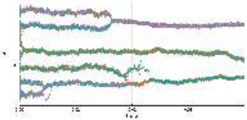

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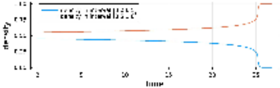

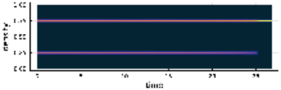

Effect IV: Microscopic reversibility

$t_{\text{reversibility}} \asymp e^{N \gamma \ell \Delta_{\mathcal{F}}}$ for some $\Delta_{\mathcal{F}} > 0$

dissolution of cluster [GS '21]

not possible

Convergence towards massive Arratia flow

$y(u,t)$ models the position of the particle starting from $u \in [0,1]$ at a time t.

Massive Arratia flow (Vitalii Konarovskyi 2017)

There exists an random element $\{y(u,t),\ u \in [0,1],\ t \in [0,T]\}$ in the Skorohod space $D([0,1], C[0,T])$ such that

(C1) for all $u \in [0,1]$, the process $y(u,\cdot)$ is a continuous square integrable martingale with respect to the filtration

$$\mathcal{F}_t = \sigma(y(u,s),\ u \in [0,1],\ s \le t), \quad t \in [0,T];$$

(C2) for all $u \in [0,1]$, $y(u,0) = u$;

(C3) for all $u < v$ from $[0,1]$ and $t \in [0,T]$, $y(u,t) \le y(v,t)$;

(C4) for all $u \in [0,1]$, the quadratic variation has the form $\langle y(u,\cdot)\rangle_t = \int_0^t \frac{ds}{m(u,s)}$, where $m(u,t) = \mathcal{L}^1\{v :\ \exists s \le t\ y(v,s) = y(u,s)\}$, $t \in [0,T]$;

(C5) for all $u, v \in [0,1]$ and $t \in [0,T]$, $\langle y(u,\cdot), y(v,\cdot)\rangle_{t\wedge\tau_{u,v}} = 0$, where $\tau_{u,v} = \inf\{t :\ y(u,t) = y(v,t)\} \wedge T$.

Conjecture: Massive Arratia flow

The system of particles

$$\mathrm{d}X_t^i = -\frac{\gamma}{N}\sum_{j=1}^{N}\nabla W\left(\frac{X_t^i - X_t^j}{\ell}\right)dt + \sqrt{2}\,\mathrm{d}B_t^i \qquad \text{for } i = 1,\dots,N$$

converges in the regime

$$N_n \to \infty, \qquad \ell_n \downarrow 0, \qquad \frac{\gamma_n \ell_n}{\log N_n} \gg 1.$$

to the massive Arratia flow (Vitalii Konarovskyi 2017): the variable $Z_{\gamma,\ell}^{N}(u,t) := X_t^{\lfloor Nu \rfloor}$ for $u \in [0,1]$ satisfies

$$Z_{\gamma_n,\ell_n}^{N_n}\left(u, \tfrac{N_n t}{2}\right) \to y(u,t) \qquad \text{as } n \to \infty\,,$$

with $y(u,t)$ the position process of the modified Arratia flow.

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Thank you for your attention!

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Appendix

Why are global minimizers analytic?

- Let ρ be a stationary state, then it is a fixed point of the Kirkwood-Monroe map

$$\rho = \frac{1}{Z(\rho)} e^{-W_{\gamma,\ell}*\rho} \qquad \text{where } Z(\rho) = \int_{[0,1]} e^{-W_{\gamma,\ell}*\rho(x)}\, \mathrm{d}x. \tag{2}$$

- ρ is smooth by (Carrillo et al. 2020). Analyticity follows if for some $C > 0$ we have

$$\left\|\rho^{(n)}\right\|_\infty \leq C^{n+1} n! \qquad \text{for all } n \in \mathbb{N}. \tag{3}$$

- By Faà di Bruno's formula[5],for $f, g \in C^n$

$$(g \circ f)^{(n)}(x) = \sum \frac{n!}{m_1! \cdot m_2! \cdots m_n!} g^{(k)}(f(x)) \prod_{j=1}^{n} \left(\frac{f^{(j)}(x)}{j!}\right)^{m_j},$$

  where the sum is over all $m_1, \dots, m_n \in \mathbb{Z}_{\geq 0}$ such that $\sum_{j=1}^n j \cdot m_j = n$.
- By (2)

$$\rho^{(n)} = \sum \frac{n!}{m_1! \cdot m_2! \cdots m_n!} \frac{\rho}{Z(\rho)} \prod_{j=1}^{n} \left(\frac{(W_{\gamma,\ell} * \rho)^{(j)}}{j!}\right)^{m_j}.$$

- $\Rightarrow$ (3) follows by induction

[5] Warren P Johnson (2002). "The curious history of Faà di Bruno's formula". In: *The American mathematical monthly* 109.3, pp. 217–234.

Fluctuating Scharfetter-Gummel scheme

Need to reintroduce noise to the McKean–Vlasov model: Dean–Kawasaki equation

$$\partial_t \rho_t = \nabla \cdot \left(\nabla \rho + \rho \nabla W * \rho + N^{-1/2} \sqrt{\rho}\, \xi_t \right)$$

with $(\xi_t)_{t \geq 0}$ space-time white noise.

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- The equation is strictly **ill-posed** in general (V. Konarovskyi, Lehmann, and Renesse 2019)
- or **trivial**: Martingale solutions on empirical measures with N atoms are equivalent to the N particle system
- In general: Suitable finite-dimensional approximations are closer to the particle system than the mean-field limit (Cornalba and Fischer 2023)

Question: Is there a fluctuating Scharfetter-Gummel scheme?

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Idea: Use stochastic cell formula in two-point flux approximation

Stochastic two-point flux approximation between volume-cell K and L at distance $h > 0$:
Solve for given $\beta > 0$, $q, \xi \in \mathbb{R}$ the boundary value problem $a, b > 0$ in $\rho : [0, h] \to \mathbb{R}$ and $j \in R$

$$j = -\beta^{-1} \partial_x \rho + \rho q + \sqrt{\rho} \xi, \qquad \rho(0) = a \quad \text{and} \quad \rho(h) = b.$$

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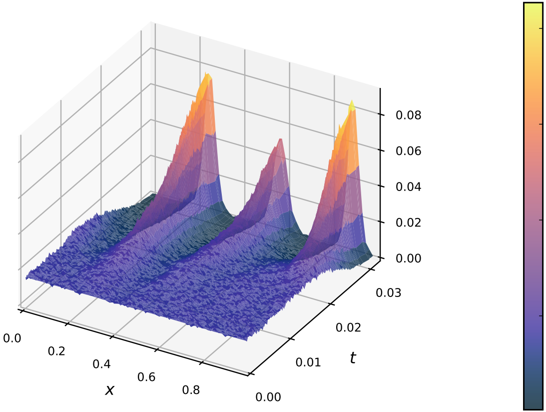
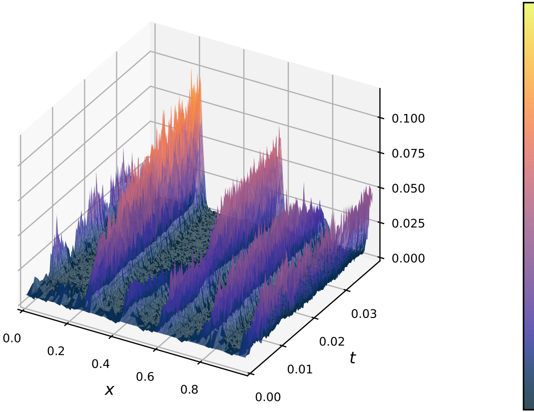
Solution is an implicit integral equation:
$\Rightarrow$ Together with time-implicit Euler, get a positivity preserving scheme!

Some numerical results

Scheme captures initial clustering regime:



Clusters merge thanks to local diffusion:



- Heuristics similar to Garnier, Papanicolaou, and Yang (2017) suggest clustering time-scale $t_{\text{cluster}} \sim \log N$
- number of clusters depends inversely on the effective range of the potential
- Clusters move like coalescing heavy Brownian motions, modified Arratia flow (Vitalii Konarovskyi 2017)