Nonlinear Aggregation-Diffusion Equations: Gradient Flows, Free Energies and Phase Transitions

J. A. Carrillo

University of Oxford

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Outline

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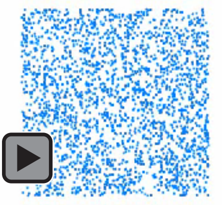
Aggregation for particles - Continuum Model

One particle attracted/repelled by a fixed location $x = a$

$$\dot{X} = -\nabla W(X-a) \qquad W(x) = W(-x), W(0) = 0\,, W \in C^1(\mathbb{R}^d/\{0\}, \mathbb{R})$$

Multiple particles attracted/repelled by one another



$$\dot{X}_i = -\sum_{j\neq i} m_j \, \nabla W(X_i - X_j)$$

$\rho(t,x) =$ density of particle at time t

$$v(x) = -\int_{\mathbb{R}^d} \nabla W(x-y)\, \rho(y) dy$$

So $\boxed{v = -\nabla W * \rho}$:

$$\begin{cases} \rho_t + \text{div}\,(\rho v) = 0 \\ v = -\nabla W * \rho \end{cases}$$

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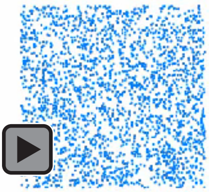

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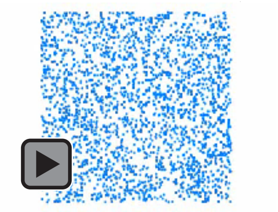

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Aggregation-Diffusion Equation

$$\begin{cases} \rho_t + \text{div}\,(\rho v) = 0 \\ v = -\nabla W * \rho - \nabla P(\rho) \end{cases}$$

$\rho(t,x)$: density
$v(t,x)$: velocity field
$x \in \mathbb{R}^d$, $t > 0$

$W : \mathbb{R}^d \to \mathbb{R}$
"interaction potential"

$-\nabla W : \mathbb{R}^d \to \mathbb{R}^d$
"attracting field"

If repulsion is modelled by diffusion, when does a balance between attraction and diffusion happen?

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Formal Gradient Flow

Basic Properties

1. **Conservation of the center of mass.**
2. **Liapunov Functional:** Gradient flow of

$$\mathcal{F}[\rho] = \frac{1}{2} \iint W(x-y)\, \rho(x)\, \rho(y)\, dxdy + \int_{\mathbb{R}^d} \Phi(\rho(x))\, dx$$

with respect to the Wasserstein distance W_2.
(C., McCann, Villani; RMI 2003, ARMA 2006).

The macroscopic equation can be rewritten as

$$\frac{\partial \rho}{\partial t}(t,x) = \operatorname{div}\left(\rho(t,x)\nabla\left[\frac{\delta \mathcal{F}}{\delta \rho}(t,x)\right]\right)$$

with $\frac{\delta \mathcal{F}}{\delta \rho} = W * \rho + \Phi'(\rho)$, $P'(\rho) = \rho \Phi''(\rho)$, and entropy dissipation:

$$\frac{\mathrm{d}}{\mathrm{d}t}\mathcal{F}[\rho(t)] = -\int_{\mathbb{R}^2} \rho(t,x)\left|\nabla \frac{\delta \mathcal{F}}{\delta \rho}(t,x)\right|^2 dx\,.$$

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Free Energy Minimization: Stable Steady States

Minimization Problem

We want to find local minimizers of the total interaction energy

$$\mathcal{F}[\rho] := \frac{1}{2} \iint_{\mathbb{R}^d \times \mathbb{R}^d} W(x-y)\rho(x)\rho(y)\, dxdy + \int_{\mathbb{R}^d} \Phi(\rho(x))\, dx\,.$$

When does a balance between attraction and repulsion (modelled either by nonlocality or diffusion) happen?

Recurrent Question in many fields:

- Statistical Mechanics & Crystallization: Typically very singular potentials at zero: Lennard-Jones.
- Semiconductors - Astrophysics - Chemotaxis: Macroscopic model obtained from Vlasov Equation under certain limits. Newtonian Potential.
- Economic Applications: Mean Field Games, Cournot-Nash Equilibria.
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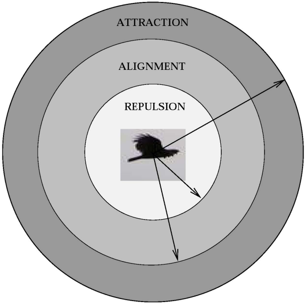
Individual Based Models (Particle models)

Swarming = Aggregation of agents of similar size and body type generally moving in a coordinated way.
Highly developed social organization: insects (locusts, ants, bees ...), fish, birds, micro-organisms,... and artificial robots for unmanned vehicle operation.

Interaction regions between individuals[a]

[a] Aoki, Helmerijk et al., Barbaro, Birnir et al.

- Repulsion Region: R_k.
- Attraction Region: A_k.
- Orientation Region: O_k.



2nd Order Model: 3-Zone Model

D'Orsogna, Bertozzi et al. (PRL 2006) + Cucker-Smale (IEEE Aut. Control 2007):

$$\begin{cases} \dfrac{dx_i}{dt} = v_i, \\ m\dfrac{dv_i}{dt} = (\alpha - \beta\,|v_i|^2)v_i - \displaystyle\sum_{j\neq i} \nabla W(|x_i - x_j|) + \sum_{j=1}^{N} a_{ij}\,(v_j - v_i)\,. \end{cases}$$

Model assumptions:

- Self-propulsion and friction terms = an asymptotic speed of $\sqrt{\alpha/\beta}$.
- Attraction/Repulsion modeled by an effective pairwise potential $W(x)$.

$$W(r) = -C_A e^{-r/\ell_A} + C_R e^{-r/\ell_R}.$$

- Communication rate: $\gamma \geq 0$ and

$$a_{ij} = a(|x_i - x_j|) = \frac{1}{(1 + |x_i - x_j|^2)^\gamma}.$$

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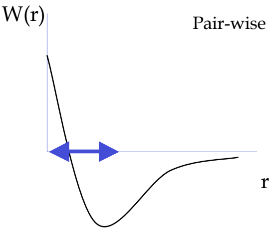

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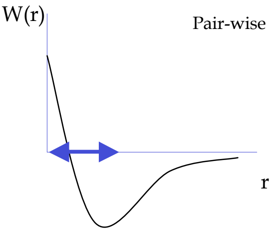

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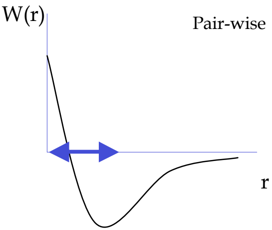

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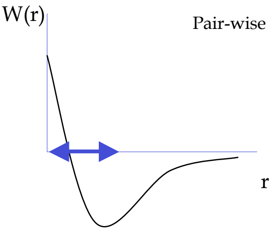

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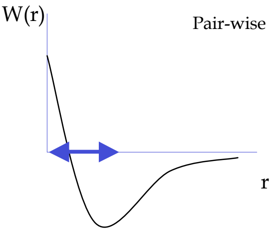
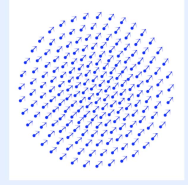
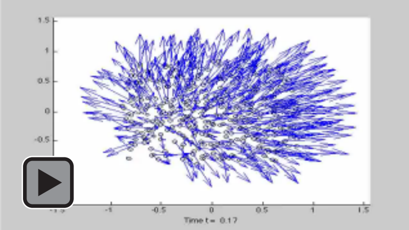
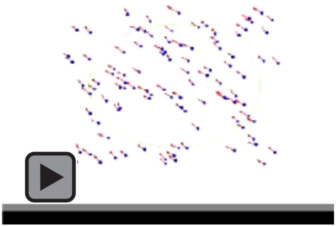


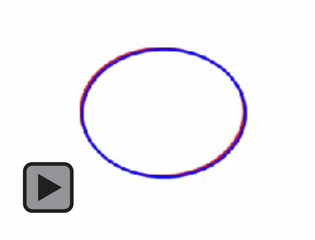
Flocking Patterns

Flocking Profiles:

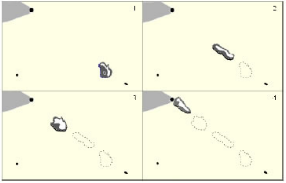


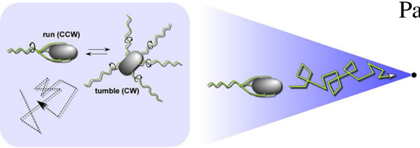






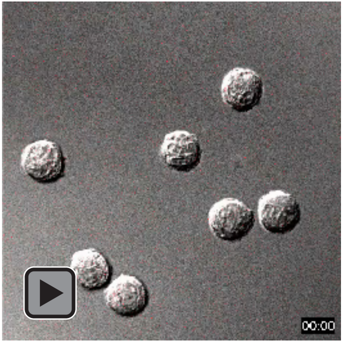
Cell/Bacteria Movement by Chemotaxis





$$
\begin{cases}
\dfrac{\partial n}{\partial t} = \Delta\Phi(n) - \chi\nabla\cdot(n\nabla c) & x\in\mathbb{R}^2,\ t>0\,, \\[2ex]
\dfrac{\partial c}{\partial t} - \Delta c = n - \alpha c & x\in\mathbb{R}^2,\ t>0\,, \\[2ex]
n(0,x) = n_0 \geq 0 & x\in\mathbb{R}^2\,.
\end{cases}
$$

Patlak (1953), Keller-Segel (1971), Nanjundiah (1973).



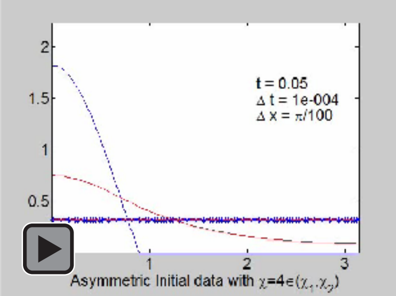
Movement and aggregation due to chemical signalling. Wikinut

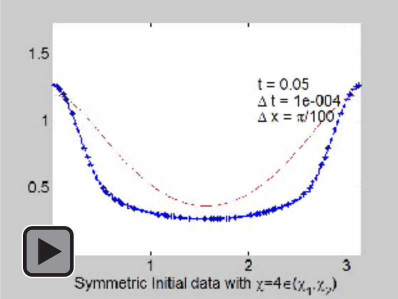
J. Saragosti etal, PLoS Comput. Biol. 2010.

S. Volpe etal, PLoS One 2012.

Phase Transitions for the Keller-Segel model on an interval [1]

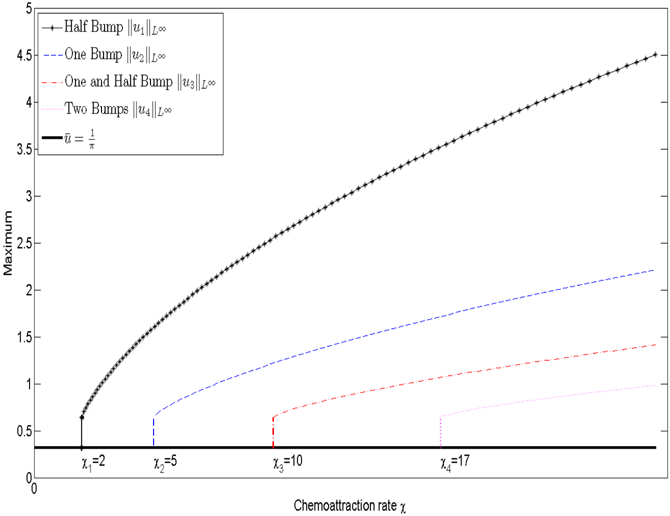
$$\begin{cases} u_t = \nabla \cdot (u\nabla u - \chi u \nabla v), & x \in \Omega, t > 0, \\ v_t = \Delta v - v + u, & x \in \Omega, t > 0, \\ \partial_\nu (u\nabla u - \chi u \nabla v) = \partial_\nu v = 0, & x \in \partial\Omega, t > 0, \\ u(x,0), v(x,0) \geq, \not\equiv 0, & x \in \Omega. \end{cases}$$





[1] C.-Chen-Wang-Wang-Zhang, SIAM J. Applied Mathematics 2020.

A bifurcation diagram



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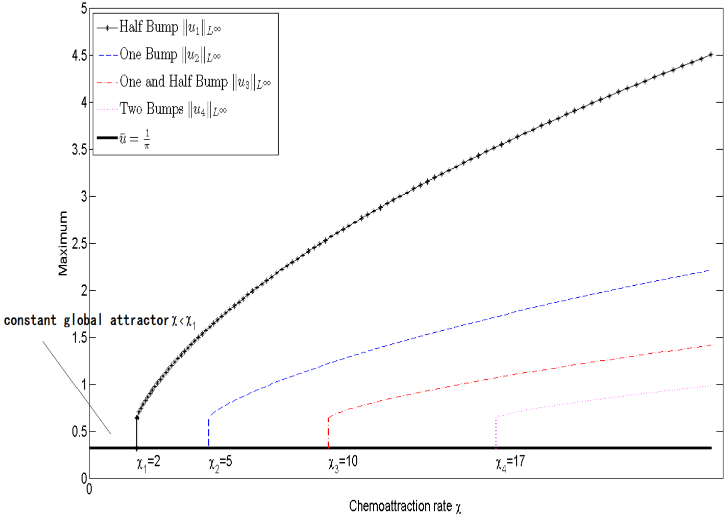

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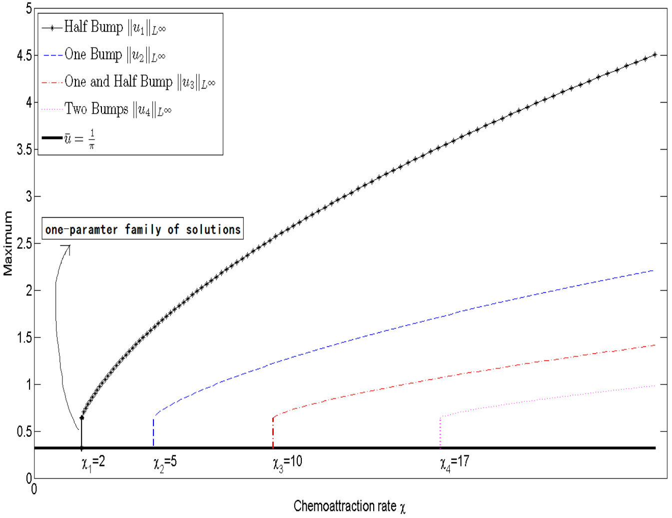

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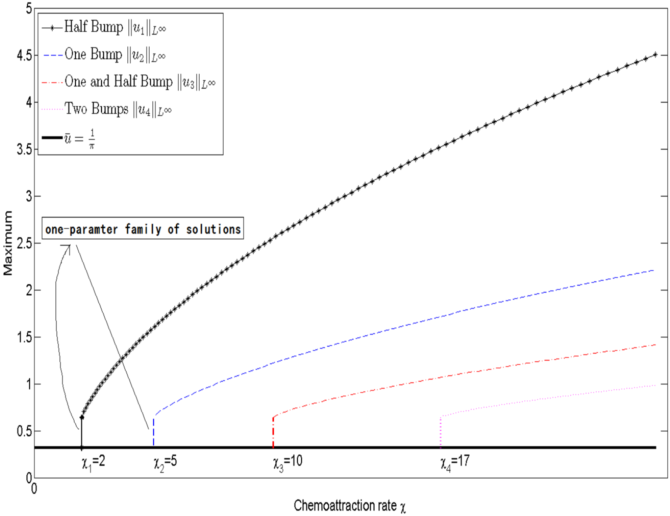

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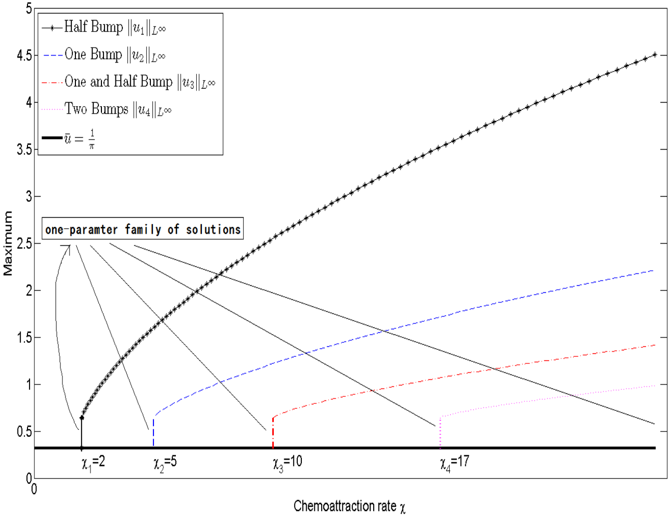

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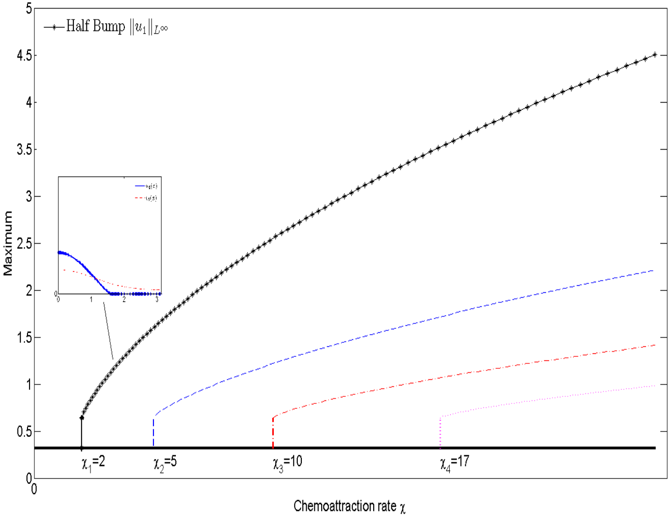

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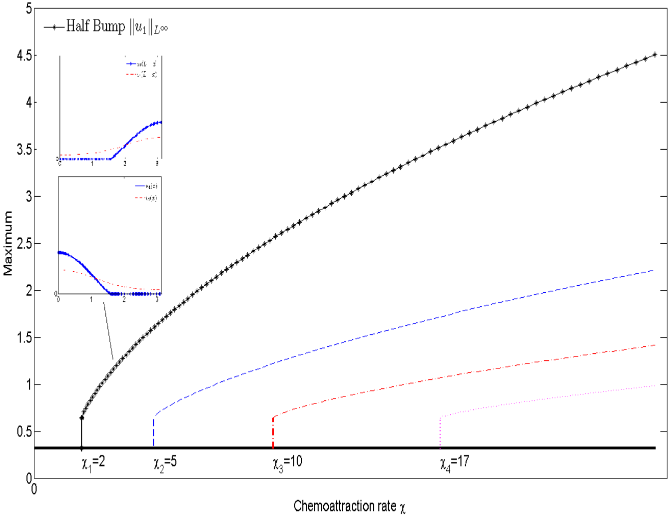

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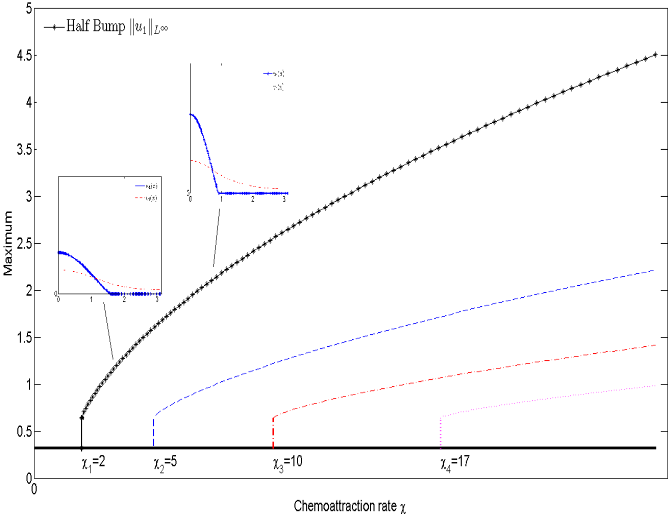

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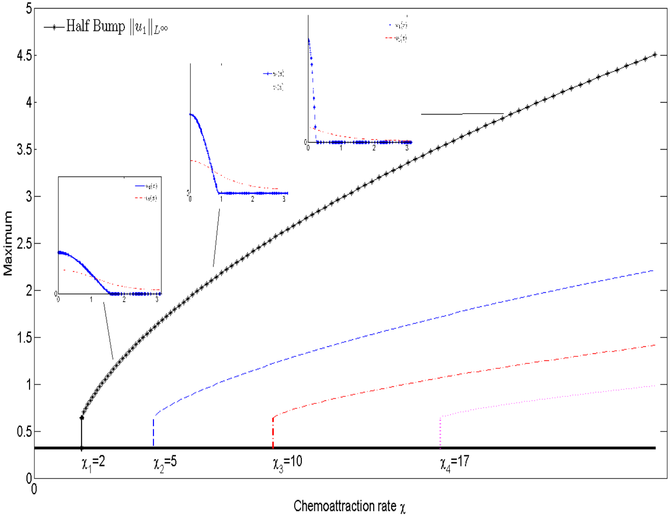

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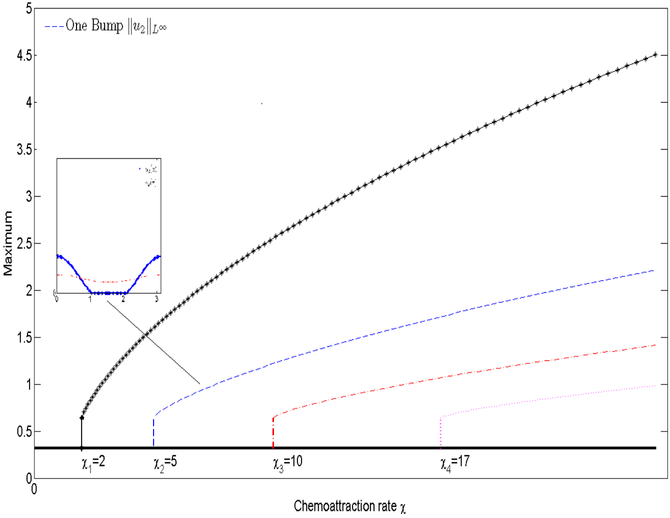

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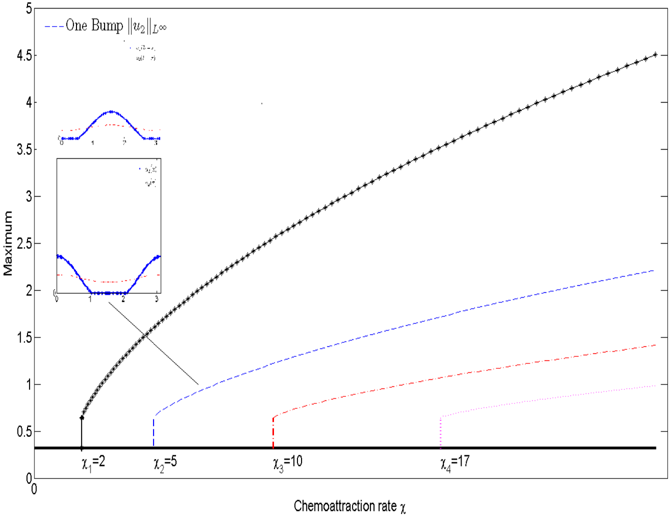

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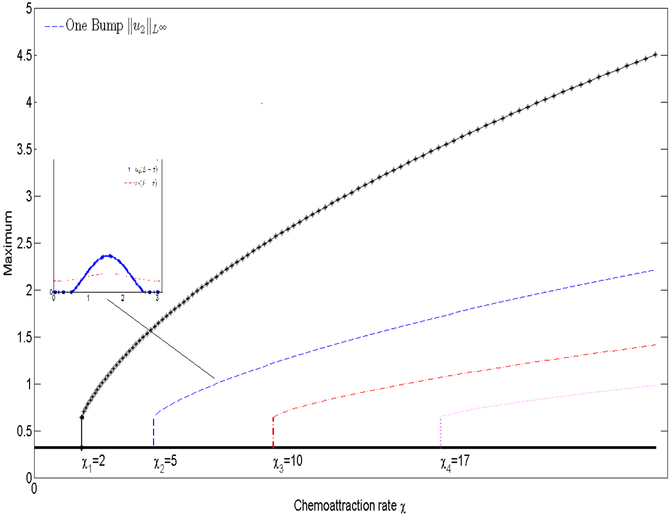

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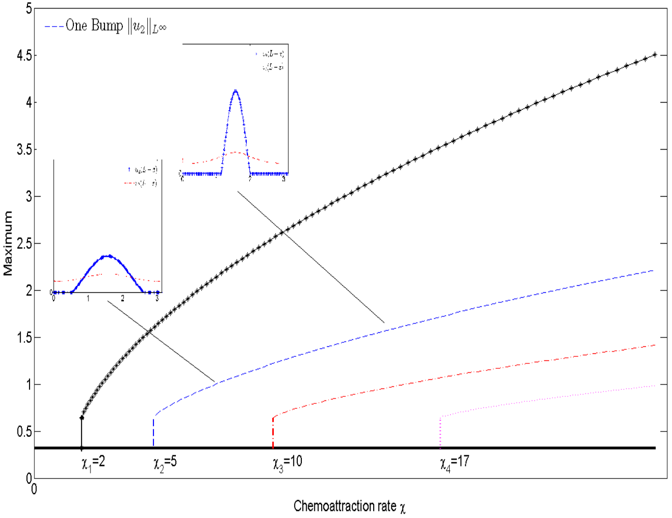

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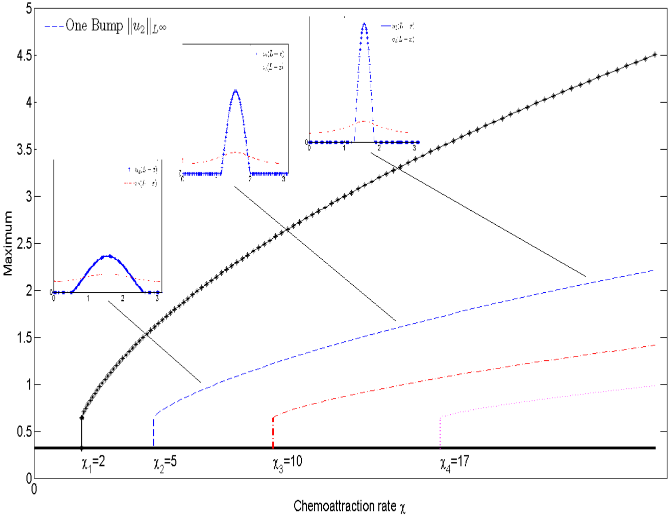

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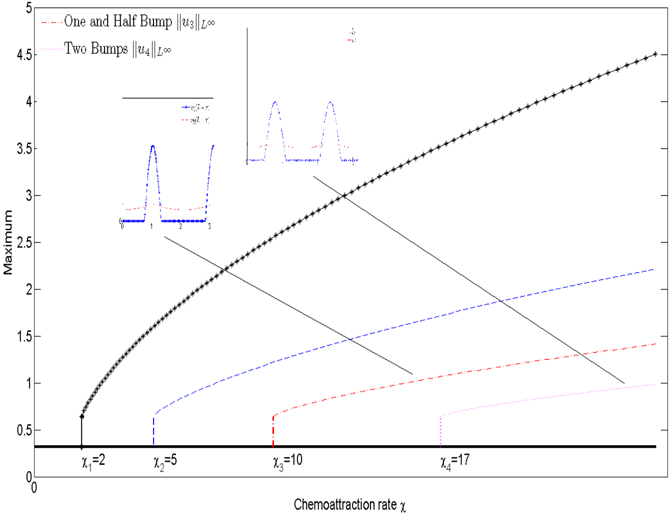

Outline

The Local Cucker-Smale model with noise

Phase Transition (Barbaro-Cañizo-C.-Degond, SIAM MMS 2016)

- We consider the following kinetic flocking model:

$$\partial_t f + v\nabla_x f = \nabla_v \cdot \Big((v - u_f) f - \alpha v(1 - |v|^2) f + D\nabla_v f \Big)\,,$$

where

$$u_f(t,x) = \frac{\int v f(t,x,v)\,dv}{\int f(t,x,v)\,dv}$$

- The first term is a Cucker-Smale-like term, encourages the velocity to align with the mean velocity
- The second term provides self-propulsion and friction, encouraging unit velocities
- The last term captures the influence of noise in the velocity

The homogeneous problem

- Looking at the spatially homogeneous problem:

$$\partial_t f = \nabla_v \cdot \Big((v - u_f) f - \alpha v (1 - |v|^2) f + D \nabla_v f \Big)$$

- We have a gradient flow structure: write the equation as $\partial_t f = \nabla_v \cdot (f \nabla_v \xi)$ with $\xi = \Phi(v) + W * f + D \log f$
  - Confinement in v: $\Phi(v) = \alpha \left(\frac{|v|^4}{4} - \frac{|v|^2}{2} \right)$
  - Interaction potential of the form $W(v) = \frac{|v|^2}{2}$
  - Linear diffusion.
- Our model is continuity equation with velocity field of the form $-\nabla_v \xi$
- Natural entropy for this equation given by the free energy of the system:

$$\mathcal{F}[f] := \int_{\mathbb{R}^d} \Phi(v) f(v)\, dv + \frac{1}{2} \int_{\mathbb{R}^d} \int_{\mathbb{R}^d} W(v - w) f(v) f(w)\, dw\, dv + D \int_{\mathbb{R}^d} f(v) \log f(v)\, dv$$
$$= \int_{\mathbb{R}^d} \left(\alpha \frac{|v|^4}{4} + (1 - \alpha) \frac{|v|^2}{2} \right) f(v)\, dv - \frac{1}{2} |u_f|^2 + D \int_{\mathbb{R}^d} f \log f(v)\, dv\,,$$

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The stationary solutions

- We consider stationary solutions of the form:

$$f(v) = \frac{1}{Z} \exp\left(\frac{-1}{D}\left[\alpha\frac{|v|^4}{4} + (1-\alpha)\frac{|v|^2}{2} - u_f \cdot v\right]\right)$$

- We see that in order for the stationary solution to exist, u_f must be a root of the equation:

$$\mathcal{H}(u, D) = \int (v-u)f(v)dv$$

- We prove that, in any dimension[2]
  - There is a region of parameter space with only one such root, namely $u = 0$
  - There is another region of parameter space with more than one root, $u = 0$ and $|u| = C_{\alpha,D} \neq 0$

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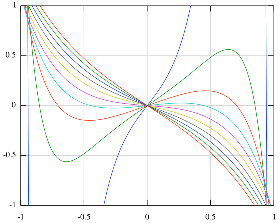
Main idea of our proof



- Our proof hinges Laplace's method and the behavior of $\mathcal{H}(u, D)$ as D varies:
  - For small D, we are able to use Laplace's Method to show that there is a nonzero stationary solution
  - For large D, $\frac{\partial \mathcal{H}}{\partial u}$ is negative for all u.
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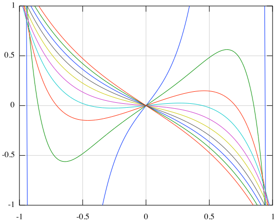

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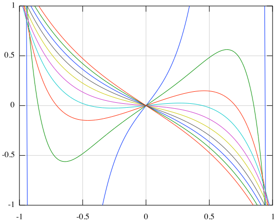

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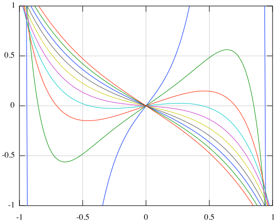

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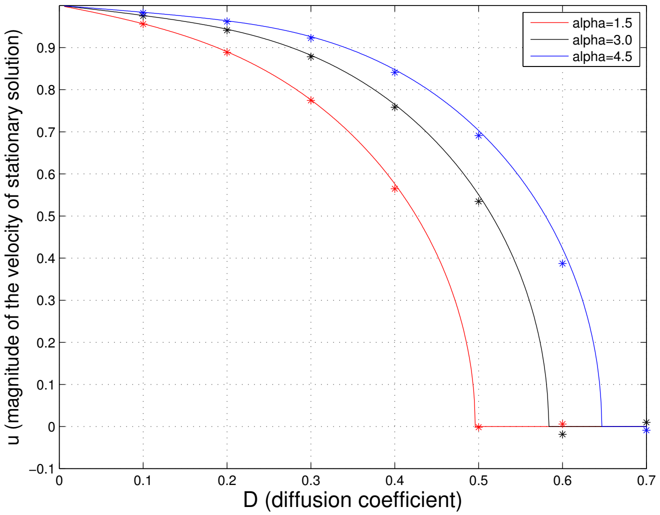
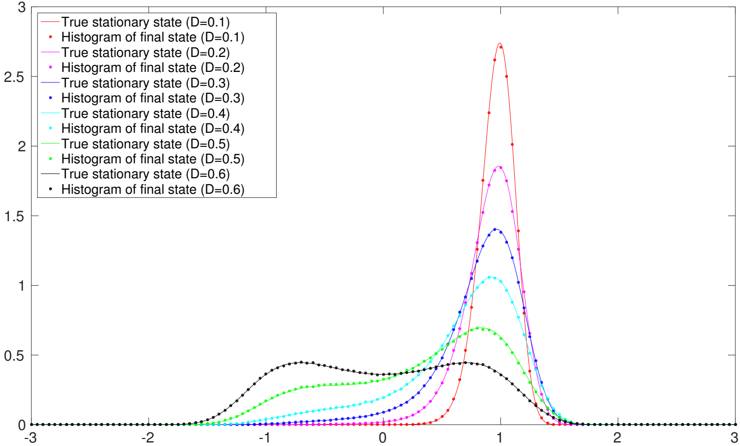
Stability of the stationary solutions in 1D



Comparing particles to f in 1D



Outline

The aggregation diffusion equation

Nonlocal (possibly) degenerate parabolic PDE

$$\partial_t \rho = \Delta \rho^m + \kappa \nabla \cdot (\rho \nabla W \star \rho) \qquad \text{in } \mathbb{T}_L^d \times (0, T]$$

with periodic boundary conditions, $\rho(\cdot, 0) = \rho_0 \in \mathcal{P}(\mathbb{T}_L^d)$, $\mathbb{T}_L^d \hat{=} \left(-\frac{L}{2}, \frac{L}{2}\right)^d = \Omega$, $1 \le m < \infty$.

- $\rho(\cdot, t) \in \mathcal{P}(\Omega)$ probability density of particles
- W coordinate-wise even, mean-zero interaction potential
- $\kappa > 0$ interaction strength (parameter)

Assume throughout that

$$W(x) \in C^2(\Omega)$$

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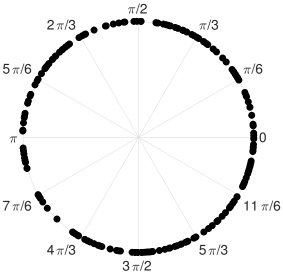
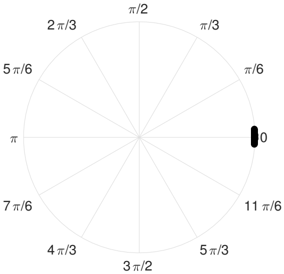
Example: The noisy Kuramoto model

The Kuramoto model:$m = 1$, $W(x) = -\sqrt{\frac{2}{L}} \cos\left(2\pi k \frac{x}{L}\right), k \in \mathbb{Z}$



$\kappa < \kappa_c$, no phase locking



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Goals and Motivation:

- Bifurcations
- Classification for continuous and discontinuous transitions
- Better understanding of the free energy landscape

H-stability

Notation: Fourier representation $\hat{f}(k) = \langle f, w_k \rangle_{L^2(\mathbb{T}_L)}$ with $k \in \mathbb{Z}^d$

$$w_k(x) = L^{-d/2}\Theta(k)\prod_{i=1}^{d} w_{k_i}(x_i) \qquad \text{with} \qquad w_{k_i}(x_i) = \begin{cases} \cos\left(\frac{2\pi k_i}{L}x_i\right) & k_i > 0, \\ 1 & k_i = 0, \\ \sin\left(\frac{2\pi k_i}{L}x_i\right) & k_i < 0, \end{cases}$$

$$\Theta(k) = 2^{\#\{i:k_i=0\}/2}$$

Definition (H-stability)

An even function $W \in L^2(\mathbb{T}_L^d)$ is H-stable, $W \in \mathbb{H}_s$, if

$$\hat{W}(k) = \langle W, w_k \rangle \geq 0, \quad \forall k \in \mathbb{Z}^d \ ,$$

Decomposition of potential W into H-stable and H-unstable part

$$W_{\mathrm{s}}(x) = \sum_{k\in\mathbb{N}^d} (\langle W, w_k \rangle)_+ w_k(x) \qquad \text{and} \qquad W_{\mathrm{u}}(x) = W(x) - W_s(x) \ .$$

Free energy

The equations have the following free energy, $\mathcal{F}_\kappa^m : \mathcal{P}(\Omega) \to \mathbb{R} \cup \{+\infty\}$, associated to them

$$\mathcal{F}_\kappa^m := \begin{cases} \frac{1}{m-1}\int_\Omega \rho^m(x)\,\mathrm{d}x - \frac{1}{m-1} + \frac{\kappa}{2}\iint_{\Omega\times\Omega} W(x-y)\rho(x)\rho(y)\,\mathrm{d}x\,\mathrm{d}y & m > 1 \\ \int_\Omega (\rho\log\rho)(x)\,\mathrm{d}x + \frac{\kappa}{2}\iint_{\Omega\times\Omega} W(x-y)\rho(x)\rho(y)\,\mathrm{d}x\,\mathrm{d}y & m = 1 \end{cases}$$

W_2-gradient flow w.r.t this energy

Theorem (Existence of minimisers)

- $m = 1$: *For $\kappa \in (0,\infty)$ the free energy $\mathcal{F}_\kappa(\rho)$ has a smooth minimiser $\rho_\kappa \in C^\infty(\Omega) \cap \mathcal{P}(\Omega)$. For $\kappa \ll 1$ or $W \in \mathbb{H}_s$, $\mathcal{F}_\kappa$ is strictly convex and ρ_∞ is the unique minimiser.*
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Characterisation of stationary solutions

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- Self-consistency equation $m > 1$

$$F_\kappa^m(\rho) = \frac{m}{m-1} \rho^{m-1} + \kappa W \star \rho - C$$

for some constant C.

Definition (Weak stationary solution)

A weak stationary solution for $m > 1$ is a bounded, measurable function

$$\rho^m \in H^1(\Omega)$$

such that

$$\int_\Omega \left(\nabla \rho^m \cdot \nabla \phi + \rho \nabla (W \star \rho) \cdot \nabla \phi \right) \mathrm{d}x = 0$$

for all $\phi \in H_0^1(\Omega)$.

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for all $\phi \in H_0^1(\Omega)$.

Characterisation of stationary solutions

Characterization of stationary states($m = 1$): TFAE

- ρ is a classical stationary solution of $\Delta\rho + \kappa\nabla \cdot (\rho\nabla W \star \rho) = 0$
- ρ is a zero of $F_\kappa(\rho)$
- ρ is a critical point of $\mathcal{F}_\kappa(\rho)$.

Characterization of stationary states($m > 1$): TFAE

- ρ is a weak stationary solution of $\Delta\rho^m + \kappa\nabla \cdot (\rho\nabla W \star \rho) = 0$
- For every connected component A of its support ρ satisfies the self-consistency equation, i.e.,

$$\frac{m}{m-1}\rho^{m-1} + \kappa W \star \rho = C(A, \rho)$$

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$\Rightarrow \rho_\infty \equiv L^{-d}$ is a stationary state for all $\kappa > 0$.

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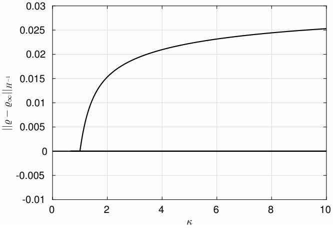
Nontrivial solutions to the stationary McKean–Vlasov eq'n?

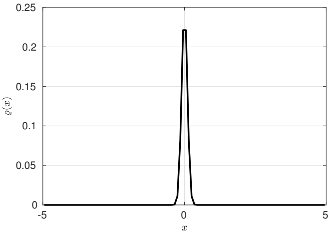
- $W \notin \mathbb{H}_s$ needs to be a necessary condition
- Numerical experiments indicate one, multiple, or possibly infinite solutions
- What determines the number of nontrivial solutions?
- Birfurcation analysis of $\rho \mapsto F_\kappa(\rho)$

Example: Kuramoto model:

$$W(x) = -\sqrt{\frac{2}{L}}\cos(2\pi x/L)$$



Bifurcation diagram for the Kuramoto model



The clustered solution

Local bifurcation result $m = 1$

$$F_\kappa(\rho) = \rho - \mathcal{T}\rho = \rho - \frac{1}{Z(\rho,\kappa)} e^{-\kappa W \star \rho}\,, \quad \text{with} \quad Z(\rho,\kappa) = \int_{\mathbb{T}_L^d} e^{-\kappa W \star \rho}\, \mathrm{d}xx\,.$$

Theorem ([C.-Gvalani-Pavliotis-Schlichting ARMA '20])

Consider $F : L^2_s(\mathbb{T}^d_L) \times \mathbb{R}_{>0} \to L^2_s(\mathbb{T}^d_L)$ *with* $F(u,\kappa) = F_\kappa(u + \rho_\infty)$ *and* $W \in L^2_s(\mathbb{T}^d_L)$ *with* $L^2_s(\mathbb{T}^d_L)$ *the subspace of coordinate-wise even functions. Assume there exists* $k^* \in \mathbb{N}^d$*, such that:*

1. $\operatorname{card}\{k \in \mathbb{N}^d : \hat{W}(k)/\Theta(k) = \hat{W}(k^*)/\Theta(k^*)\} = 1$
2. $\hat{W}(k^*) < 0$

Then, $(0,\kappa_*)$ *is a bifurcation point of* $F(u,\kappa) = 0$*, where,* $\kappa_* = -\frac{L^{\frac{d}{2}}\Theta(k^*)}{\hat{W}(k^*)}$ *. The branch of solutions* $(\rho^*_s, \kappa(s))$ *has the following form*

$$\rho^*_s = \rho_\infty + s w_{k^*} + r(\kappa(s), s)\,.$$

for $s \in (-\delta,\delta)$ *and* $r \sim o(s)$*. Also,* $\kappa(0) = \kappa_*$*,* $\kappa'(0) = 0$*, and* $\kappa''(0) = 1$*.*

Use Crandall–Rabinowitz theorem and Look at higher order Fréchet derivatives of F to study structure of the branch

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Local bifurcation result $m > 1$

Define the map, $F : H^n_{0,s}(\Omega) \times \mathbb{R}_+ \to H^n_{0,s}(\Omega)$ for $n > d/2$ which is given by

$$F(\eta, \kappa) := \frac{m}{m-1}(\rho_\infty + \eta)^{m-1} + \kappa W \star \eta - \frac{m}{|\Omega|\,(m-1)} \|\rho_\infty + \eta\|^{m-1}_{L^{m-1}(\Omega)} \ .$$

Theorem ([C.-Gvalani, preprint])

Consider the map $F : H^n_{0,s}(\Omega) \times \mathbb{R}_+ \to H^n_{0,s}(\Omega)$ *for* $n > d/2$ *as defined above with its trivial branch* $(0, \kappa)$*. Assume there exists* $k^* \in \mathbb{N}^d, k \neq 0$ *such that the following two conditions are satisfied*

1. $\hat{W}(k^*) < 0$
2. $\mathrm{card}\left\{k \in \mathbb{N}^d, k \neq 0 : \frac{\hat{W}(k)}{\Theta(k)} = \frac{\hat{W}(k^*)}{\Theta(k^*)}\right\} = 1 \quad ,$

then $(0, \kappa_*)$ *is a bifurcation point of* $(0, \kappa)$ *with* $\kappa_* = -\frac{\sqrt{2}m\rho_\infty^{m-3/2}}{\hat{W}(k^*)}$ *, there exists a neigbourhood* N *of* $(0, \kappa_*)$ *and a curve* $(\eta(s), \kappa(s)) \in N, s \in (-\delta, \delta), \delta > 0$ *such that* $F(\eta(s), \kappa(s)) = 0$*. Additionally* $\eta(s)$ *has the form*

$$\eta(s) = s e_{k_*} + r(s e_{k_*}, \kappa s)\,, \tag{1}$$

where $\|r\|_{H^n_{0,s}(\Omega)} = o(s)$ *as* $s \to 0$*.*

Examples of birfucations results

- Kuramoto-type of models: $W(x) = -w_k(x)$ in $d = 1$

$$\hat{W}(k) = -1,$$

satisfying both conditions. Thus we have that $\kappa_* = \sqrt{2L}$

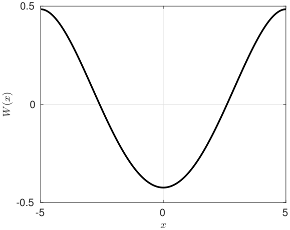
- For $W(x) = \frac{x^2}{2}$ holds

$$\hat{W}(k) = \frac{L^{5/2}\cos(\pi k)}{2\sqrt{2}\pi k^2}$$

satisfying both conditions for odd values of k. Hence, every odd k is birfucation point $\kappa_* = \frac{4k^2}{L^2}$.

- $W^s(x) = -\sum_{k=1}^{\infty} \frac{1}{k^{2s+2}} w_k(x)$

For $s \geq 1 : W^s(x) \in H^s(\mathbb{T}_L^d)$
$\forall k > 0$: conditions (1) and (2) ok
Infinitely many bifurcation points



Further examples of bifurcation results

Corollary (Keller–Segel)

Consider the stationary parabolic-elliptic Keller–Segel equation, i.e., $W \star \rho = -(-\Delta)^{-s}\rho$. For $d \leq 2$ and $s \in (\frac{1}{2}, 1]$, it has smooth solutions and its trivial branch (ρ_∞, κ) has infinitely many bifurcation points.

Corollary (Liquid crystals)

We have the following results for $W_\ell(x) = |*| \sin(2\pi x/L)^\ell, \ell \in \mathbb{N}$:

- *The trivial branch of the Onsager model, $W_1(x)$, has infinitely many bifurcation points.*
- *The trivial branch of the Maiers–Saupe model, $W_2(x)$, has exactly one bifurcation point.*
- *The trivial branch of the model $W_\ell(x)$ for ℓ even has at least $\frac{\ell}{4}$ bifurcation points if $\frac{\ell}{2}$ is even and $\frac{\ell}{4} + \frac{1}{2}$ bifurcation points if $\frac{\ell}{2}$ is odd.*
- *The trivial branch of the model $W_\ell(x)$ for ℓ odd has infinitely many bifurcation points if $\frac{\ell-1}{2}$ is even and at least $\frac{\ell+1}{4}$ bifurcation points if $\frac{\ell-1}{2}$ is odd.*

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- *The trivial branch of the model $W_\ell(x)$ for ℓ odd has infinitely many bifurcation points if $\frac{\ell-1}{2}$ is even and at least $\frac{\ell+1}{4}$ bifurcation points if $\frac{\ell-1}{2}$ is odd.*

Outline

Transition points: Change in the set of minimizers

New stationary solutions obtain via local bifurcation need not be new minimisers.

Question: When do we get new minimisers?

Definition (Transition point [Chayes-Panferov '10])

A parameter value $\kappa_c > 0$ is said to be a transition point of an energy E_κ if it satisfies the following conditions,

1. *For $0 < \kappa < \kappa_c$: ρ_∞ is the unique minimiser of $E_\kappa(\rho)$*
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Definition (Continuous and discontinuous transition point)

A transition point $\kappa_c > 0$ is a continuous transition point of $\mathcal{F}_\kappa$ if

1. *For $\kappa = \kappa_c$: ρ_∞ is the unique minimiser of $E_\kappa(\rho)$*
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Basic properties of transition points, $m = 1$

Summary of critical points:

- κ_c transition point
- κ_* bifurcation point
- $\kappa_\sharp$ point of linear stability, i.e., $\kappa_\sharp = -\frac{L^{\frac{d}{2}}}{\min_k \hat{W}(k)/\Theta(k)}$.

  If $k_\sharp = \arg\min \hat{W}(k)$ is unique, then $\kappa_\sharp = \kappa_*$ is a bifurcation point.

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

- $\mathcal{F}_\kappa$ has a transition point κ_c iff $W \notin \mathbb{H}_s$
- $\min \mathcal{F}_\kappa$ is non-increasing as a function of κ
- If for some κ' : ρ_∞ is no longer the unique minimiser, then $\forall \kappa > \kappa'$: ρ_∞ is no longer a minimizer
- If κ_c is continuous, then $\kappa_c = \kappa_\sharp$

Conclusion:

- To prove a discontinuous transition: Show ρ_∞ is no longer global minimizer at $\kappa_\sharp$.
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Conditions for continuous and discontinuous phase transition

Theorem ([C.-Gvalani-Pavliotis-Schlichting ARMA '20])

Let $W(x) \in \mathbb{H}_s^c$.

- *If there exist (near)-resonating dominant modes:*
  That is for δ small enough

$$k^a, k^b, k^c \in \left\{ k' \in \mathbb{N}^d : \frac{\hat{W}(k')}{\Theta(k')} \leq \min_{k \in \mathbb{N}^d} \frac{\hat{W}(k)}{\Theta(k)} + \delta \right\} := K^\delta$$

  satisfying $k^a = k^b + k^c$, then there exists a discontinuous transition point $\kappa_c < \kappa_\sharp$.

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

$$\alpha \tilde{W}(k^\sharp) \leq \tilde{W}(k) \qquad \textit{for all } k \neq k^\sharp : \tilde{W}(k) < 0 \,,$$

  then the transition point $\kappa_c = \kappa_\sharp = \kappa_*$ is continuous.

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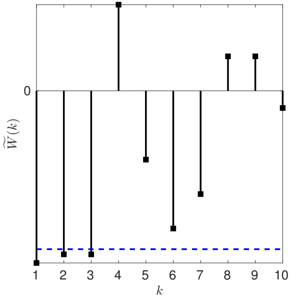
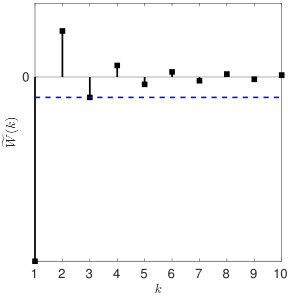


The near resonating dominant modes scenario



The dominant mode scenario

What can we say for $m > 1$?

Can we reproduce the results obtained with linear diffusion?

Proposition ([C.-Gvalani, preprint])

Assume that $W \in \mathbb{H}_s^c$. Then $\mathcal{F}_\kappa^m$ has a transition point at some $\kappa_c \leq \kappa_\sharp$ where $\kappa_\sharp = -\frac{\sqrt{2}m\rho_\infty^{m-3/2}}{\min_{k\in\mathbb{N}} \hat{W}(k)}$ is the point of linear stability. If κ_c is continuous, then $\kappa_c = \kappa_\sharp$.

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Assume κ_c is a discontinuous transition point. Then, there exists $\rho_{\kappa_c} \neq \rho_\infty$ such that $\mathcal{F}_{\kappa_c}^m(\rho_{\kappa_c}) = \mathcal{F}_{\kappa_c}^m(\rho_\infty)$, i.e., there exists a nontrivial minimiser at $\kappa = \kappa_c$.

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Theorem (Stability of discontinuous transition points around $m = 1$)

Let W be such that $\mathcal{F}^m_\kappa$ has a discontinuous transition point for $m = 1$ and $\kappa_c < \kappa^1_\sharp$. Then for $1 \le m < 1 + \varepsilon$ for some $\varepsilon > 0$ small enough, $\mathcal{F}^m_\kappa$ has a discontinuous transition point at $\kappa^m_c < \kappa^m_\sharp$.

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Assume $W \in \mathbb{H}^c_s$ such that β_c is a transition point of $\mathcal{F}^m_\beta$. Then if $m \in [2, 3]$, β_c is a discontinuous transition point.

No general conditions for continuous transition points. We give examples of continuous phase transitions for a large class of potentials for $m = 4$.

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$$k^a, k^b, k^c \in \left\{ k' \in \mathbb{N}^d : \frac{\hat{W}(k')}{\Theta(k')} \leq \min_{k \in \mathbb{N}^d} \frac{\hat{W}(k)}{\Theta(k)} + \delta \right\} := K^\delta$$

satisfying $k^a = k^b + k^c$, then there exists a discontinuous transition point $\kappa_c < \kappa_\sharp$.

Assume $W \in \mathbb{H}_s^c$ such that β_c is a transition point of $\mathcal{F}_\beta^m$. Then if $m \in [2, 3]$, β_c is a discontinuous transition point.

No general conditions for continuous transition points. We give examples of continuous phase transitions for a large class of potentials for $m = 4$.

What can we say for $m > 1$?

Theorem (Stability of discontinuous transition points around $m = 1$)

Let W be such that $\mathcal{F}_\kappa^m$ has a discontinuous transition point for $m = 1$ and $\kappa_c < \kappa_\sharp^1$. Then for $1 \le m < 1 + \varepsilon$ for some $\varepsilon > 0$ small enough, $\mathcal{F}_\kappa^m$ has a discontinuous transition point at $\kappa_c^m < \kappa_\sharp^m$.

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Conclusions

- Aggregation-diffusion equations can lead to complicated phase transitions and bifurcations diagrams.
- General conditions for continuous or discontinuous phase transitions depending on the interaction potential.
- Nonlinear diffusion lead to particular effects: persistence of discontinuous phase transitions and one parameter families of solutions a bifurcation points.
- References:
  1. Barbaro-Cañizo-C.-Degond (SIAM MMS 2016).
  2. C.-Chen-Wang-Wang-Zhang (SIAM J. Applied Mathematics 2020).
  3. C.-Gvalani-Pavliotis-Schlichting (ARMA 2020).
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