Collective dynamics in life sciences

Lecture 3. Phase transitions in the Vicsek model

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Summary

1. Phase transitions in the Vicsek model

Particle system

self-propelled $\Rightarrow$ constant velocity

align with their neighbours up to a certain noise

Time-discrete model

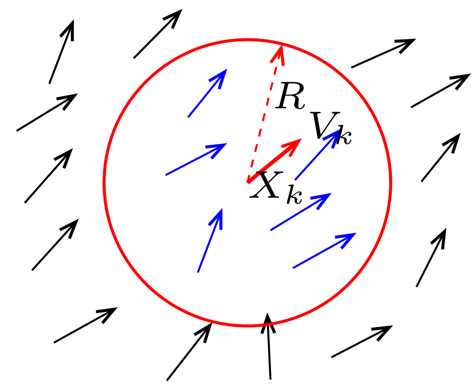
k-th particle position X_k^n, velocity V_k^n, at time $t^n = n\Delta t$

$$|V_k^n| = 1$$

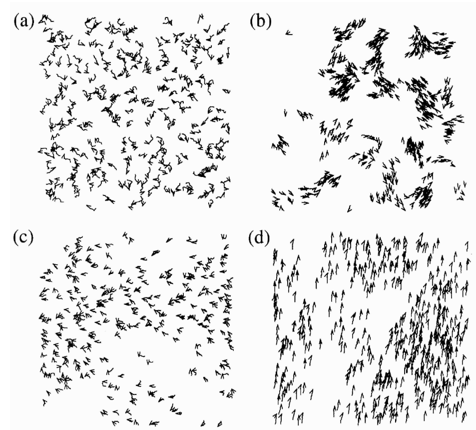
$$X_k^{n+1} = X_k^n + V_k^n \Delta t,$$

$$\bar{V}_k^n = \frac{\mathcal{J}_k^n}{|\mathcal{J}_k^n|}, \quad \mathcal{J}_k^n = \sum_{j, |X_j^n - X_k^n| \leq R} V_j^n$$

$$\arg(V_k^{n+1}) = \arg(\bar{V}_k^n + \tau_k^n)$$



τ_k^n drawn uniformly in $[-\tau, \tau]$; $R =$ interaction range



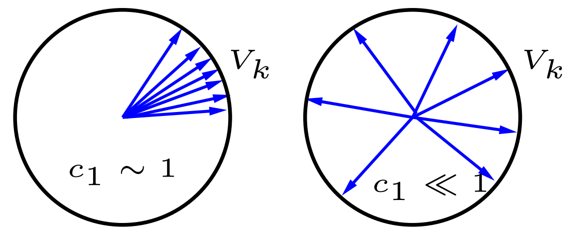
Phase transition

disordered → aligned state

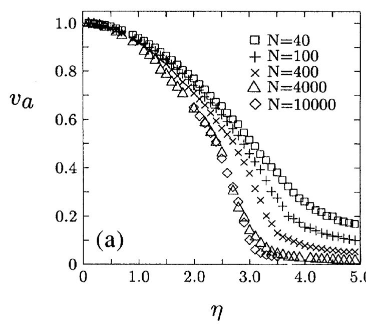
Symmetry breaking

Order parameter measures alignment

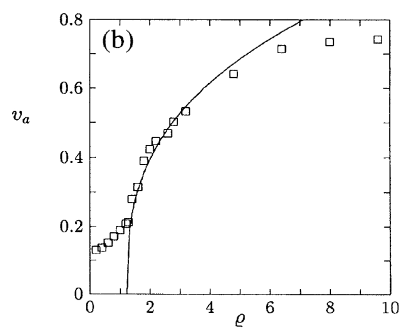
$$c_1 = \left| N^{-1} \sum_j V_j \right|, \quad 0 \le c_1 \le 1$$



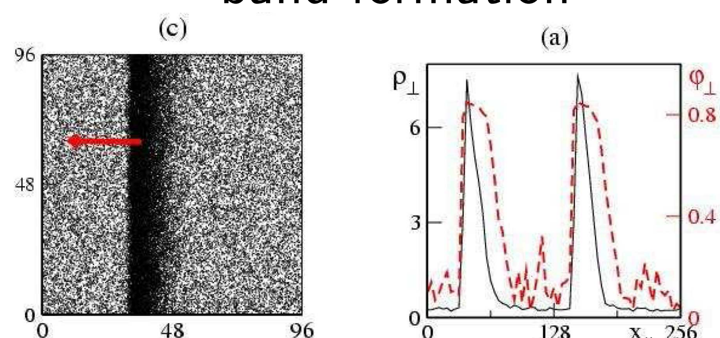
c_1 vs noise



c_1 vs density



band formation



after [Chaté et al, PRE 2008]

2. Mathematical analysis of the phase transitions

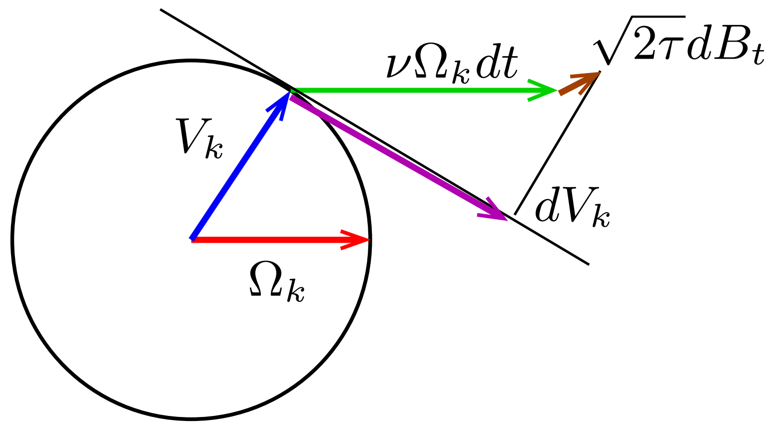
$$\dot{X}_k(t) = V_k(t), \qquad |V_k(t)| = 1$$

$$dV_k(t) = P_{V_k^\perp}(\nu\,\bar{V}_k dt + \sqrt{2\tau} \circ dB_t^k), \quad P_{V_k^\perp} = \mathrm{Id} - V_k \otimes V_k$$

$$\bar{V}_k = \frac{\mathcal{J}_k}{|\mathcal{J}_k|}, \quad \mathcal{J}_k = \sum_{j, |X_j - X_k| \leq R} V_j$$

ν collision frequency τ noise intensity

$P_{V_k^\perp}$ maintains $|V_k(t)| = 1$

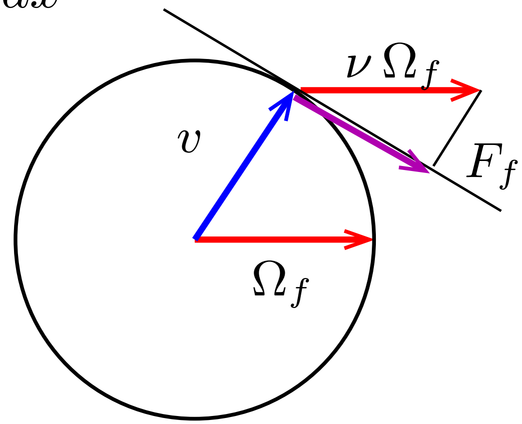


$f(x,v,t) =$ 1-particle proba distr. $(v \in \mathbb{R}^n,\ |v| = 1)$

$$\partial_t f + v \cdot \nabla_x f = -\nabla_v \cdot (F_f f) + \tau \Delta_v f$$

$$F_f = \nu\, P_{v^\perp} \bar v_f, \quad P_{v^\perp} = (\mathrm{Id} - v \otimes v), \quad \bar v_f = \frac{\mathcal{J}_f}{|\mathcal{J}_f|}$$

$$\mathcal{J}_f = \int_{(x',v')} K\Big(\frac{|x'-x|}{R}\Big)\, f(x',v',t)\, v'\, dv'\, dx'$$



$\bar v_f =$ direction of locally averaged flux

Here, we assume:

$$\nu = \nu(|\mathcal{J}_f|)\ , \quad \tau = \tau(|\mathcal{J}_f|)$$

Forget the space-variable: $\nabla_x \equiv 0$

Motivation: medium-scale size observations

Find the equilibria

Use them as LTE in hydrodynamic expansion

Local Thermodynamic Equilibria

Global existence result in [Figalli, Kang, Morales, arXiv:1509.02599]

Spatially homogeneous system: $f(v,t), \quad v \in \mathbb{R}^n, \quad |v| = 1$

$$\partial_t f = -\nabla_v \cdot (F_f f) + \tau(|J_f|)\, \Delta_v f := Q(f)$$

$$F_f = \nu(|J_f|)\, P_{v^\perp} u_f, \quad u_f = \frac{J_f}{|J_f|}, \quad J_f = \int_{v'} f(v',t)\, v'\, dv'$$

Note that $\partial_t \rho = 0$

$$\rho(t) = \int f(v,t)\, dv = \text{Constant}$$

Equilibria are functions $f(v)$ such that $Q(f) := 0$

$$Q(f) = \tau(|J_f|)\nabla_v \cdot \big[- k(|J_f|)\, P_{v^\perp} u_f\, f + \nabla_v f \big] \quad \text{with} \quad k(|J|) = \frac{\nu(|J|)}{\tau(|J|)}$$

Von Mises-Fisher (VMF) distribution $M_{\kappa u}$:

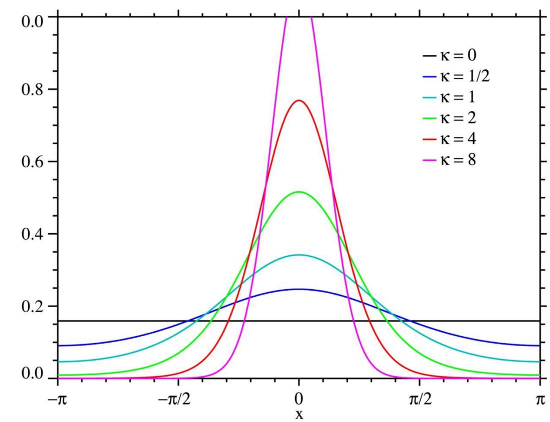
$$M_{\kappa u}(v) = \frac{e^{\kappa\, u \cdot v}}{\int e^{\kappa\, u \cdot v}\, dv}$$

$\kappa > 0$: concentration parameter ; $u \in \mathbb{R}^n$, $|u| = 1$: orientation

Order parameter: $c_1(\kappa) = \int M_{\kappa u}(v)\, (u \cdot v)\, dv$

$$\kappa \overset{\nearrow}{\longrightarrow} c_1(\kappa), \quad 0 \leq c_1(\kappa) \leq 1$$

Flux: $\int M_{\kappa u}(v)\, v\, dv = c_1(\kappa) u$



Compatibility condition

Equilibria are of the form $\quad f(v) = \rho\, M_{\kappa u}(v)$

where $\rho > 0$ and $u \in \mathbb{R}^n$ s.t. $|u| = 1$ are arbitrary

Current given by: $|J_f| = \rho c_1(\kappa)$

From expression of Q, κ must be equal to $k(|J_f|)$

Leads to compatibility condition

$$\kappa = k(\rho c_1(\kappa)) \quad \text{or equivalently} \quad \rho = \frac{j(\kappa)}{c_1(\kappa)}$$

where $j(\kappa)$ is the inverse function of $k(|J|)$ $\quad (|J| \xrightarrow{\nearrow} k(|J|))$:

$$\kappa = k(|J|) \Longleftrightarrow |J| = j(\kappa)$$

Number of roots and local monotony of $\frac{j(\kappa)}{c_1(\kappa)}$

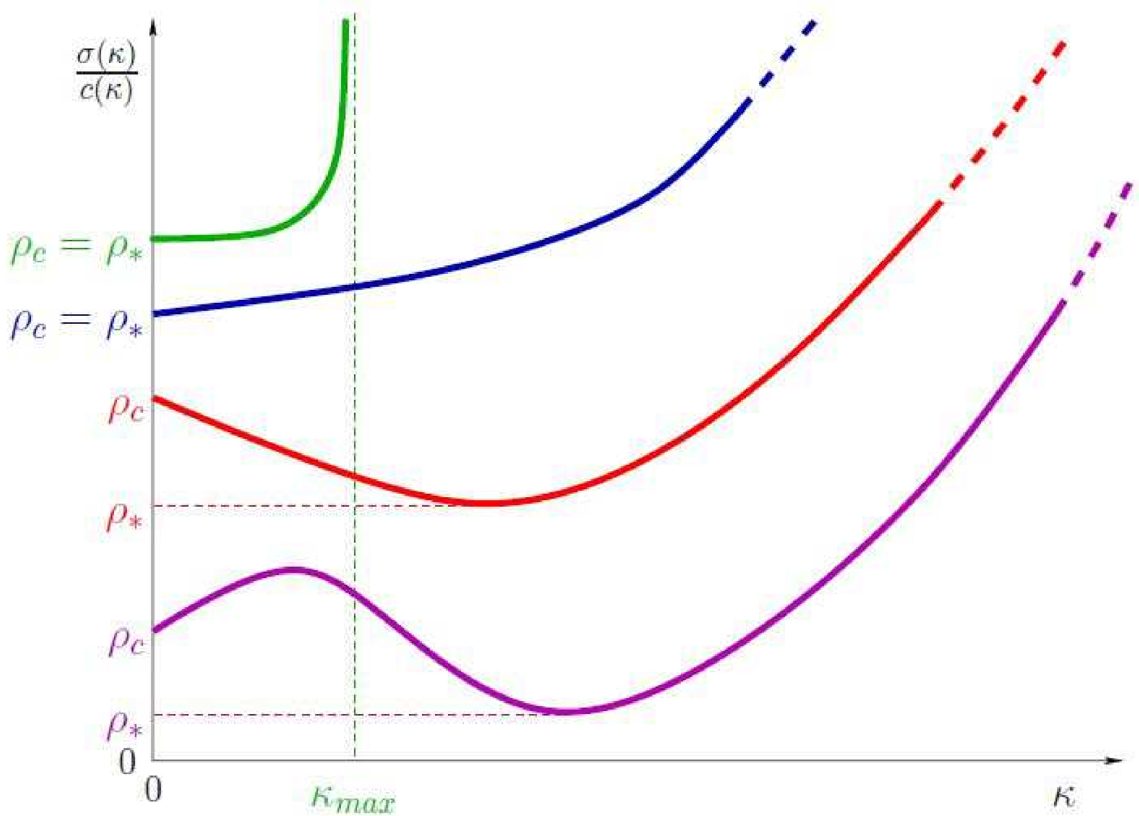
determine number of equilibria and their stability

The function $\kappa \to \frac{j(\kappa)}{c(\kappa)}$

We assume $|J| \to \tau(|J|)$ and $|J| \to \frac{\nu(|J|)}{|J|}$ smooth

Define $\rho_* = \min_{\kappa>0} \frac{j(\kappa)}{c_1(\kappa)}$, $\rho_c = \lim_{\kappa\to 0} \frac{j(\kappa)}{c_1(\kappa)}$, $\rho_* \leq \rho_c$

But monotony of $\kappa \to \frac{j(\kappa)}{c_1(\kappa)}$ can be arbitrary



$\kappa = 0$ (uniform distribution) always a solution

If $\rho < \rho_*$, the only equilibrium

If $\rho > \rho_*$, $\exists$ non-isotropic equilibria

Number of classes of non-isotropic equilibria (different κ's)

$= $ number of roots of $\frac{j(\kappa)}{c_1(\kappa)} = \rho$

Stability:

Isotropic equilibria are stable if $\rho < \rho_c$, unstable if $\rho > \rho_c$

Non-isotropic equilibria are stable if $\frac{j(\kappa)}{c_1(\kappa)} \nearrow$, unstable if $\searrow$

In non-isotropic case, stability means that:

if f_0 is close to equilibrium $f_{\text{eq}} = \rho M_{\kappa u}$

solution $f(t) \to \tilde{f}_{\text{eq}} = \rho M_{\kappa \tilde{u}}$ as $t \to \infty$

but $\tilde{u}$ may be $\neq u$

Free energy

Free energy

$$\mathcal{F}(f) = \int f \, \ln f \, dv - \Phi(|J_f|) \quad \text{with} \quad \Phi' = k$$

Free energy dissipation

$$\mathcal{D}(f) = \tau(|J_f|) \int f \left| \nabla_v f - k(|J_f|)(v \cdot u_f) \right|^2 dv \quad \text{with} \quad u_f = \frac{J_f}{|J_f|}$$

Free energy dissipation identity $\quad \frac{d}{dt}\mathcal{F}(f) = -\mathcal{D}(f) \leq 0$

Free energy decays with time

f is an equilibrium iff $\mathcal{D}(f) = 0$

Stability / Instability of isotropic equilibria

Behavior determined by first spherical harmonics, i.e. by J_f

$$\frac{d}{dt} J_f = -(n-1)\tau_0 \Big(1 - \frac{\rho}{\rho_c}\Big) J_f + \text{h. o. t.} \quad \text{with} \quad \tau_0 = \tau\big|_{|J|=0}$$

In stable case, convergence to equilibrium with rate λ_0

$$\lambda_0 = (n-1)\tau_0 \Big(1 - \frac{\rho}{\rho_c}\Big)$$

Instability of non-isotropic equilibria proved by showing:

In any neighborhood of an unstable equilibrium $f_{\text{eq}} = \rho M_{\kappa u}$,

$\exists\ f_0$ with $\mathcal{F}(f_0) < \mathcal{F}(f_{\text{eq}})$

Then $\mathcal{F}(f(t)) \leq \mathcal{F}(f_0) < \mathcal{F}(f_{\text{eq}})$

$f(t)$ cannot converge to any equilibrium of the same family

$\tilde{f}_{\text{eq}} = \rho M_{\kappa \tilde{u}}$ with any $\tilde{u}$ since $\mathcal{F}(\tilde{f}_{\text{eq}}) = \mathcal{F}(f_{\text{eq}})$

Stability / instability (2)

Stability of non-isotropic equilibrium uses that

if $\left(\frac{j}{c_1}\right)' > 0$, we have

$$\|f(t) - \rho M_{\kappa u_{f(t)}}\|_{L^2}^2 \sim \mathcal{F}(f(t)) - \mathcal{F}(\rho M_{\kappa u_{f(t)}})$$

and this quantity is decreasing

Convergence to limit equilibrium with rate λ_κ

$$\lambda_\kappa = \frac{c_1 \tau(j)}{j'}(\kappa)\ \Lambda_\kappa \left(\frac{j}{c_1}\right)'(\kappa)$$

where Λ_κ is the best Poincaré constant for

$$\int |\nabla_v g|^2 \, M_{\kappa u}(v) dv \geq \Lambda_\kappa \int |g - \langle g \rangle|^2 \, M_{\kappa u}(v) dv, \quad \langle g \rangle = \int g(v) M_{\kappa u}(v) dv$$

Relies on estimate on the free energy dissipation

$$\mathcal{D}(f) \geq 2\lambda_\kappa (\mathcal{F}(f) - \mathcal{F}(M_{\kappa u})) + \mathcal{O}\big((\mathcal{F}(f) - \mathcal{F}(M_{\kappa u}))^{1+\varepsilon}\big)$$

Assume $\kappa \to \frac{j(\kappa)}{c_1(\kappa)}$ increasing: then $\rho_c = \rho_*$

If $\rho < \rho_c$: isotropic distribution = only equilibrium and stable

If $\rho > \rho_c$: isotropic distribution is unstable

$\exists$ only one class of non-isotropic equilibria and is stable

Order parameter: $c_1(\rho) = c_1(\kappa(\rho))$, with $\frac{j}{c_1}(\kappa(\rho)) = \rho$

Then $c_1(\rho) \sim \tilde{c}_{10}(\rho - \rho_c)^\beta$ as $\rho \xrightarrow{>} \rho_c$; β = critical exponent

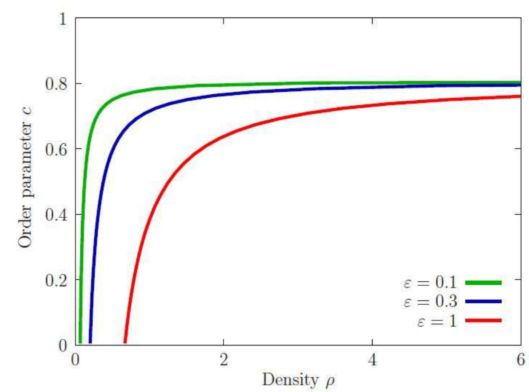
Assume $\frac{k(|J|)}{|J|} = \frac{n}{\rho_c} - a|J|^q + o(|J|^q)$ as $|J| \to 0$ then:

If $q < 2$, $\beta = \frac{1}{q} > \frac{1}{2}$

If $q > 2$, $\beta = \frac{1}{2}$

If $q = 2$, $0 < \beta \leq \frac{1}{2}$

Phase diagram for $k(|J|) = \frac{|J|}{\varepsilon + |J|}$:



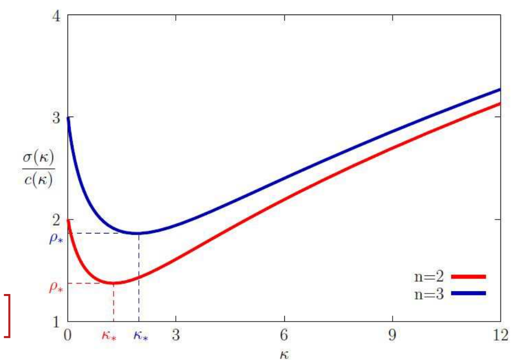
Example 2: first-order phase transition

Assume $k(|J|) = |J| + |J|^2$

Uniform equilib. stable for $\rho \in [0, \rho_c]$

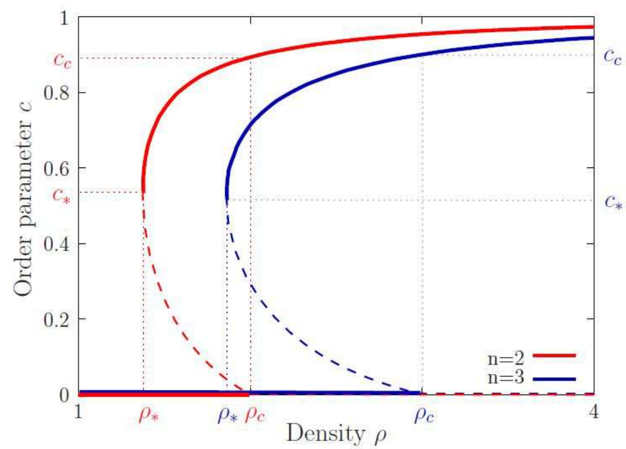
Non-isotropic equilibria with maximal κ stable for $\rho \in [\rho_*, \infty]$

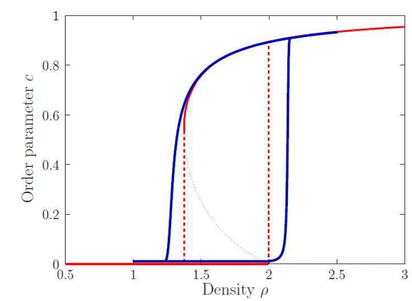
Second class of unstable non-isotropic equilibria for $\rho \in [\rho_*, \rho_c]$



Function $\kappa \to \frac{j}{c_1}(\kappa)$

Phase diagram





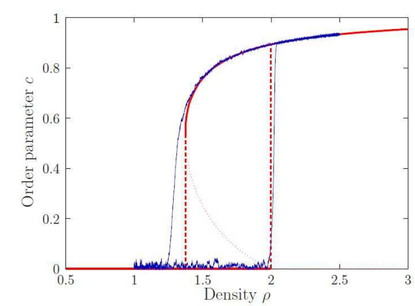
Kinetic simulation

Hysteresis

Numerical computation of hysteresis loop

Using the kinetic model

Using the particle model



Particle simulation

3. Self-organized Hydrodynamics (SOH)

Space-inhomogeneous case

Scaling assumptions: let ε, $\eta \ll 1$ with $\eta = \eta(\varepsilon)$

Social force and noise are large: ν, $\tau = \mathcal{O}(\frac{1}{\varepsilon})$

Interaction radius is small: $R = \mathcal{O}(\eta)$

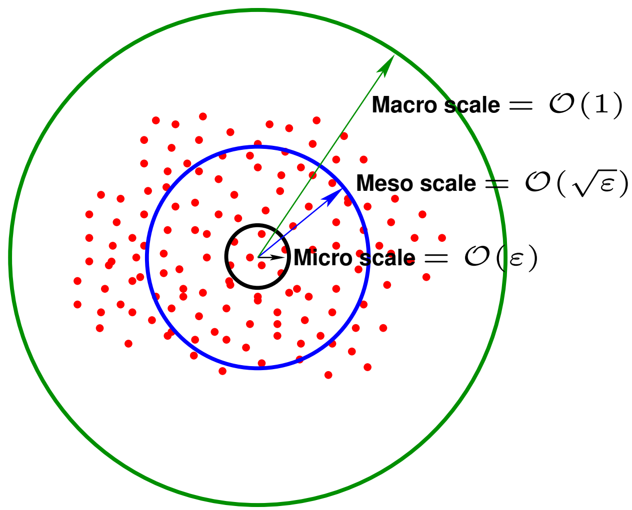
$$\varepsilon(\partial_t f^\varepsilon + v \cdot \nabla_x f^\varepsilon) + \eta^2 \nabla_v \cdot (F^{(1)}_{f^\varepsilon} f^\varepsilon) = Q(f^\varepsilon)$$

$F^{(1)}_f$ = First order term in the expansion of F_f in η^2

Two types of scaling

$\eta = O(\varepsilon)$: microscopic interaction radius

$\eta = O(\sqrt{\varepsilon})$: mesoscopic interaction radius



Macroscopic model

Macroscopic limit $\varepsilon \to 0$: $f^\varepsilon \to$ local equilibrium f_{eq}:

$$f_{\text{eq}}(x,v,t) = \rho(x,t) M_{\kappa(\rho(x,t))u(x,t)}(v), \quad \text{with} \quad |u(x,t)| = 1$$

locally around (x,t), a branch of stable equilibria is chosen

question: what equations for $\rho(x,t)$ and $u(x,t)$?

Two cases: either $\kappa(\rho) = 0$: isotropic equilibria

or $\kappa(\rho) \neq 0$: non-isotropic equilibria

Limit $\varepsilon \to 0$: Mass conservation eq.

obtained by integrating kinetic eq. w.r.t. v

and closing the flux $\int f(v)\, v\, dv$ with $f = f_{\text{eq}}$

$$\partial_t \rho + \nabla \cdot (c_1(\rho) \rho u) = 0$$

Case $\kappa(\rho) = 0$: isotropic equilibria

Then $c_1(\rho) = c_1(\kappa(\rho)) = 0$: flux vanishes

Leads to $\partial_t \rho = 0$

To get non-trivial dynamics, requires $\mathcal{O}(\varepsilon)$ terms

Gives diffusion model

$$\partial_t \rho^\varepsilon = \frac{\varepsilon}{(n-1)n\tau_0} \nabla_x \cdot \big(\frac{1}{1 - \frac{\rho^\varepsilon}{\rho_c}} \nabla_x \rho^\varepsilon \big)$$

Note: stability of isotropic equilibria requires $1 - \frac{\rho^\varepsilon}{\rho_c} > 0$

Case $\kappa(\rho) \neq 0$: non-isotropic equilibria

Now, $c_1(\rho) = c_1(\kappa(\rho)) \neq 0$: flux does not vanish

Requires an equation for $u(x,t)$

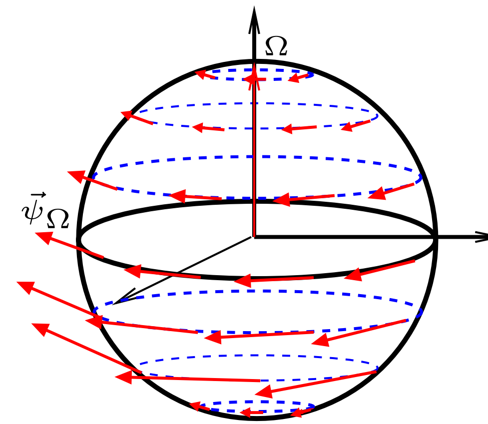
Problem: no momentum conservation

Requires new concept: Generalized Collision Invariants (GCI)

Fix u and require 'momentum' conservation only for f such that $J_f \parallel u$

This special 'momentum' $\vec{\psi}_u$ is the GCI

Not explicit: solves a PDE related to Q^*



Yields 'Self-Organized Hydrodynamics' (SOH)

$$\partial_t \rho + \nabla_x \cdot (c_1 \rho u) = 0$$

$$\rho\, (\partial_t u + c_2 (u \cdot \nabla_x) u) + \Theta\, P_{u^\perp} \nabla_x \rho = \delta P_{u^\perp} \Delta_x (c_1 \rho u)$$

$|u| = 1$; c_1, c_2, Θ, δ functions of ρ; $\delta = 0$ if $\eta = \mathcal{O}(\varepsilon)$

Similar to Compressible Navier-Stokes

First-order part hyperbolic under some conditions on the data

But major differences:

Geometric constraint $|u| = 1$

Non-conservative projection $P_{u^\perp}$ and factors c, Θ, δ

$c_2 \neq c_1$: loss of Galilean invariance

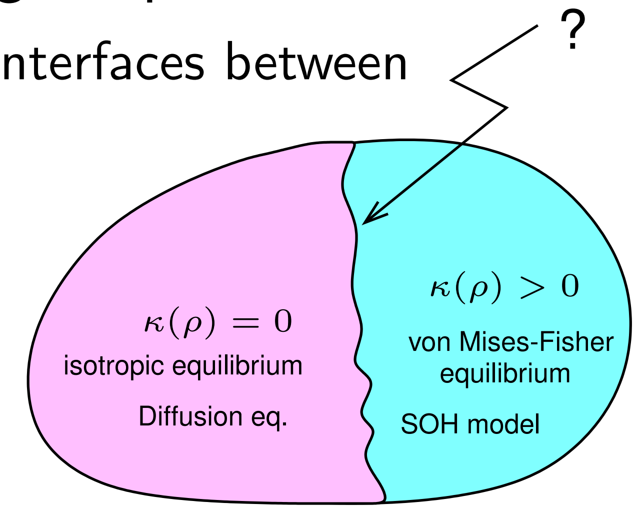
Phase interface when disordered and aligned phases coexist

Connection conditions between models at interfaces between

region $\kappa(\rho) = 0$ (diffusion eq.)

and region $\kappa(\rho) \neq 0$ (SOH)

are unknown



Numerical treatment:

Relaxation 'super-model' (no diffusion case)

$$\partial_t \rho + \nabla_x \cdot (\rho v) = 0 \qquad p'(\rho) = c_1(\rho)\,\Theta(\rho)$$

$$\partial_t(\rho v) + \nabla_x \cdot \big(\frac{c_2}{c_1} \rho v \otimes v\big) + \nabla_x p(\rho) = \frac{1}{\alpha} \rho v \big(c_1(\rho)^2 - |v^2|\big)$$

As $\alpha \to 0$ super-model tends to [PD, H. Yu, S. Merino-Aceituno, WIP]

SOH (if $c_1(\rho) > 0$)

Diffusion eq (if $c_1(\rho) = 0$)

4. Conclusion

Summary & Perspectives

Complete characterization of phase transitions

- in kinetic models of self-propelled particles with alignment
- Order of phase transition fully determined
- Occurrence of hysteresis in case of first-order phase transitions

Derivation of macroscopic models of Self-Propelled particles

- Diffusion in regions where isotropic equilibria are stable
- New hydrodynamics in regions of anisotropic equilibria
- Opens new challenges in analysis and numerical simulation

Model has potential validity for large class of phenomena

- can be improved $\rightarrow$ attraction/repulsion, volume exclusion . . .