# 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
2. Mathematical analysis of the phase transitions
3. Self-organized Hydrodynamics (SOH)
4. Conclusion

## 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 $t^{n}=n \Delta t$

$$
\begin{aligned}
& \left|V_{k}^{n}\right|=1 \\
& X_{k}^{n+1}=X_{k}^{n}+V_{k}^{n} \Delta t, \\
& \bar{V}_{k}^{n}=\frac{\mathcal{J}_{k}^{n}}{\left|\mathcal{J}_{k}^{n}\right|}, \quad \mathcal{J}_{k}^{n}=\sum_{j,\left|X_{j}^{n}-X_{k}^{n}\right| \leq R} V_{j}^{n} \\
& \arg \left(V_{k}^{n+1}\right)=\arg \left(\bar{V}_{k}^{n}+\tau_{k}^{n}\right)
\end{aligned}
$$


$\tau_{k}^{n}$ drawn uniformly in $[-\tau, \tau] ; \quad R=$ interaction range

## Phase transition

disordered $\rightarrow$ aligned state
Symmetry breaking


Order parameter measures alignment

$$
c_{1}=\left|N^{-1} \sum_{j} V_{j}\right|, \quad 0 \leq c_{1} \leq 1
$$


$c_{1}$ vs noise


band formation


after [Chaté et al, PRE 2008]

## 2. Mathematical analysis of the phase transitions

$$
\begin{aligned}
& \dot{X}_{k}(t)=V_{k}(t), \quad\left|V_{k}(t)\right|=1 \\
& d V_{k}(t)=P_{V_{k}^{\perp}}\left(\nu \bar{V}_{k} d t+\sqrt{2 \tau} \circ d B_{t}^{k}\right), \quad P_{V_{k}^{\perp}}=\mathrm{ld}-V_{k} \otimes V_{k} \\
& \bar{V}_{k}=\frac{\mathcal{J}_{k}}{\left|\mathcal{J}_{k}\right|}, \quad \mathcal{J}_{k}=\sum_{j,\left|X_{j}-X_{k}\right| \leq R} V_{j}
\end{aligned}
$$

$\nu$ collision frequency $\quad \tau$ noise intensity

$$
P_{V_{k}^{\perp}} \text { maintains }\left|V_{k}(t)\right|=1
$$


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

$$
\begin{aligned}
& \partial_{t} f+v \cdot \nabla_{x} f=-\nabla_{v} \cdot\left(F_{f} f\right)+\tau \Delta_{v} f \\
& F_{f}=\nu P_{v^{\perp}} \bar{v}_{f}, \quad P_{v^{\perp}}=(\operatorname{ld}-v \otimes v), \quad \bar{v}_{f}=\frac{\mathcal{J}_{f}}{\left|\mathcal{J}_{f}\right|} \\
& \mathcal{J}_{f}=\int_{\left(x^{\prime}, v^{\prime}\right)} K\left(\frac{\left|x^{\prime}-x\right|}{R}\right) f\left(x^{\prime}, v^{\prime}, t\right) v^{\prime} d v^{\prime} d x^{\prime} \\
& \bar{v}_{f}=\text { direction of locally averaged flux } \\
& \text { Here, we assume: } \\
& \nu=\nu\left(\left|\mathcal{J}_{f}\right|\right), \quad \tau=\tau\left(\left|\mathcal{J}_{f}\right|\right)
\end{aligned}
$$

## Spatially homogeneous case

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

$$
\begin{aligned}
& \partial_{t} f=-\nabla_{v} \cdot\left(F_{f} f\right)+\tau\left(\left|J_{f}\right|\right) \Delta_{v} f:=Q(f) \\
& F_{f}=\nu\left(\left|J_{f}\right|\right) P_{v} u_{f}, \quad u_{f}=\frac{J_{f}}{\left|J_{f}\right|}, \quad J_{f}=\int_{v^{\prime}} f\left(v^{\prime}, t\right) v^{\prime} d v^{\prime}
\end{aligned}
$$

Note that $\partial_{t} \rho=0$

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

## Equilibria

Equilibria are functions $f(v)$ such that $Q(f):=0$
$Q(f)=\tau\left(\left|J_{f}\right|\right) \nabla_{v} \cdot\left[-k\left(\left|J_{f}\right|\right) P_{v^{\perp}} u_{f} f+\nabla_{v} f\right] \quad$ with $\quad k(|J|)=\frac{\nu(|J|)}{\tau(|J|)}$
Von Mises-Fisher (VMF) distribution $M_{\kappa u}$ :

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

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

Order parameter: $\quad c_{1}(\kappa)=\int M_{\kappa u}(v)(u \cdot v) d v$

$$
\begin{aligned}
& \kappa \xrightarrow{\nearrow} c_{1}(\kappa), \quad 0 \leq c_{1}(\kappa) \leq 1 \\
& \text { Flux: } \quad \int M_{\kappa u}(v) v d v=c_{1}(\kappa) u
\end{aligned}
$$



## Compatibility condition

Equilibria are of the form $f(v)=\rho M_{\kappa u}(v)$
where $\rho>0$ and $u \in \mathbb{R}^{n}$ s.t. $|u|=1$ are arbitrary
Current given by: $\left|J_{f}\right|=\rho c_{1}(\kappa)$
From expression of $Q, \kappa$ must be equal to $k\left(\left|J_{f}\right|\right)$
Leads to compatibility condition

$$
\kappa=k\left(\rho c_{1}(\kappa)\right) \quad \text { or equivalently } \quad \rho=\frac{j(\kappa)}{c_{1}(\kappa)}
$$

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 $\frac{j(\kappa)}{c_{1}(k)}$
determine number of equilibria and their stability

We assume $|J| \rightarrow \tau(|J|)$ and $|J| \rightarrow \frac{\nu(|J|)}{|J|}$ smooth
Define $\quad \rho_{*}=\min _{\kappa>0} \frac{j(\kappa)}{c_{1}(\kappa)}, \quad \rho_{c}=\lim _{\kappa \rightarrow 0} \frac{j(\kappa)}{c_{1}(\kappa)}, \quad \rho_{*} \leq \rho_{c}$
But monotony of $\kappa \rightarrow \frac{j(\kappa)}{c_{1}(\kappa)}$ 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 $\kappa$ '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 $\frac{j(\kappa)}{c_{1}(\kappa)}$, 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 $f(t) \rightarrow \tilde{f}_{\mathrm{eq}}=\rho M_{\kappa \tilde{u}}$ as $t \rightarrow \infty$
but $\tilde{u}$ may be $\neq u$

Free energy

$$
\mathcal{F}(f)=\int f \ln f d v-\Phi\left(\left|J_{f}\right|\right) \quad \text { with } \quad \Phi^{\prime}=k
$$

Free energy dissipation

$$
\mathcal{D}(f)=\tau\left(\left|J_{f}\right|\right) \int f\left|\nabla_{v} f-k\left(\left|J_{f}\right|\right)\left(v \cdot u_{f}\right)\right|^{2} d v \quad \text { with } \quad u_{f}=\frac{J_{f}}{\left|J_{f}\right|}
$$

Free energy dissipation identity $\quad \frac{d}{d t} \mathcal{F}(f)=-\mathcal{D}(f) \leq 0$ Free energy decays with time
$f$ is an equilibrium iff $\mathcal{D}(f)=0$

## Stability / instability

## Stability / Instability of isotropic equilibria

Behavior determined by first spherical harmonics, i.e. by $J_{f}$

$$
\frac{d}{d t} J_{f}=-(n-1) \tau_{0}\left(1-\frac{\rho}{\rho_{c}}\right) J_{f}+\text { h. o. t. } \quad \text { with } \quad \tau_{0}=\left.\tau\right|_{|J|=0}
$$

In stable case, convergence to equilibrium with rate $\lambda_{0}$

$$
\lambda_{0}=(n-1) \tau_{0}\left(1-\frac{\rho}{\rho_{c}}\right)
$$

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 $\mathcal{F}\left(f_{0}\right)<\mathcal{F}\left(f_{\text {eq }}\right)$
Then $\mathcal{F}(f(t)) \leq \mathcal{F}\left(f_{0}\right)<\mathcal{F}\left(f_{\text {eq }}\right)$
$f(t)$ cannot converge to any equilibrium of the same family
$\tilde{f}_{\text {eq }}=\rho M_{\kappa \tilde{u}}$ with any $\tilde{u}$ since $\mathcal{F}\left(\tilde{f}_{\text {eq }}\right)=\mathcal{F}\left(f_{\text {eq }}\right)$

## Stability of non-isotropic equilibrium uses that

if $\left(\frac{j}{c_{1}}\right)^{\prime}>0$, we have

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

and this quantity is decreasing
Convergence to limit equilibrium with rate $\lambda_{\kappa}$

$$
\lambda_{\kappa}=\frac{c_{1} \tau(j)}{j^{\prime}}(\kappa) \Lambda_{\kappa}\left(\frac{j}{c_{1}}\right)^{\prime}(\kappa)
$$

where $\Lambda_{\kappa}$ is the best Poincaré constant for

$$
\int\left|\nabla_{v} g\right|^{2} M_{\kappa u}(v) d v \geq \Lambda_{\kappa} \int|g-\langle g\rangle|^{2} M_{\kappa u}(v) d v, \quad\langle g\rangle=\int g(v) M_{\kappa u}(v) d v
$$

Relies on estimate on the free energy dissipation

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

Assume $\kappa \rightarrow \frac{j(\kappa)}{c_{1}(\kappa)}$ 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: $\quad c_{1}(\rho)=c_{1}(\kappa(\rho))$, with $\frac{j}{c_{1}}(\kappa(\rho))=\rho$
Then $c_{1}(\rho) \sim \tilde{c}_{10}\left(\rho-\rho_{c}\right)^{\beta}$ as $\rho \xrightarrow{>} \rho_{c} ; \beta=$ critical exponent
Assume $\frac{k(|J|)}{|J|}=\frac{n}{\rho_{c}}-a|J|^{q}+o\left(|J|^{q}\right) \quad$ as $|J| \rightarrow 0$ then:

$$
\begin{aligned}
& \text { If } q<2, \beta=\frac{1}{q}>\frac{1}{2} \\
& \text { If } q>2, \beta=\frac{1}{2} \\
& \text { If } q=2,0<\beta \leq \frac{1}{2}
\end{aligned}
$$

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 $\rho \in\left[0, \rho_{c}\right]$
Non-isotropic equilibria with maximal $\kappa$ stable for $\rho \in\left[\rho_{*}, \infty\right]$
Second class of unstable non-isotropic equilibria for $\rho \in\left[\rho_{*}, \rho_{c}\right]$
Phase diagram

Hysteresis



Function $\kappa \rightarrow \frac{j}{c_{1}}(\kappa)$

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 $\varepsilon, \eta \ll 1$ with $\eta=\eta(\varepsilon)$
Social force and noise are large: $\nu, \tau=\mathcal{O}\left(\frac{1}{\varepsilon}\right)$
Interaction radius is small: $R=\mathcal{O}(\eta)$

$$
\varepsilon\left(\partial_{t} f^{\varepsilon}+v \cdot \nabla_{x} f^{\varepsilon}\right)+\eta^{2} \nabla_{v} \cdot\left(F_{f^{\varepsilon}}^{(1)} f^{\varepsilon}\right)=Q\left(f^{\varepsilon}\right)
$$

$F_{f}^{(1)}=$ First order term in the expansion of $F_{f}$ in $\eta^{2}$
Two types of scaling
$\eta=O(\varepsilon)$ : microscopic interaction radius
$\eta=O(\sqrt{\varepsilon})$ : mesoscopic interaction radius


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

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

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 $\varepsilon \rightarrow 0$ : Mass conservation eq.
obtained by integrating kinetic eq. w.r.t. $v$ and closing the flux $\int f(v) v d v$ with $f=f_{\text {eq }}$

$$
\partial_{t} \rho+\nabla \cdot\left(c_{1}(\rho) \rho u\right)=0
$$

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

Then $c_{1}(\rho)=c_{1}(\kappa(\rho))=0$ : flux vanishes
Leads to $\quad \partial_{t} \rho=0$
To get non-trivial dynamics, requires $\mathcal{O}(\varepsilon)$ terms
Gives diffusion model

$$
\partial_{t} \rho^{\varepsilon}=\frac{\varepsilon}{(n-1) n \tau_{0}} \nabla_{x} \cdot\left(\frac{1}{1-\frac{\rho^{\varepsilon}}{\rho_{c}}} \nabla_{x} \rho^{\varepsilon}\right)
$$

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 $J_{f} \| u$ This special 'momentum' $\vec{\psi}_{u}$ is the GCI Not explicit: solves a PDE related to $Q^{*}$

Yields 'Self-Organized Hydrodynamics' (SOH)

$$
\begin{aligned}
& \partial_{t} \rho+\nabla_{x} \cdot\left(c_{1} \rho u\right)=0 \\
& \rho\left(\partial_{t} u+c_{2}\left(u \cdot \nabla_{x}\right) u\right)+\Theta P_{u^{\perp}} \nabla_{x} \rho=\delta P_{u^{\perp}} \Delta_{x}\left(c_{1} \rho u\right) \\
& |u|=1 ; \quad c_{1}, c_{2}, \Theta, \delta \text { functions of } \rho ; \quad \delta=0 \text { if } \eta=\mathcal{O}(\varepsilon)
\end{aligned}
$$

## 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 $c, \Theta, \delta$
$c_{2} \neq c_{1}$ : loss of Galilean invariance

## Motion of phase interfaces

Phase interface when disordered and aligned phases coexist
Connection conditions between models at interfaces between
region $\kappa(\rho)=0$ (diffusion eq.)
and region $\kappa(\rho) \neq 0(\mathrm{SOH})$
are unknown

## Numerical treatment:

Relaxation 'super-model' (no diffusion case)


$$
\begin{aligned}
& \partial_{t} \rho+\nabla_{x} \cdot(\rho v)=0 \quad p^{\prime}(\rho)=c_{1}(\rho) \Theta(\rho) \\
& \partial_{t}(\rho v)+\nabla_{x} \cdot\left(\frac{c_{2}}{c_{1}} \rho v \otimes v\right)+\nabla_{x} p(\rho)=\frac{1}{\alpha} \rho v\left(c_{1}(\rho)^{2}-\left|v^{2}\right|\right)
\end{aligned}
$$

As $\alpha \rightarrow 0$ 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...

