

Coarse-graining dry aligning active matter

The BGL approach

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ACTIVE20 – Tutorials

(California dreaming...)



Introduction: active matter

Active particles are able to **extract and dissipate energy** from their surroundings to produce **systematic and coherent motion**

- Energy enters and exits the system → out of equilibrium
- Energy is spent to perform actions, typically move (self-propel) in a non-thermal way
- In active systems, energy is injected and dissipated in the bulk, not from the boundaries, in a way that does not explicitly break any symmetry

What are we interested into ?

Collective effects	Single swimmer properties
<p data-bbox="481 686 981 790">Particle interactions are relevant</p> <p data-bbox="407 933 1052 1157">Typically, local interactions leads to (non-trivial) emergent phenomena on much larger scales</p>	<p data-bbox="1160 686 1796 790">Inter-particles interactions are negligible/non-existent</p>

Here we discuss collective effects!

Some fundamental distinctions

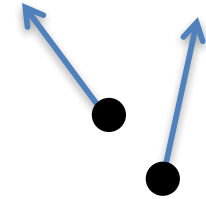
Momentum is NOT conserved DRY (hydro interaction DO NOT matter)	Momentum is conserved WET (hydro interactions DO matters)
Crawling critters Quasi-2D suspensions Relatively high Reynolds numbers (birds, fish) ? (i.e.: inertial effects dominates viscosity)	3D suspensions Especially at low Reynolds (i.e.. Stokes regime)

Here we stay dry!

Warming up -- Simplest model for active particles ?

An (almost trivial) active system

No alignment between particles: active Brownian particles (ABP)



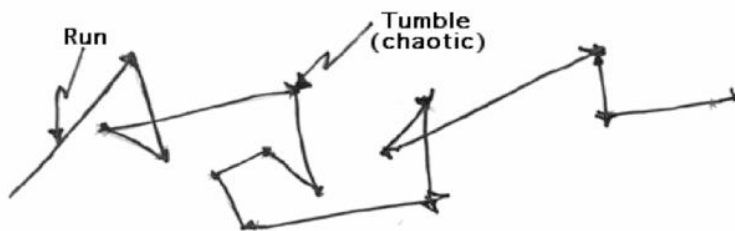
$$\dot{\mathbf{r}}_i = \hat{\mathbf{v}}_i v_0$$

$$\dot{\theta}_i = \eta_i \quad \hat{\mathbf{v}}_i = (\cos \theta_i, \sin \theta_i)$$

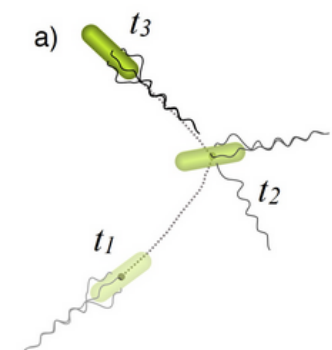
Zero mean noise with delta-correlations

$$\langle \eta_i(t) \eta_j(t') \rangle = 2D_R \delta_{ij} \delta(t - t')$$

Equivalent system (at large scales): Run & Tumble particles



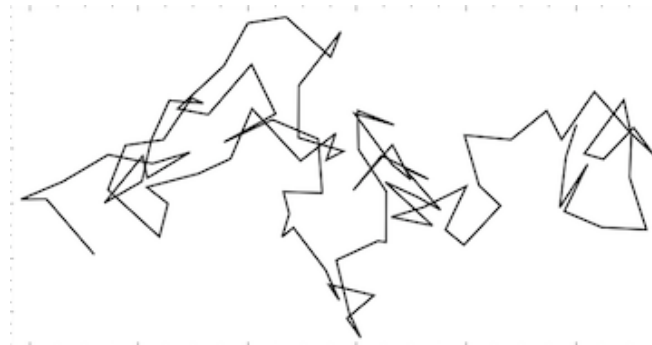
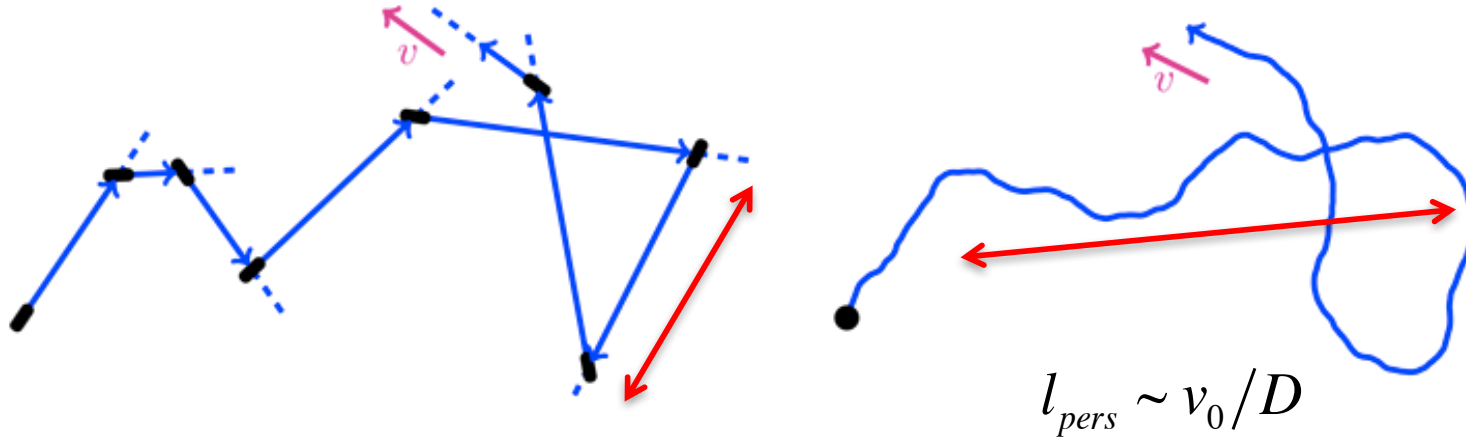
"Run-tumble" paradigm for taxis
Berg and Brown, Nature, (1972)



Run-and-tumble

Warming up -- Simplest model for active particles ?

Persistent random walkers



At length scales $\gg l_{pers}$
undistinguishable from
a standard random walk

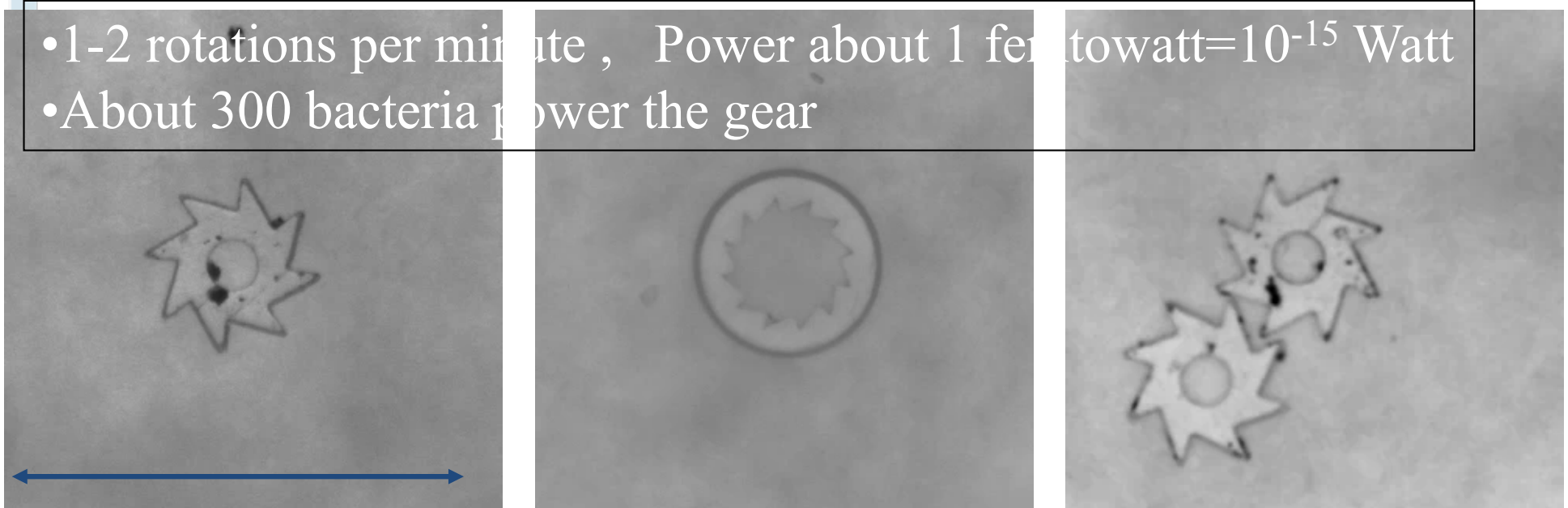
Life is hard: II Law of thermodynamics

At equilibrium you cannot rectify (i.e. extract work from thermal fluctuations)

Active particles are out of equilibrium!!

Throw in something below the persistence length scale

- 1-2 rotations per minute, Power about 1 femtowatt = 10^{-15} Watt
- About 300 bacteria power the gear



1 mm

Active Brownian particles can rectify a-thermal motion

PNAS

Swimming bacteria power microscopic gears

Andrey Sokolov^{a,b}, Mario M. Apodaca^c, Bartosz A. Grzybowski^{c,d,1}, and Igor S. Aranson^{a,e,1}

^aMaterials Science Division, Argonne National Laboratory, Argonne, IL 60439; ^bDepartment of Ecology and Evolutionary Biology, Princeton University, Princeton, NJ 08543; and ^cDepartments of Chemistry, ^dChemical and Biological Engineering, and ^eEngineering Sciences and Applied Mathematics, Northwestern University, 2145 Sheridan Rd, Evanston, IL 60208

PNAS

Bacterial ratchet motors

R. Di Leonardo^{a,1}, L. Angelani^a, D. Dell'Arciprete^b, G. Ruocco^b, V. Iebba^c, S. Schippa^c, M. P. Conte^c, F. Mecarini^{d,e}, F. De Angelis^{d,e}, and E. Di Fabrizio^{d,e}

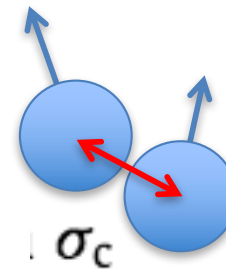
^aConsiglio Nazionale delle Ricerche-Istituto per i Processi Chimico-Fisici, c/o Università di Roma "Sapienza," I-00185, Rome, Italy; ^bDipartimento di Fisica, Università di Roma "Sapienza," I-00185, Rome, Italy; ^cDipartimento Scienze di Sanità Pubblica, Università di Roma "Sapienza," I-00185, Rome, Italy; ^dNanobioscience Department, Italian Institute of Technology, I-16163, Genova, Italy; and ^eBionanotechnology and Engineering for Medicine Laboratory, Università della Magna Graecia, I-88100, Catanzaro, Italy

II. Repulsion interactions: Motility induced phase separation (MIPS)

Add simple short range repulsion to ABPs

$$\dot{\mathbf{r}}_i = \hat{\nu}_i v_0 + \mu \sum_{j \neq i} \mathbf{F}_{ij} + \boldsymbol{\eta}_i^T$$

$$\dot{\theta}_i = \eta_i$$



$$\mathbf{F}_{ij} = -f(r_{ij}) \hat{\mathbf{r}}_{ij}$$

Zero mean noise with delta-correlations

$$\langle \eta_i(t) \eta_j(t') \rangle = 2D_R \delta_{ij} \delta(t - t')$$

$$\langle \eta_{i\alpha}^T(t) \eta_{j\beta}^T(t') \rangle = 2D \delta_{ij} \delta_{\alpha\beta} \delta(t - t')$$

$$D = k_B T \mu$$

$$\therefore D_R = 3D / \sigma_c^2$$

2 main control parameters

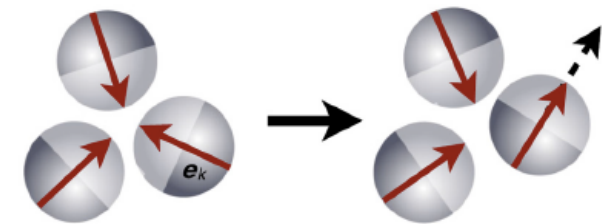
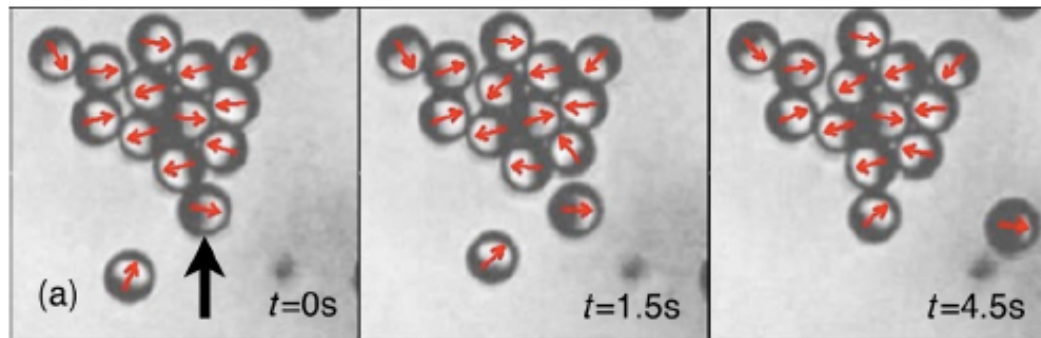
$$Pe = \frac{\sigma_c v_0}{k_B T \mu}$$

Peclet number (ratio between advection and diffusion rates)

$$\phi_0 = N \frac{S_c}{S}$$

Occupied surface fraction

Clustering effects



MIPS: the Physical mechanism in a nutshell

In high density regions, crowding slows down the active particles effective speed

$$v \sim e^{-\lambda\rho/2} v_0$$

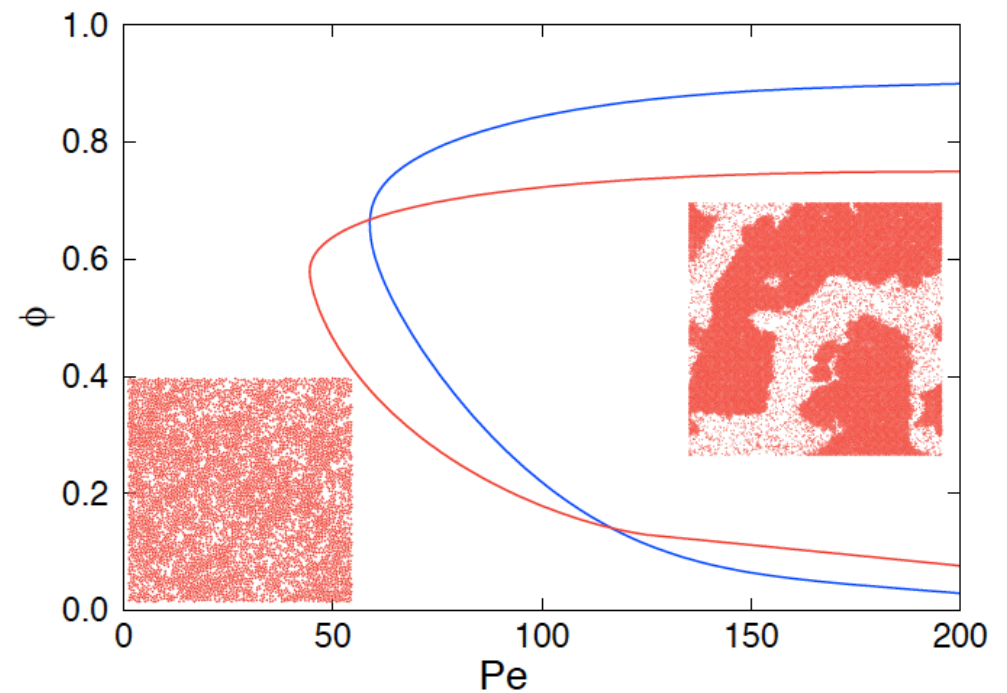
1. Fluctuations can spontaneously produce high and low density regions
2. Self-propelled particles accumulate where they move slower (think of pedestrians in a busy street)
3. Positive feedback between effective slowing down and increasing density
4. A (different w.r.t. alignment dominated systems) instability mechanism leading to phase segregation (without order)

Simple models for active particles

Interacting particles: short range repulsion (avoid your neighbours)

The system can undergo spontaneous phase separation and show clusters

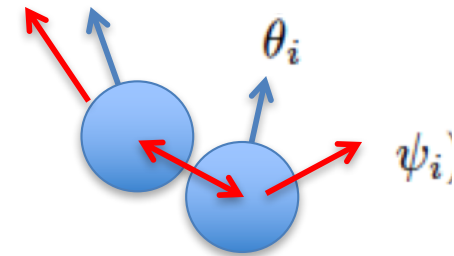
Motility Induced Phase Separation (MIPS)



Go with the flow: Collisional Vicsek model

$$\dot{\mathbf{r}}_i = v_0 \hat{\mathbf{n}}(\theta_i) + \beta \sum_j^{N_0} \mathbf{F}_{ij}$$

$$\dot{\theta}_i = \frac{1}{\tau} (\theta_i - \psi_i) + \xi_i$$



$$\mathbf{v}_i \equiv \dot{\mathbf{r}}_i = v_i (\cos \psi_i, \sin \psi_i)$$

**A transition to collective motion!
(when τ small enough)**

Szabo B, Szollosi GJ, Gonci B, Juranyi Z, Selmeczi D and Vicsek T 2006 *Phys. Rev. E* 74(6) 061908

Henkes S, Fily Y and Marchetti M C 2011 *Phys. Rev. E* 84(4) 040301

Flocking active matter

spontaneous symmetry breaking to collective motion



Starlings flock - Predation attempt in Rome

thanks to STARFLAG Project & Claudio Carere, Istituto Superiore di Sanità - Roma - Italy

Some fundamental distinctions

Isotropic	Symmetry Breaking e.g.: Polar and nematic collective motion
-----------	--

Go and look at your system.

Do they show a **symmetry breaking phase transition to collective motion as parameters (density, motility, environmental noise, etc...) are changed?**

Question checklist about your system

- **Equilibrium or out-of-equilibrium**
- **How equilibrium is broken? Inherently Active particles**
yes, you are probably dealing with an active matter problem
- **Other conservation laws (particle number, momentum (wet vs. dry systems, ...))**
- **Fundamental symmetries (e.g: to break or not to break the rotational symmetry)**

These determines hydrodynamic slow fields

- **Relevant lengths- and time-scales (is there more than hydrodynamics?)**

Some fundamental distinctions

Momentum is NOT conserved DRY (hydro interaction DO NOT matter)	Momentum is conserved WET (hydro interactions DO matters)
Crawling critters Quasi-2D suspensions Relatively high Reynolds numbers (birds, fish) ? (i.e.: inertial effects dominates viscosity)	3D suspensions Especially at low Reynolds (i.e.. Stokes regime)

Some fundamental distinctions

Isotropic	Symmetry Breaking e.g.: Polar and nematic collective motion
-----------	--

Go and look at your system. Typically, many systems show a **symmetry breaking phase transition** to collective motion as parameters (density, motility, environmental noise, etc...) are changed

- **Much more complications** pops up almost everywhere – life far from equilibrium is complicated !!

One of the simplest examples:

Flocking in DRY active matter systems

Which are these essential ingredients ?

- 1. Particles are self propelled**
- 2. A continuous symmetry can be spontaneously broken**
- 3. Particles number conservation**

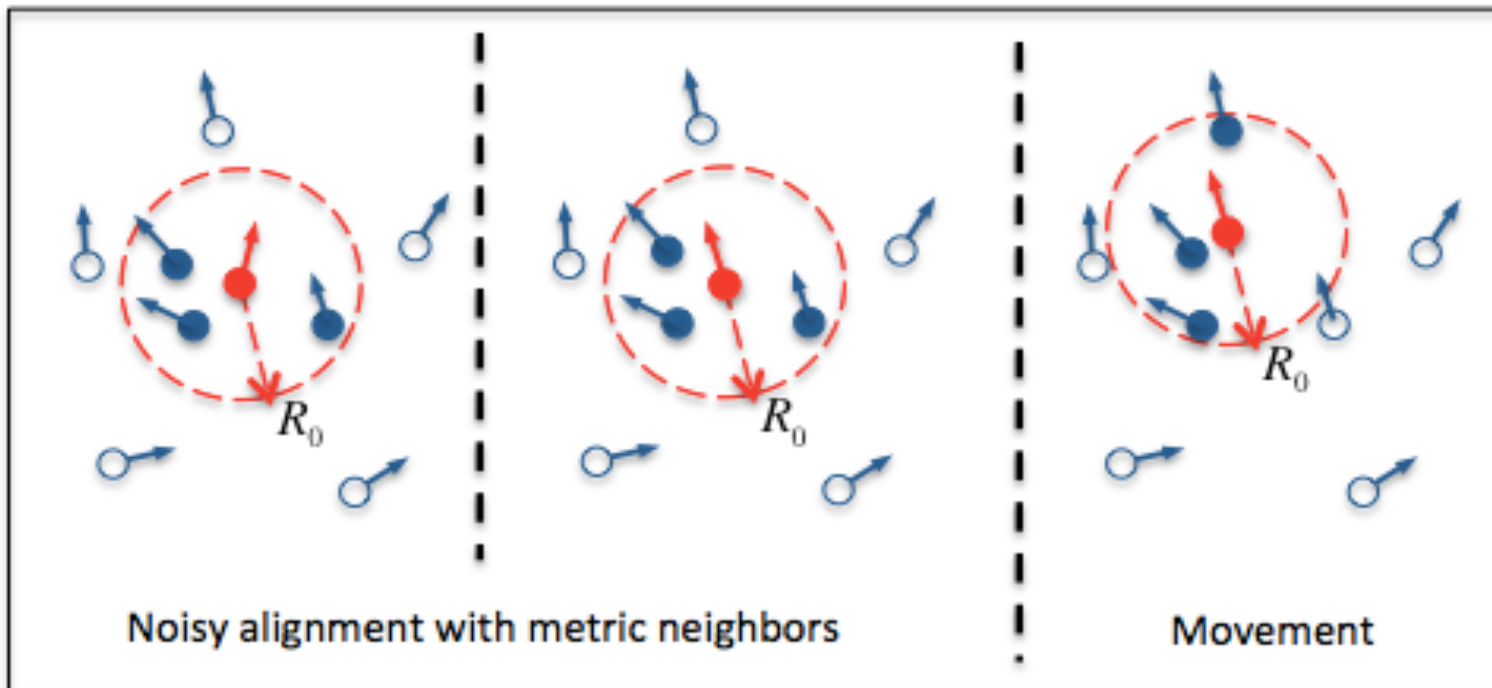
**A lot of physics is actually determined
by these facts alone !!**

The Vicsek model (“moving XY spins”)

Vicsek et al, PRL (1995)

- Off lattice self propelled particles that move with constant speed v_0
- Local *ferromagnetic (or polar)* alignment with local neighbors (inside a metric range R_0 .)
- Environmental **white noise**

In $d=2$ one may write the VM as

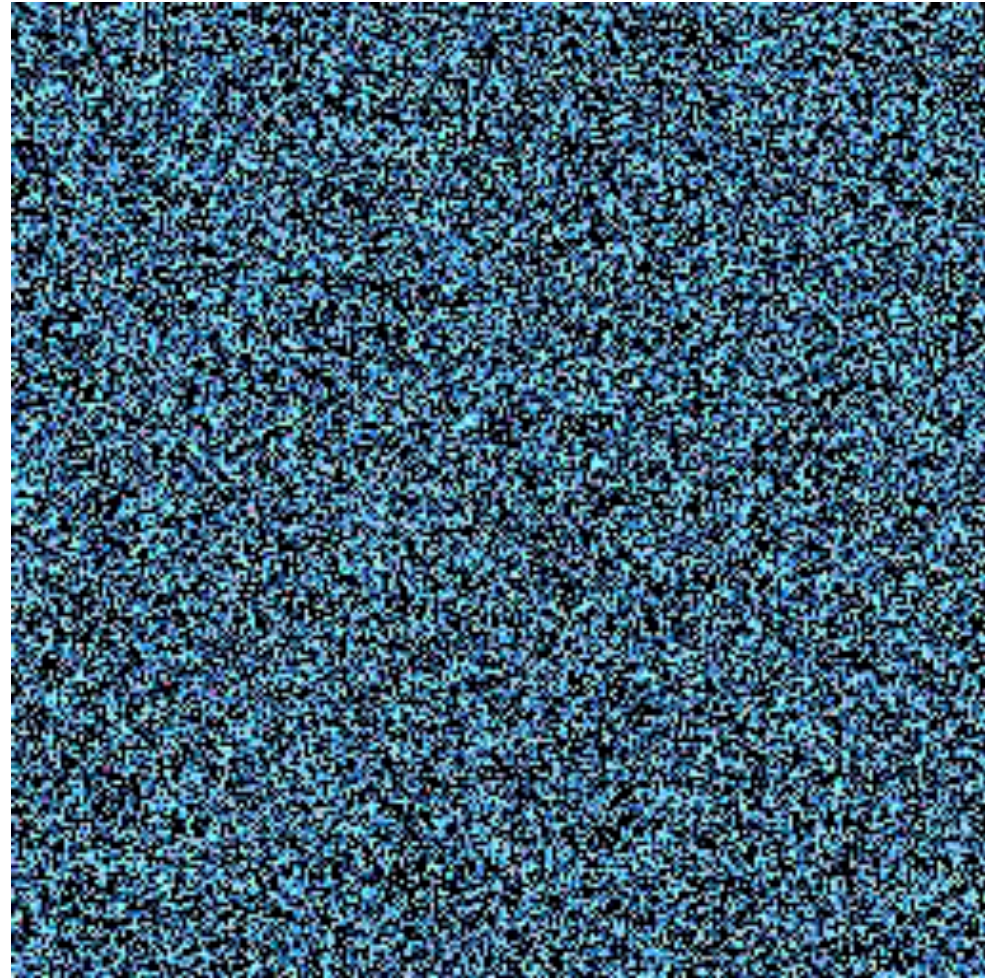


Numerical simulations

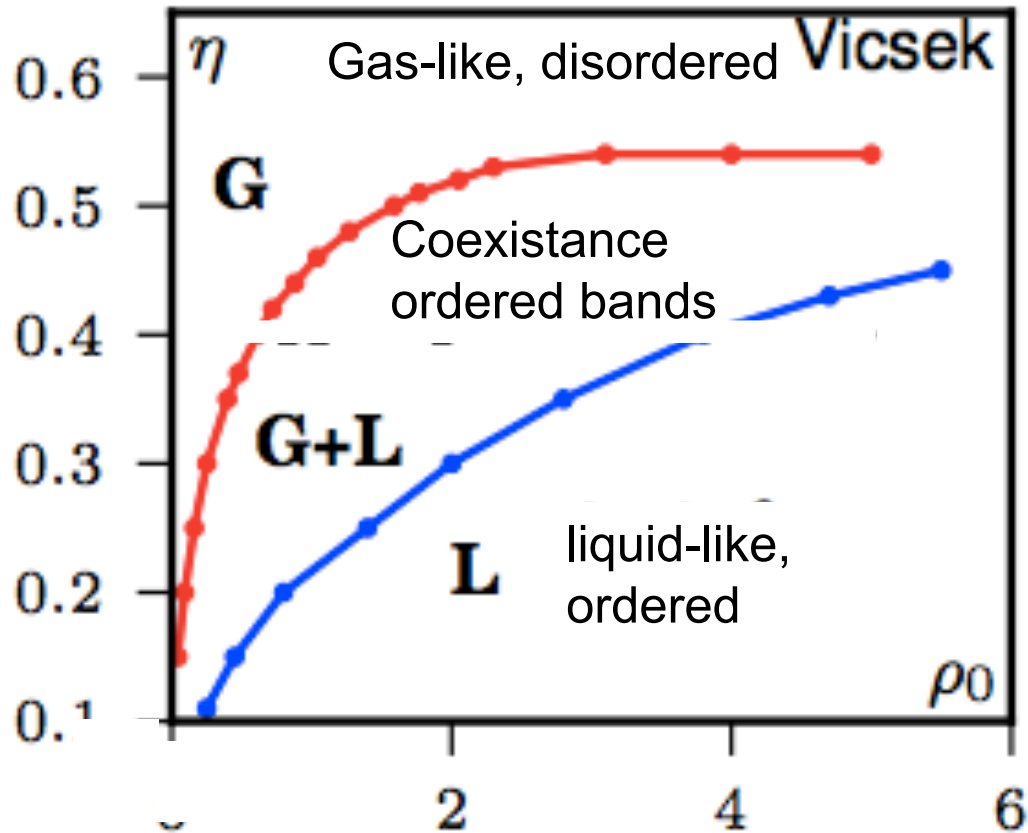
Strong noise: disorder, random walks

Quench into ordered phase
(coarse-grained density field)
 $L=16384$, $\rho=1/8$ (32M particles)

Low noise: **order**



The VM phase diagram



Generic to all Vicsek-like models with metric interactions

Polar order parameter

$$\varphi(t) = \frac{1}{N} \sum_{i=1}^N s_i^t$$

$\left\{ \begin{array}{l} |\phi| \sim \frac{1}{\sqrt{N}} \text{ disordered} \\ |\phi| \sim 1 \text{ ordered} \end{array} \right.$

Vicsek-like dry active matter models

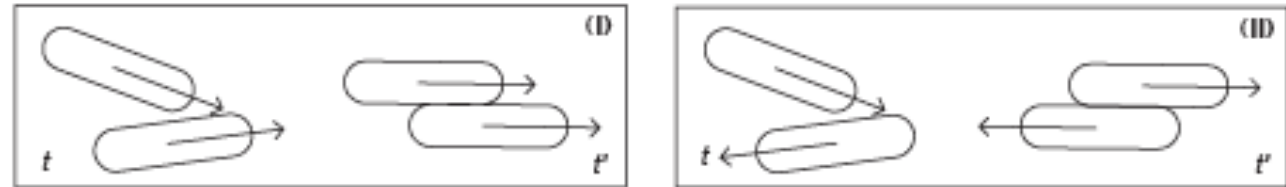
$$\vartheta \rightarrow \vartheta + \pi$$

Active nematics

$$\mathbf{x}_j^{t+\Delta t} = \mathbf{x}_j^t + d_0 \kappa_j^t \hat{\mathbf{n}}_j^t, \quad \theta_j^{t+\Delta t} = \frac{1}{2} \text{Arg} \left[\sum_{k \in V_j} e^{i2\theta_k^t} \right] + \eta \xi_i^t$$

$$\kappa_j^t = \pm 1$$

Polar rods



$$\theta_j^{t+1} = \arg \left[\sum_{k \sim j} \text{sign}[\cos(\theta_k^t - \theta_j^t)] e^{i\theta_k^t} \right] + \eta \xi_j^t$$

$$\mathbf{r}_j^{t+1} = \mathbf{r}_j^t + v_0 e^{i\theta_k^{t+1}},$$

Coarse-graining towards hydrodynamic theory

- **Hydrodynamic** theories describe **the long wavelength, long time behavior** of the system
- Dynamics of the **slow modes** of our problem, i.e. the hydrodynamic fields. *The idea is that all other modes have a much faster dynamics, and quickly relax to values determined by the slow modes. i.e. on the hydrodynamic timescales are **enslaved** to the slow modes.*
- Slow modes are related to **conservation laws** and **symmetry breaking**
- **Density $\rho(\mathbf{r}, t)$ and coarse-grained velocity $\mathbf{v}(\mathbf{r}, t)$**

E.g.: Toner & Tu theory for polar flocks

$$\partial_t \rho + \nabla \cdot (\mathbf{v} \rho) = 0 \quad \text{continuity eq.}$$

$$\partial_t \mathbf{v} + \Lambda [\nabla \mathbf{v} \mathbf{v}] = U(\rho, |\mathbf{v}|) \mathbf{v} + \mathbf{D} [\nabla \nabla \mathbf{v}] + \mathbf{F}_P + \mathbf{f}$$

advective

$$\Lambda [\nabla \mathbf{v} \mathbf{v}] \equiv \lambda_1 (\mathbf{v} \cdot \nabla) \mathbf{v} + \lambda_2 (\nabla \cdot \mathbf{v}) \mathbf{v} + \lambda_3 \nabla (|\mathbf{v}|^2)$$

Some kind of material derivative (time + convective derivatives), but with extra terms since Galileian invariance is broken

Can be derived either by:

1. Phenomenological hydrodynamics
2. Direct coarse-graining: e.g. Kinetic approaches
(Boltzmann-Ginzburg-Landau approach)

E.g.: Toner & Tu theory for polar flocks

$$\partial_t \rho + \nabla \cdot (\mathbf{v} \rho) = 0$$

$$\partial_t \mathbf{v} + \Lambda [\nabla \mathbf{v} \mathbf{v}] = U(\rho, |\mathbf{v}|) \mathbf{v} + \mathbf{D} [\nabla \nabla \mathbf{v}] + \mathbf{F}_P + \mathbf{f}$$

Diffusive, viscous terms

$$\mathbf{D} [\nabla \nabla \mathbf{v}] \equiv D_1 \nabla (\nabla \cdot \mathbf{v}) + D_2 (\mathbf{v} \cdot \nabla)^2 \mathbf{v} + D_3 \nabla^2 \mathbf{v};$$

Can be derived either by:

1. Phenomenological hydrodynamics
2. Direct coarse-graining: e.g. Kinetic approaches
(Boltzmann-Ginzburg-Landau approach)

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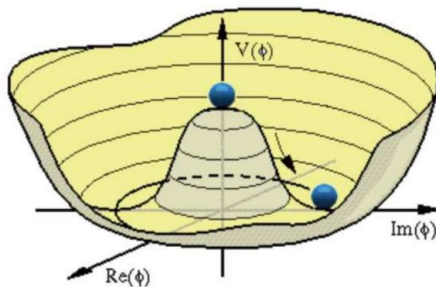
Spontaneous
symmetry
breaking

pressure

$$\mathbf{F}_P \equiv -\nabla P_1 - \mathbf{v} (\dot{\mathbf{v}} \cdot \nabla P_2)$$

$$P_i(\rho) = P_i^0 + \sum_{n=1}^{\infty} \sigma_{i,n} (|\bar{\mathbf{v}}|) \delta \rho^n,$$

$$U \mathbf{v} = \left(\mu - \beta |\mathbf{v}|^2 \right) \mathbf{v}$$



Force term derived by a quartic potential V

$$v_0(0) = \sqrt{\mu/\beta},$$

E.g.: Toner & Tu theory for polar flocks

$$\partial_t \rho + \nabla \cdot (\mathbf{v} \rho) = 0$$

$$\partial_t \mathbf{v} + \Lambda [\nabla \mathbf{v} \mathbf{v}] = U(\rho, |\mathbf{v}|) \mathbf{v} + \mathbf{D} [\nabla \nabla \mathbf{v}] + \mathbf{F}_P + \mathbf{f}$$

$$\langle f_i(\mathbf{r}, t) f_j(\mathbf{r}', t') \rangle = \Delta \delta_{ij} \delta^d(\mathbf{r} - \mathbf{r}') \delta(t - t')$$

Can be derived either by:

1. Phenomenological hydrodynamics
2. Direct coarse-graining: e.g. Kinetic approaches
(Boltzmann-Ginzburg-Landau approach)

Coarse-grained theory

The Boltzmann-Ginzburg-Landau (BGL) approach

- We want to derive a continuous, mesoscopic theory for the relevant hydrodynamic fields, like local density $\rho(\mathbf{r}, t)$ and local momentum $\mathbf{w}(\mathbf{r}, t) = \rho \mathbf{v}$
- Spatial **coarse-grain**. For instance $\rho(\mathbf{r}, t)$ is the local density at time t computed in a volume $\Delta V(\mathbf{r})$ centered on \mathbf{r} , which is much smaller than the macroscopic dimensions of the system, but large enough to contain many particles.
- We shall consider scales much larger than the linear size of the volume ΔV , so that it can be treated as infinitesimal.

$$\Delta V \rightarrow dV$$

We are describing the large scale physics of our system

- We follow the so-called **kinetic approach**, where we are interested in the single particle probability distribution function

$$f(\mathbf{r}, \theta, t) dV d\theta$$

$$\left[\begin{array}{l} f(\mathbf{r}, \theta, t) = f(\mathbf{r}, \theta + m\pi, t) \\ \frac{1}{\bar{V}} \int_V d\mathbf{r} \int_{-\pi}^{\pi} d\theta f(\mathbf{r}, \theta, t) = \rho_0 \end{array} \right]$$

which, at a given time t gives the number of particles with orientation between θ and $\theta + d\theta$ which are in the volume dV centered on \mathbf{r}

Our strategy

$$f(\mathbf{r}, \theta, t) dV d\theta$$

Single particle PDF



Binary collisions and molecular chaos approximations



(generalized) **Boltzmann equation**



Fourier space representation: fields (density, momentum, nematic field)



Truncation strategy a-la Ginzburg-Landau, **enslaving** of the fast modes



Slow modes, **hydrodynamic-like description**

Evolution of f for free ballistic particles (free Boltzmann equation)

$$f(\mathbf{r}, \theta, t + dt) = f(\mathbf{r} - dt v_0 \mathbf{e}(\theta), \theta, t) \quad [\mathbf{e}(\theta) \equiv (\cos \theta, \sin \theta)]$$

we expand to first order

$$f(\mathbf{r} - dt v_0 \mathbf{e}(\theta), \theta, t) \approx f(\mathbf{r}, \theta, t) - dt v_0 \mathbf{e}(\theta) \cdot \nabla f(\mathbf{r}, \theta, t)$$

$$\Rightarrow f(\mathbf{r}, \theta, t + dt) - f(\mathbf{r}, \theta, t) = -dt v_0 \mathbf{e}(\theta) \cdot \nabla f(\mathbf{r}, \theta, t) = 0$$

And finally, dividing by dt and taking dt as infinitesimal (this means we are considering timescales much larger than the microscopic timescale):

$$\partial_t f(\mathbf{r}, \theta, t) + v_0 \mathbf{e}(\theta) \cdot \nabla f(\mathbf{r}, \theta, t) = 0$$

Diffusion may be included

Generalized displacement, random \mathbf{v}

$$\mathbf{r}(t + \Delta t) = \mathbf{r}(t) + \mathbf{v} \Delta t$$

$$\mathbf{v} = v \mathbf{n}(\theta) \equiv v(\cos \theta, \sin \theta) \quad d=2 \text{ for simplicity}$$

$\Phi_{v_0}(v, \theta - \theta_0)$ distribution function (given by dynamics) for \mathbf{v}

Pure ballistic (Vicsek)


$$\Phi_{v_0}(v, \theta - \theta_0) = \delta(v - v_0)\delta(\theta - \theta_0)$$

Axial diffusion (Active nematics)

$$\Phi_{v_0}(v, \theta - \theta_0) = \frac{1}{2}\delta(v - v_0)\delta(\theta - \theta_0) + \frac{1}{2}\delta(v - v_0)\delta(\theta + \theta_0)$$

Diffusion may be included

$$f(\mathbf{r}, \theta, t + \Delta t) = \int d\mathbf{v} \Phi(v, \theta_v - \theta) f(\mathbf{r} - \mathbf{v}\Delta t, \theta, t).$$


$$\frac{\partial f}{\partial t} = -\langle v_\alpha \rangle \partial_\alpha f(\mathbf{r}, \theta, t) + \frac{1}{2} \langle \delta v_\alpha \delta v_\beta \rangle \Delta t \partial_\alpha \partial_\beta f(\mathbf{r}, \theta, t)$$

$$\langle v_\alpha \rangle = \int_0^\infty dv \int_{-\pi}^\pi d\theta_v v n_\alpha(\theta_v) \Phi(v, \theta_v - \theta)$$

$$\langle \delta v_\alpha \delta v_\beta \rangle = \int_0^\infty dv \int_{-\pi}^\pi d\theta_v \delta v_\alpha(\theta_v) \delta v_\beta(\theta_v) \Phi(v, \theta_v - \theta)$$

Diffusion may be included

$$\frac{\partial f}{\partial t} = -v_0 n_\alpha \partial_\alpha f + D_0 \Delta f + D_1 g_{\alpha\beta} \partial_\alpha \partial_\beta f$$

$$v_0 = \langle v \cos \delta\theta \rangle$$

Drift

$$\delta\theta \equiv \theta_v - \theta_0$$

$$D_0 = \frac{1}{4} (\langle v^2 \rangle - v_0^2) \Delta t$$

Isotropic diffusion

$$D_1 = \frac{1}{2} (\langle v^2 \cos 2\delta\theta \rangle - v_0^2) \Delta t$$

anisotropic diffusion

$$g_{\alpha\beta} = n_\alpha n_\beta - \frac{1}{2} \delta_{\alpha\beta}$$

$$\langle \delta v_\alpha \delta v_\beta \rangle = \frac{1}{2} \langle v^2 (1 - \cos 2\delta\theta) \rangle \delta_{\alpha\beta} + (\langle v^2 \cos 2\delta\theta \rangle - v_0^2) n_\alpha(\theta) n_\beta(\theta)$$

D_0

D_1

$$\delta v_\alpha = v_\alpha - \langle v_\alpha \rangle$$

The Boltzmann equation

$$\frac{\partial f}{\partial t} + v_0 n_\alpha \partial_\alpha f = D_0 \Delta f + D_1 g_{\alpha\beta} \partial_\alpha \partial_\beta f + I_{\text{diff}}[f] + I_{\text{col}}[f]$$

Self diffusion, aka orientational noise

- Self diffusion term (linear in f)

$$I_{\text{diff}}[f] = -\lambda f(\mathbf{r}, \theta, t) + \lambda \int_{-\pi}^{\pi} d\theta' f(\mathbf{r}, \theta', t) \int_{-\infty}^{+\infty} d\xi P(\xi) \delta_{2\pi}(\theta - \theta' - \xi)$$

- P is the noise probability distribution. It has to be symmetric $P(\xi) = P(-\xi)$ and, in the following, without loss of generality (due to central limit theorem) we will consider it Gaussian with standard deviation η

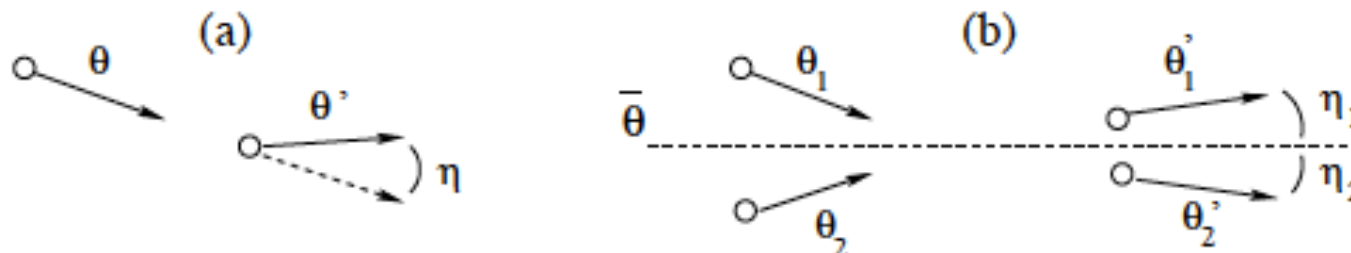
$$P(\xi) = \frac{e^{-\xi^2/2\sigma^2}}{\sigma\sqrt{2\pi}}$$

- $\delta_{m\pi}(\theta - \theta' - \xi)$ is a generalized Dirac's delta with a $m\pi$ periodic argument
- λ is the self-diffusion rate; note we can always rescale time units to set $\lambda = 1$

How to treat noise and alignment interactions : the dilute gas limit

$$\rho_0 \ll 1/d_0 \Rightarrow \langle l \rangle = 1/\sqrt{\rho_0} \gg d_0$$

- Orientation dynamics is dominated by (a) self diffusion events (no interaction just noise) and (b) binary interactions (aka binary “collisions”). Higher order interactions involving more than 2 particles at once can be neglected



- A further important hypothesis is the total decorrelation of orientations between consecutive collisions (this is known as *molecular chaos* hypothesis), which to a certain extent is also justifiable at low densities.

$$f_2(\mathbf{r}, \theta_1, \theta_2, t) \approx f(\mathbf{r}, \theta_1, t) f(\mathbf{r}, \theta_2, t)$$

Interaction part

General microscopic rule

$$\mathbf{r}(t + \Delta t) = \mathbf{r}(t) + \mathbf{v} \Delta t$$

$$\theta' = \Psi^{(p)}(\theta, \theta_{i_1}, \theta_{i_2}, \dots, \theta_{i_p}) + \eta$$

Binary collision approximation

$$\theta'_1 = \Psi(\theta_1, \theta_2) + \eta_1, \quad \theta'_2 = \Psi(\theta_2, \theta_1) + \eta_2$$

Symmetry and isotropy

$$\Psi(\theta_1, \theta_2) \text{ is } n\pi\text{-periodic,} \quad \Psi(\theta_1 + \phi, \theta_2 + \phi) = \Psi(\theta_1, \theta_2) + \phi [n\pi].$$

arbitrary rotation

Choosing $\phi = -\theta_1$ and $\theta_2 = \theta_1 + \Delta$, one obtains

$$\Psi(\theta_1, \theta_1 + \Delta) = \theta_1 + \Psi(0, \Delta) [n\pi].$$

No chirality, symmetric interactions

$$\Psi(0, \Delta) = -\Psi(0, -\Delta)$$

The alignment rule

- Other symmetries for the interaction rule change the symmetry of h . For instance, nematic symmetry $\theta \rightarrow \theta + \pi$ requires h and f to be π periodic, not just 2π .
- E.g.: In the **Vicsek model**, we have simply

$$\Psi(\theta_1, \theta_2) = \text{Arg}[e^{i\theta_1} + e^{i\theta_2}]$$

so that (you can show it as an exercise)

$$\Psi(0, \Delta) = \text{Arg}[1 + e^{i\Delta}] = \frac{\Delta}{2} = \frac{\theta_2 - \theta_1}{2} \quad \text{for } \theta_2 - \theta_1 \in [-\pi, \pi]$$

and we have the half-angle collision rule

$$\theta_1 \rightarrow \frac{\theta_1 + \theta_2}{2} \quad \theta_2 \rightarrow \frac{\theta_1 + \theta_2}{2} \quad \text{for } \theta_2 - \theta_1 \in [-\pi, \pi]$$

The Boltzmann equation - Interaction

$$\frac{\partial f}{\partial t} + v_0 n_\alpha \partial_\alpha f = D_0 \Delta f + D_1 g_{\alpha\beta} \partial_\alpha \partial_\beta f + I_{\text{diff}}[f] + I_{\text{col}}[f]$$

Collision part

Collision Kernel

$$I_{\text{col}}[f] = -f(\mathbf{r}, \theta, t) \int_{-\pi}^{\pi} d\theta' K(\theta' - \theta) f(\mathbf{r}, \theta', t) + \int_{-\pi}^{\pi} d\theta_1 \int_{-\pi}^{\pi} d\theta_2 \int_{-\infty}^{\infty} d\eta P_\sigma(\eta) \\ \times K(\theta_2 - \theta_1) f(\mathbf{r}, \theta_1, t) f(\mathbf{r}, \theta_2, t) \delta_{m\pi}(\Psi(\theta_1, \theta_2) + \eta - \theta)$$

Alignment rule

The collision kernel

- Which is the probability that two particles laying in the same volume centered on position \mathbf{r} actually collide in a unit time interval ?
- Rotational invariance and lack of chirality requires

$$K(\theta_1, \theta_2) = K(\theta_2 - \theta_1) = K(\Delta) \quad \text{and} \quad K(\Delta) = K(-\Delta)$$

- For **self-propelled** particles the kernel can be computed in the reference frame of the first particle, where

$$\mathbf{v}_2' = v_0(\mathbf{e}_2 - \mathbf{e}_1) \quad \mathbf{e}_i = (\cos \theta_i, \sin \theta_i)$$

- The number of colliding particle per unit density is then given by (using elementary trigonometry) Incoming flux

$$K(\theta_2 - \theta_1) = \underbrace{2d_0}_{d=2 \text{ cross section}} \underbrace{v_0 |\mathbf{e}_2 - \mathbf{e}_1|}_{\text{Incoming flux}} = 4d_0 v_0 \sin \left| \frac{\theta_2 - \theta_1}{2} \right| = \alpha \left| \sin \frac{\Delta}{2} \right|$$

- α is a collision rate; note we can always rescale length units to set $\alpha = 1$

Hydrodynamic equations

- In $d = 2$ hydrodynamic fields can be accessed via Fourier coefficients of f

$$f(\mathbf{r}, \theta, t) = \frac{1}{2\pi} \sum_{k=-\infty}^{\infty} \hat{f}_k(\mathbf{r}, t) e^{-ik\theta} \quad \text{and} \quad \hat{f}_k(\mathbf{r}, t) = \int_{-\pi}^{\pi} d\theta f(\mathbf{r}, \theta, t) e^{ik\theta}$$

- In particular, for $k = 0$ we have the **local density**

$$\left[\hat{f}_k^* = \hat{f}_{-k} \right]$$

$$\rho(\mathbf{r}, t) \equiv \hat{f}_0(\mathbf{r}, t) = \int_{-\pi}^{\pi} d\theta f(\mathbf{r}, \theta, t)$$

- And for $k = 1, 2$ the **local momentum** and the **nematic tensor**

$$\rho \mathbf{P} = \begin{pmatrix} \text{Re } f_1 \\ \text{Im } f_1 \end{pmatrix}$$

$$\rho \mathbf{Q} = \frac{1}{2} \begin{pmatrix} \text{Re } f_2 & \text{Im } f_2 \\ \text{Im } f_2 & -\text{Re } f_2 \end{pmatrix}$$

$$P_\alpha = \langle n_\alpha \rangle_l,$$

$$Q_{\alpha\beta} = \langle n_\alpha n_\beta \rangle_l - \delta_{\alpha\beta}/2$$

Fourier Expansion of Boltzmann Eq.

$$\frac{\partial f_k}{\partial t} + \frac{v_0}{2} (\nabla f_{k-1} + \nabla^* f_{k+1}) = -(1 - P_k) f_k + D_0 \Delta f_k + \frac{D_1}{4} (\nabla^2 f_{k-2} + \nabla^{*2} f_{k+2})$$

$$+ \sum_{q=-\infty}^{\infty} (P_k I_{k,q} - I_{0,q}) f_q f_{k-q}$$

with

$$I_{k,q} = \frac{1}{2\pi} \int_{-\pi}^{\pi} d\Delta K(\Delta) e^{-iq\Delta + ikH(\Delta)} \quad H(\Delta) \equiv \Psi(0, \Delta)$$

$$P_k(\sigma) = e^{-\sigma^2 k^2 / 2}.$$

And complex gradients

$$\nabla = \partial_x + i\partial_y \quad \Delta = \nabla \nabla^*$$

$$\nabla^* = \partial_x - i\partial_y \quad \nabla^2 = (\partial_x + i\partial_y)^2$$

Fourier Expansion of Boltzmann Eq.

$$\frac{\partial f_k}{\partial t} + \frac{v_0}{2}(\nabla f_{k-1} + \nabla^* f_{k+1}) = -(1 - P_k)f_k + D_0\Delta f_k + \frac{D_1}{4}(\nabla^2 f_{k-2} + \nabla^{*2} f_{k+2})$$
$$+ \sum_{q=-\infty}^{\infty} (P_k I_{k,q} - I_{0,q}) f_q f_{k-q}$$

$k = 0$ gives continuity equation

$$\frac{\partial \rho}{\partial t} + v_0 \text{Re}(\nabla^* f_1) = D_0 \Delta \rho + \frac{D_1}{2} \text{Re}(\nabla^{*2} f_2).$$

= 0 for $k = 0$



But $k > 0$ infinite hierarchy, truncation needed

The Ginzburg-Landau ansatz for self-propelled particles

- At this level, our infinite hierarchy is fully equivalent to the Boltzmann equation we started with. Indeed to numerically study it, the best strategy is to numerically solve the above hierarchy for a large (but necessarily finite) number of modes. To proceed further analytically, we need a closure strategy which leaves only with the hydrodynamic, relevant modes.
- Our **ballistic** ansatz assumes that Fourier modes change slowly in space and time (this imply our theory will be correct only on large space and time scales),

$$\nabla \sim \epsilon, \quad \partial_t \sim \epsilon \quad \epsilon \ll 1$$

- Note that **we scale space and time equally**, since our propagation mechanism is **ballistic**, linear in time, rather than diffusive or quadratic in time (e.g. **active nematics**)

$$\nabla \sim \epsilon, \quad \partial_t \sim \epsilon^2.$$

The Ginzburg-Landau ansatz for self-propelled particles

- Note that the **homogeneous disordered solution** $\hat{f}_0 = \rho$ $\hat{f}_k = 0$ $k > 0$ is always a solution of our hierarchy. Fluctuations can lead to a nonzero k Fourier modes only if one has $\mu_k(\rho, \sigma) > 0$

Suppose f_j is the first non damped Fourier mode (the **order parameter**)

$$\mu_j > 0 \quad \mu_k < 0 \quad k < j$$

$$\rho - \rho_0 \sim \epsilon,$$

Slow field, particle conservation

$$f_k \sim \epsilon \quad 0 < k \leq j$$

$$f_k \sim \epsilon^2 \quad j < k \leq 2j$$

$$j = 2 / n$$

$$f_k \sim \epsilon^3 \quad 2j < k \leq 3j$$

Controlled by symmetry!

Truncation strategy: find the order parameter and enslave higher orders

Linearize around the homogeneous solution $f_0 = \rho_0, f_k = 0 \ (k \geq 1)$

$$\frac{\partial f_k}{\partial t} = [-(1 - P_k) + \omega_k \rho_0] f_k \equiv \mu_k f_k \quad k > 0$$

$$\omega_k = P_k(I_{k,k} + I_{k,0}) - (I_{0,k} + I_{0,0}).$$

$$\mu_k(\sigma, \rho_0) \equiv -(1 - P_k) + \omega_k \rho_0.$$

Zero noise limit $P_k \rightarrow 1 \quad \mu_k \approx \omega_k^{(0)} \rho_0$

$$\omega_k^{(0)} = \frac{1}{\pi} \int_0^\pi d\Delta K(\Delta) [\cos k(H(\Delta) - \Delta) + \cos kH(\Delta) - \cos k\Delta - 1]$$

Controls the sign of the linear term

Truncation strategy: find the order parameter and enslave higher orders

$$\frac{\partial f_k}{\partial t} + \frac{v_0}{2}(\nabla f_{k-1} + \nabla^* f_{k+1}) = -(1 - P_k)f_k + D_0 \Delta f_k + \frac{D_1}{4}(\nabla^2 f_{k-2} + \nabla^{*2} f_{k+2})$$

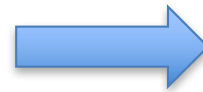
$$+ \sum_{q=-\infty}^{\infty} (P_k I_{k,q} - I_{0,q}) f_q f_{k-q}$$

For $k > j$

$$\partial_t f_k \ll f_k$$

For $\partial_t f_k \approx 0$

$$\partial_t f_k = \mu f_k + \dots$$



$$f_k \approx -\frac{1}{\mu_k} [\dots]$$



Enslaved to lower order terms

Plug back into eqs. For $k \leq j$ and ignore terms of order 4 or higher

Example: Vicsek model

Full polar symmetry, $n = m = 2$

$$K(\theta_2 - \theta_1) = 4d_0v_0 \sin \frac{|\theta_2 - \theta_1|}{2}$$

$$\Psi(0, \theta_2 - \theta_1) \equiv H(0, \theta_2 - \theta_1) = \frac{\theta_2 - \theta_1}{2}$$



$$I_{k,q} = \frac{1}{2\pi} \int_{-\pi}^{\pi} d\Delta K(\Delta) e^{-iq\Delta + ikH(\Delta)}$$

- And after (somehow lengthy calculations) to lowest k 's

$$k = 0 \quad \overset{2}{\partial_t \hat{f}_0} + \frac{v_0}{2} \left[\overset{2}{\tilde{\nabla} \hat{f}_1^*} + \overset{2}{\tilde{\nabla}^* \hat{f}_1} \right] = 0$$

$$k = 1 \quad \overset{2}{\partial_t \hat{f}_1} + \frac{v_0}{2} \left[\overset{2}{\tilde{\nabla} \hat{f}_0} + \overset{3}{\tilde{\nabla}^* \hat{f}_2} \right] = \overset{1+2?}{\mu_1(\rho, \sigma)} \overset{3}{\hat{f}_1} + b_1 \overset{3}{\hat{f}_1^* \hat{f}_2}$$

$$k = 2 \quad \overset{3}{\partial_t \hat{f}_2} + \frac{v_0}{2} \overset{2}{\tilde{\nabla} \hat{f}_1} = \overset{2}{\mu_2(\rho, \sigma)} \overset{2}{\hat{f}_2} + b_2 \overset{2}{\hat{f}_1 \hat{f}_1}$$

- Computing explicitly (it's a good exercise) one sees that $\mu_2(\rho, \sigma) < 0 \quad \forall \rho, \eta$ while $\mu_1(\rho, \sigma)$ changes sign over some critical line $\rho_c(\sigma)$

- The term $\overset{3}{\partial_t \hat{f}_2} \ll \varepsilon^2$ can be neglected, and one sees immediately that \hat{f}_2 is **enslaved** to \hat{f}_1

$$\hat{f}_2 \approx \frac{1}{\mu_2} \left[\frac{v_0}{2} \tilde{\nabla} \hat{f}_1 - b_2 \hat{f}_1 \hat{f}_1 \right]$$

- This allows to close our equation at the $k = 1$ level

$$\partial_t \rho + \frac{v_0}{2} [\tilde{\nabla} \hat{f}_1^* + \tilde{\nabla}^* \hat{f}_1] = 0$$

$$\begin{aligned} \partial_t \hat{f}_1 = & \left[\mu_1(\rho, \sigma) - \frac{b_1 b_2}{\mu_2} |\hat{f}_1|^2 \right] \hat{f}_1 - \frac{v_0}{2} \tilde{\nabla} \rho - \frac{v_0^2}{4\mu_2} \tilde{\nabla} \tilde{\nabla}^* \hat{f}_1 \\ & + \frac{v_0 b_2}{\mu_2} \hat{f}_1 \tilde{\nabla}^* \hat{f}_1 + \frac{v_0 b_1}{2\mu_2} \hat{f}_1^* \tilde{\nabla} \hat{f}_1 \end{aligned}$$

- The equations above are invariant under rotations, in our complex language under the transformation

$$\begin{aligned} \hat{f}_1 &\rightarrow e^{i\phi} \hat{f}_1 & \tilde{\nabla} &\rightarrow e^{i\phi} \tilde{\nabla}_1 \\ \hat{f}_1^* &\rightarrow e^{-i\phi} \hat{f}_1^* & \tilde{\nabla}^* &\rightarrow e^{-i\phi} \tilde{\nabla}^* \end{aligned}$$

- The only other term (up to third order) allowed by symmetry non present here is

$$\hat{f}_1 \tilde{\nabla} \hat{f}_1^*$$

Hydrodynamic equations in vectorial notations

$$\frac{\partial \mathbf{w}}{\partial t} + \gamma(\mathbf{w} \cdot \nabla) \mathbf{w} = -\frac{v_0}{2} \nabla \rho + \frac{\kappa}{2} \nabla \mathbf{w}^2 + (\mu - \xi \mathbf{w}^2) \mathbf{w} + \nu \nabla^2 \mathbf{w} - \kappa(\nabla \cdot \mathbf{w}) \mathbf{w}$$

$$\frac{\partial}{\partial t} \rho + v_0 \nabla \cdot \mathbf{w} = 0 \quad [\mathbf{w} = \rho \mathbf{v}]$$

- With transport coefficients (in non rescaled units), for the Vicsek case

$$\nu = \frac{v_0^2}{4} \left[\lambda \left(1 - e^{-2\sigma_0^2} \right) + \frac{16}{3\pi} d_0 v_0 \rho \left(\frac{7}{5} + e^{-2\sigma^2} \right) \right]^{-1}, \quad [\sigma_0 \equiv \sigma]$$

$$\gamma = \frac{16\nu d_0}{\pi} \left(\frac{16}{15} + 2e^{-2\sigma^2} - e^{-\sigma^2/2} \right), \quad \mu = \frac{8}{\pi} d_0 v_0 \rho \left(e^{-\sigma^2/2} - \frac{2}{3} \right) - \lambda \left(1 - e^{-\sigma_0^2/2} \right),$$

$$\kappa = \frac{16\nu d_0}{\pi} \left(\frac{4}{15} + 2e^{-2\sigma^2} + e^{-\sigma^2/2} \right), \quad \xi = \frac{256\nu d_0^2}{\pi^2} \left(e^{-\sigma^2/2} - \frac{2}{5} \right) \left(\frac{1}{3} + e^{-2\sigma^2} \right).$$

- This equations are formally valid **near threshold and for large length and time scales**. The same equations can be derived only from symmetry considerations (Toner & Tu theory, *J. Toner & Y. Tu, Phys Rev Lett 75 4326 (1995)*). However, this approach does not allow to compute transport coefficients and their fields dependence

Study of the homogeneous solution

- First consider an homogeneous solution (density is fixed in time by particle conservations)

$$\rho(\mathbf{r}, t) = \rho_0 \quad \mathbf{w}(\mathbf{r}, t) = \mathbf{w}(t)$$

- First consider an homogeneous solution (density is fixed in time by particle conservations). Our hydrodynamic equations simplifies to

$$\partial_t \mathbf{w} = (\mu - \xi \mathbf{w}^2) \mathbf{w}$$

$$\mu = \mu(\rho, \sigma)$$

$$\xi(\rho, \sigma) > 0 \quad \text{if} \quad \mu(\rho, \sigma) > 0$$

This guarantees the dynamics does not blow up, as for large \mathbf{w} the r.h.s. will always turn negative

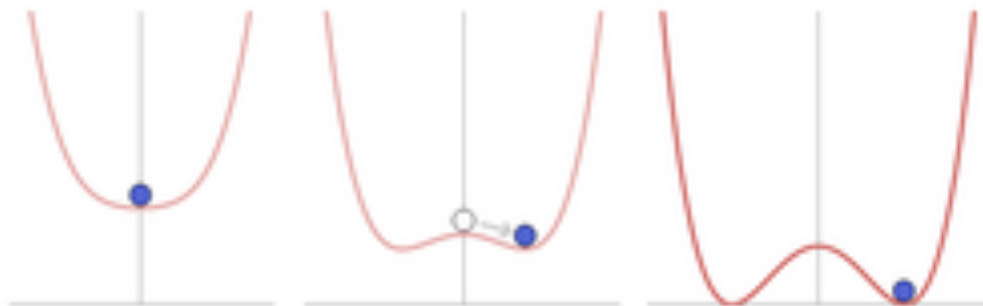
Study of the homogeneous solution – spontaneous symmetry breaking

- There are two possible stationary solution, so that $\partial_t \mathbf{w} = 0$
- The first is the disordered, isotropic solution, where it is stable for $\mu < 0$ and unstable for $\mu > 0$
- The second exist only if $\mu > 0$, and it is the ordered, spontaneously symmetry broken solution. It is stable in the direction of the modulo (**hard mode**) and marginal in the direction of the phase (**soft mode**)

$$\mathbf{w}_0 = 0$$

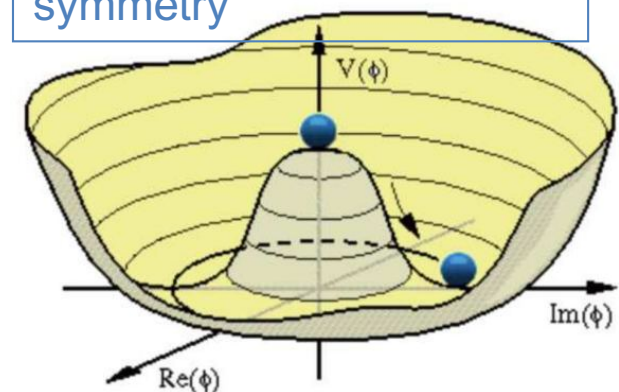
Orientation
(randomly chosen)

$$\mathbf{w}_0 = \sqrt{\frac{\mu}{\xi}} \mathbf{e}$$



Breaking of a discrete symmetry (ising like)

Breaking of a continuous symmetry



Linear stability analysis – spontaneous symmetry breaking

- First understanding is given by **linear stability analysis**, i.e. linearizing the homogeneous equation around the given solution, i.e. considering the small perturbation $\mathbf{w}_0 \rightarrow \mathbf{w}_0 + \delta \mathbf{w}$ and keeping only linear terms in the perturbation.

- Around the isotropic solution one has:

$$\partial_t \delta \mathbf{w} = \mu \delta \mathbf{w}$$

and the stability depends on the sign of μ (positive: perturbations grows, negative, perturbations are damped)

- Perturb the ordered solution (assume the solution is oriented in the x direction), and decompose the perturbation in the parallel and perpendicular directions

$$\mathbf{w}_0 = \left(\sqrt{\mu/\xi}, 0 \right) \quad \delta \mathbf{w} = \left(\delta w_{//}, \delta w_{\perp} \right)$$

- One has

$$\partial_t \delta w_{//} = -2\mu \delta w_{//} \quad \text{and} \quad \partial_t \delta w_{\perp} = 0$$

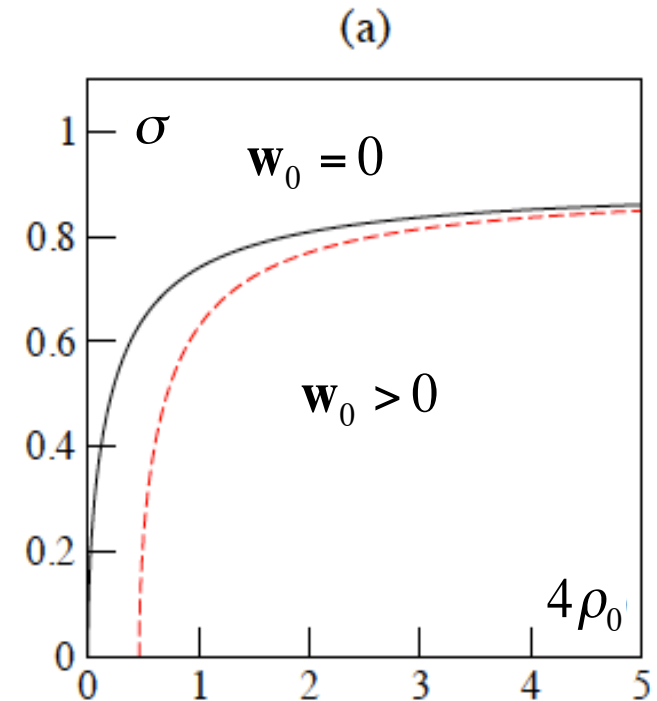
so that perturbations parallel to the ordered solution (in the modulo direction) are damped (a hard mode), while perpendicular ones, along the phase (a soft mode) are marginal and undamped.

Phase diagram

- We are now able to draw a phase diagram in the (σ, ρ) plane, with a transition from the disordered to the ordered homogeneous phases (black line)

note that near the transition we have

$$\varepsilon \sim |\mathbf{w}_0| = \sqrt{\frac{\mu}{\xi}} \Rightarrow \mu \sim \varepsilon^2$$



- What we do not know, is whether these phases are stable against **spatial perturbations** (non homogeneous)

Linear stability with respect to non-homogeneous perturbations

- First of all, we have to linearize our full set of hydrodynamic equations with respect to non-homogeneous small perturbations.

$$\rho_0 \rightarrow \rho_0 + \delta \rho(\mathbf{r}, t) \quad \text{and} \quad \mathbf{w}_0 \rightarrow \mathbf{w}_0 + \delta \mathbf{w}(\mathbf{r}, t)$$

$$\left[\int_S \delta \rho(\mathbf{r}, t) dV = 0 \right]$$

- Again, this implies discarding all terms higher than linear in the perturbations, to get

$$\frac{\partial}{\partial t} \delta \rho + v_0 \nabla \cdot \delta \mathbf{w} = 0$$

$$\begin{aligned} \frac{\partial}{\partial t} \delta \mathbf{w} + \gamma (\mathbf{w}_0 \cdot \nabla) \delta \mathbf{w} &= -\frac{v_0}{2} \nabla \delta \rho + \kappa \nabla (\mathbf{w}_0 \cdot \delta \mathbf{w}) \\ &+ [(\mu' - \xi' \mathbf{w}_0^2) \delta \rho - 2\xi \mathbf{w}_0 \cdot \delta \mathbf{w} - \kappa \nabla \cdot \delta \mathbf{w}] \mathbf{w}_0 \\ &+ (\mu - \xi \mathbf{w}_0^2) \delta \mathbf{w} + \nu \nabla^2 \delta \mathbf{w}, \end{aligned}$$

$$\mu' = \frac{\partial \mu}{\partial \rho} \quad \xi' = \frac{\partial \xi}{\partial \rho}$$

Linear stability with respect to non-homogeneous perturbations

- To study spatial perturbations, we chose the following ansatz

$$\delta \rho(\mathbf{r}, t) = \delta \rho(\mathbf{r}) e^{st} \quad \text{and} \quad \delta \mathbf{w}(\mathbf{r}, t) = \delta \mathbf{w}(\mathbf{r}) e^{st}$$

where s is a complex number. The sign of its real part controls whether perturbations grow or are damped in time, thus the stability to such perturbations.

- Furthermore, we proceed expanding the spatial perturbations in Fourier modes

$$\delta \rho(\mathbf{r}) \sim \sum_q \delta \rho_q e^{-i\mathbf{q}\cdot\mathbf{r}} \quad \text{and} \quad \delta \mathbf{w}(\mathbf{r}) \sim \sum_q \delta \mathbf{w}_q e^{-i\mathbf{q}\cdot\mathbf{r}}$$

with $\mathbf{q} = (q_x, q_y)$ being the wavevector (the inverse of a spatial length).

- We will analyze the stability of one mode at the time; in principle one unstable mode is enough to destabilize the homogeneous solution. We are particularly interested in long-wavelength modes, $\mathbf{q} \ll \mathbf{1}$

$$\delta \rho(\mathbf{r}, t) = \delta \rho_q e^{st - i\mathbf{q}\cdot\mathbf{r}} \quad \text{and} \quad \delta \mathbf{w}(\mathbf{r}, t) = \delta \mathbf{w}_q e^{st - i\mathbf{q}\cdot\mathbf{r}}$$

Linear stability with respect to non-homogeneous perturbations

- Our ansatz implies

$$\nabla \delta \mathbf{w}(\mathbf{r}, t) = -i\mathbf{q} \delta \mathbf{w}(\mathbf{r}, t) \quad \partial_t \delta \mathbf{w}(\mathbf{r}, t) = s \delta \mathbf{w}(\mathbf{r}, t)$$

$$\nabla \delta \rho(\mathbf{r}, t) = -i\mathbf{q} \delta \rho(\mathbf{r}, t) \quad \partial_t \delta \rho(\mathbf{r}, t) = s \delta \rho(\mathbf{r}, t)$$

so that the linearized equations become

$$s \delta \rho_q = -i v_0 \mathbf{q} \cdot \delta \mathbf{w}_q$$

$$s \delta \mathbf{w}_q = \left[(\mu - \xi \mathbf{w}_0^2) - i\gamma(\mathbf{q} \cdot \mathbf{w}_0) - \nu \mathbf{q}^2 \right] \delta \mathbf{w}_q + i\kappa \mathbf{q} (\mathbf{w}_0 \cdot \delta \mathbf{w}_q) + \\ - \mathbf{w}_0 \left((2\xi \mathbf{w}_0 + i\kappa \mathbf{q}) \cdot \delta \mathbf{w}_q \right) + \left[\mathbf{w}_0 (\mu' - \xi' \mathbf{w}_0^2) - i\mathbf{q} \frac{v_0^2}{2} \right] \delta \rho_q$$

- Which is just an eigenvalues problem,

$$\mathbf{M}(\mathbf{q}, \mathbf{w}_0) \delta \mathbf{v}_q = s \delta \mathbf{v}_q \quad \delta \mathbf{v}_q = \left(\delta \rho_q, [\delta \mathbf{w}]_x, [\delta \mathbf{w}]_y \right)^T$$

with the stability being controlled by the sign of the largest eigenvalue

$$\text{Re}[s_+(\mathbf{q})] > 0 \Rightarrow \text{unstable mode}$$

Linear stability with respect to non-homogeneous perturbations

- We begin from the **disordered phase** $\mathbf{w}_0 = 0$, $\mu < 0$ which simplifies the linearized equations to

$$s\delta\rho_q = -iv_0\mathbf{q} \cdot \delta\mathbf{w}_q$$

$$s\delta\mathbf{w}_q = \left[\mu - \nu\mathbf{q}^2\right]\delta\mathbf{w}_q - i\mathbf{q}\frac{v_0}{2}\delta\rho_q$$

- Since $\delta\mathbf{w}$ and \mathbf{q} are parallel, it is possible to simplify, getting the quadratic equation

$$s^2 + (\nu q^2 - \mu)s + \frac{v_0^2}{2}q^2 = 0.$$

which, for $\mu < 0$ has both eigenvalues with a **negative real part** for any finite \mathbf{q}

So, for $\mu < 0$ **the disordered phase is stable** against spatial perturbations

Linear stability with respect to non-homogeneous perturbations

- We now consider the **ordered phase** $|\mathbf{w}_0| = \sqrt{\mu/\xi}$, $\mu > 0$

- We can write explicitly the 3x3 matrix of our eigenvalue problem in term of the angle ϕ between \mathbf{q} and \mathbf{w}_0 :

$$[w_0 = |\mathbf{w}_0| , q = |\mathbf{q}|]$$

$$\mathbf{M} = \begin{pmatrix} 0 & -iv_0q \cos \phi & -iv_0q \sin \phi \\ w_0(\mu' - \xi' w_0^2) - i\frac{v_0}{2}q \cos \phi & -2\mu - i\gamma w_0q \cos \phi - q^2\nu & -i\kappa w_0q \sin \phi \\ -i\frac{v_0}{2}q \sin \phi & i\kappa w_0q \sin \phi & -i\gamma w_0q \cos \phi - q^2\nu \end{pmatrix}$$

The problem greatly simplifies for parallel \mathbf{q} and \mathbf{w}_0 !!

Linear stability with respect to non-homogeneous perturbations

$$\mathbf{M} = \begin{pmatrix} 0 & -iv_0q & 0 \\ w_0(\mu' - \xi' w_0^2) - i\frac{v_0}{2}q & -2\mu - i\gamma w_0q - q^2\nu & 0 \\ 0 & 0 & -i\gamma w_0q - q^2\nu \end{pmatrix}$$

- The eigenvalues are thus $s_3 = -q^2\nu < 0$
and the two solutions of the quadratic equation with complex coefficients

$$s^2 + s \left[(\nu q^2 + 2\mu) + iq\gamma w_1 \right] + \left[\frac{q^2 v_0^2}{2} + iqw_1 (\mu' - \xi' w_1^2) \right] = 0,$$

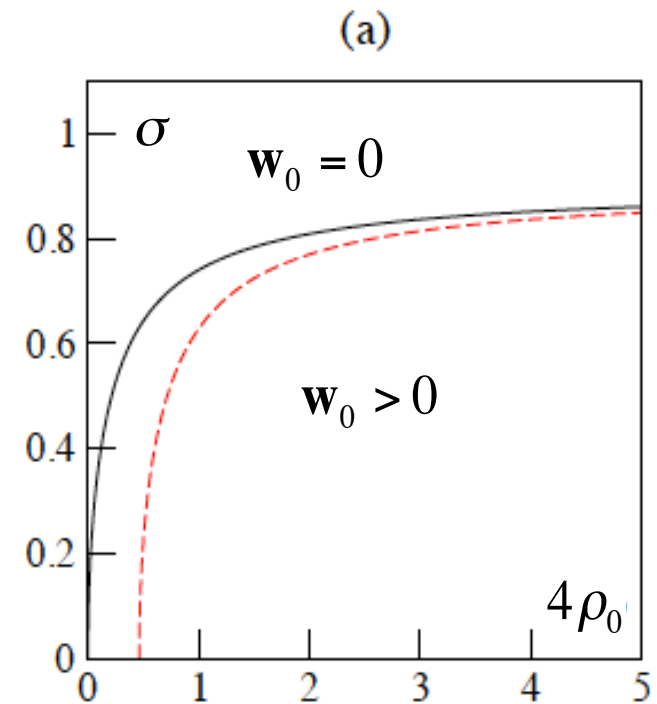
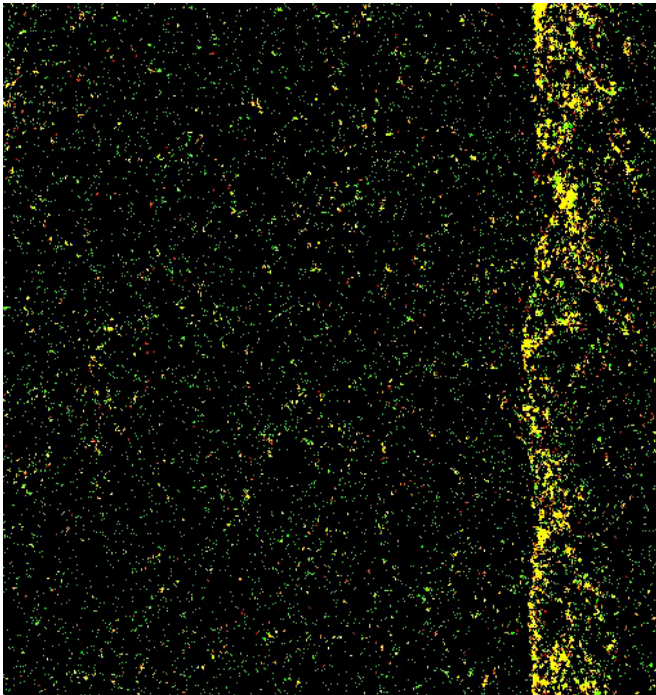
- The largest eigenvalue can be easily computed near threshold $\mu \ll 1$ and in the long wavelength limit $q \ll 1$

$$\Re[s_+] = \frac{\mu'^2}{8\xi\mu^2} q^2$$

Linear stability with respect to non-homogeneous perturbations

$$\Re[s_+] = \frac{\mu'^2}{8\xi\mu^2} q^2$$

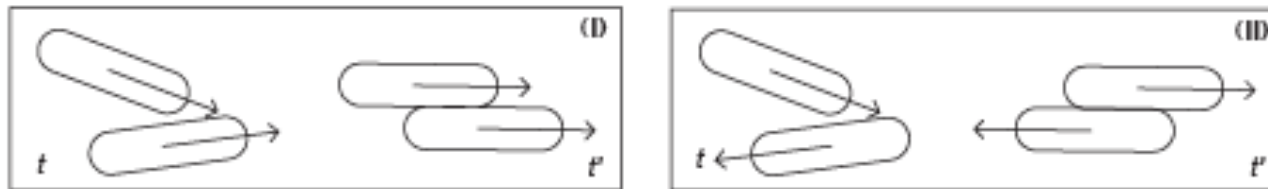
- Since $\mu' > 0$, the largest eigenvalue is positive, and near threshold the homogeneous ordered solution is unstable to long-wavelength perturbations along the longitudinal direction (w.r.t. order parameter)



Example II

Nematic interactions with polar self propulsion:

Self propelled rods

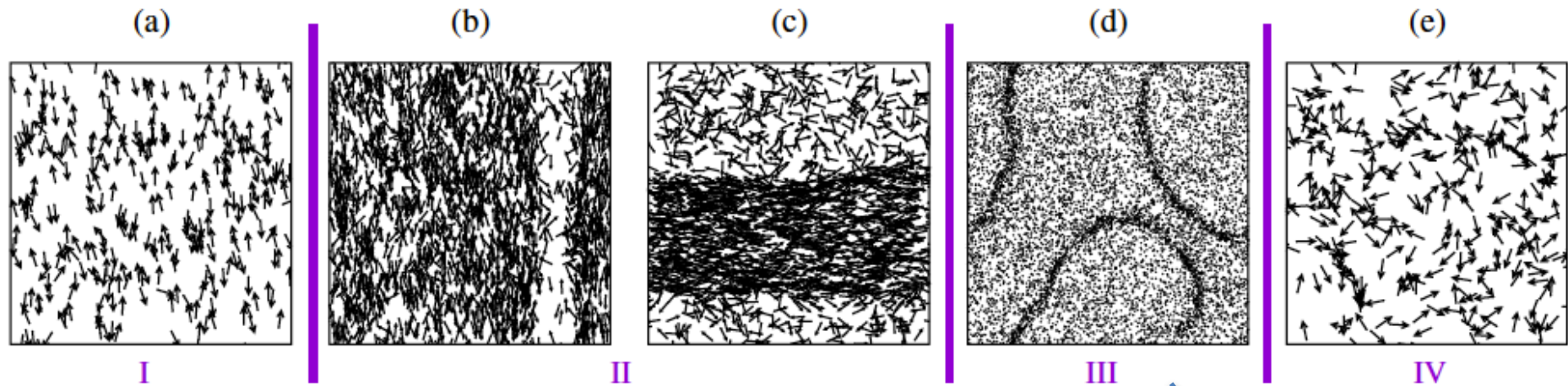


$$\vartheta \rightarrow \vartheta + \pi$$

$$\theta_j^{t+1} = \arg \left[\sum_{k \sim j} \text{sign}[\cos(\theta_k^t - \theta_j^t)] e^{i\theta_k^t} \right] + \eta \xi_j^t \quad i \sim j \quad \text{if} \quad |\vec{r}_i^t - \vec{r}_j^t| < 1$$

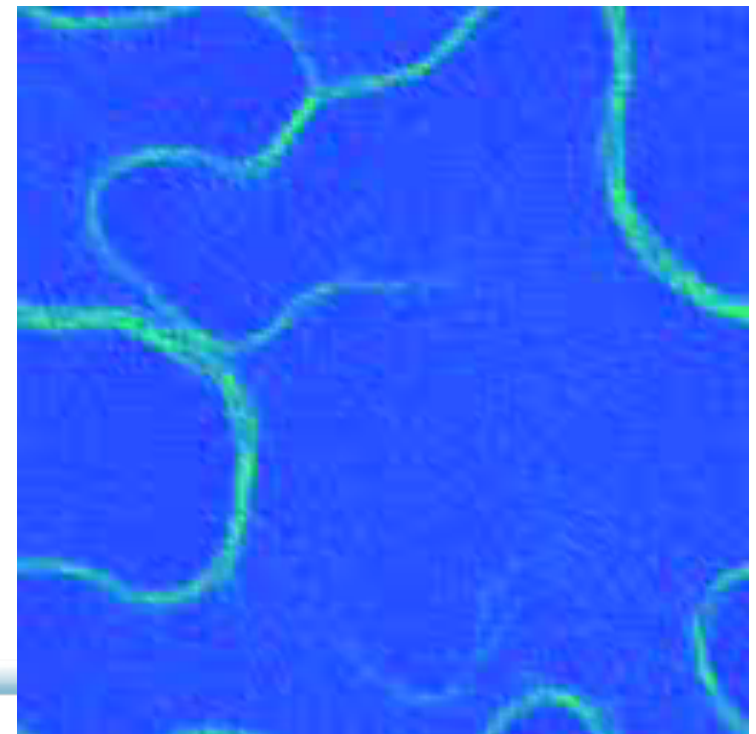
$$\mathbf{r}_j^{t+1} = \mathbf{r}_j^t + v_0 e^{i\theta_j^{t+1}}, \quad \langle \xi_j^t \xi_i^{t'} \rangle \sim \delta_{ij} \delta_{tt'}$$

4 different phases, 2 ordered and 2 disordered



η

- I. Homogeneous long range nematic order
(typical fluctuating HO phase properties)
- II. Spontaneous phase segregation,
nematically ordered bands
- III. Long wavelength instability leads to
Band chaos
- IV. Disordered



Hydrodynamic equations (BGL Kinetic approach):

Boltzmann equation

$$\partial_t f(\mathbf{r}, \theta, t) + v_0 \mathbf{e}(\theta) \cdot \nabla f(\mathbf{r}, \theta, t) = I_{diff}[f] + I_{coll}[f]$$

Fourier expansion

$$\hat{f}_k(\mathbf{r}, t) = \int_{-\pi}^{\pi} d\theta f(\mathbf{r}, \theta, t) e^{ik\theta}$$

Truncation, due to symmetry and ballistic displacement

$$\rho - \rho_0 \sim \epsilon, \quad \{f_{2k-1}, f_{2k}\}_{k \geq 1} \sim \epsilon^k, \quad \nabla \sim \epsilon, \quad \partial_t \sim \epsilon.$$

Hydrodynamic equations (BGL Kinetic approach):

$$\frac{\partial \rho}{\partial t} = -\text{Re}[\bar{\nabla} f_1]$$

$$\begin{aligned} \frac{\partial f_1}{\partial t} = & -\frac{1}{2} \nabla \rho - \frac{1}{2} \bar{\nabla} f_2 + \frac{\gamma}{2} \bar{f}_2 \nabla f_2 \\ & - \left(\alpha - \beta |f_2|^2 \right) f_1 - \epsilon \bar{f}_1 f_2 \end{aligned}$$

$$\begin{aligned} \frac{\partial f_2}{\partial t} = & -\frac{1}{2} \nabla f_1 + \frac{\nu}{4} \Delta f_2 - \frac{\kappa}{2} \bar{f}_1 \nabla f_2 - \frac{\chi}{2} \bar{\nabla} f_1 f_2 \\ & - \left(\mu(\rho) - \xi |f_2|^2 \right) f_2 - \omega f_1^2 + \tau |f_1|^2 f_2 \end{aligned}$$

where $\nabla \equiv \partial_x + i\partial_y$ and $\bar{\nabla} \equiv \partial_x - i\partial_y$ ($\Delta \equiv \nabla \bar{\nabla}$)

Hydrodynamics modes are lowest Fourier modes

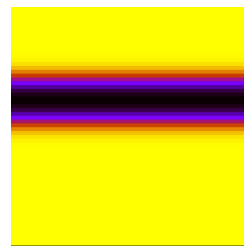
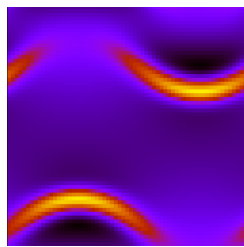
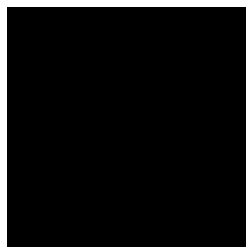
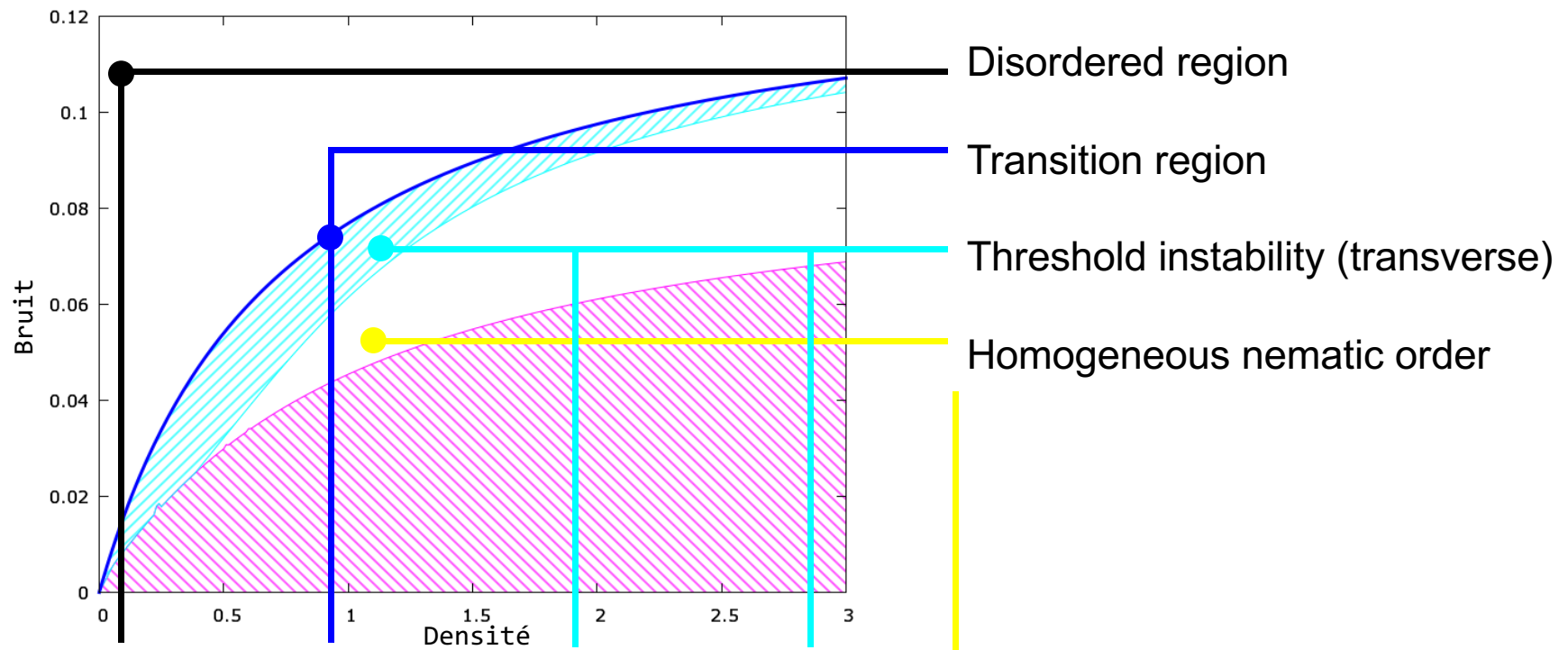
$$\rho = f_0 \quad \mathbf{w} = \rho \mathbf{v} = \begin{pmatrix} \text{Re } f_1 \\ \text{Im } f_1 \end{pmatrix} \quad \rho \mathbf{Q} = \frac{1}{2} \begin{pmatrix} \text{Re } f_2 & \text{Im } f_2 \\ \text{Im } f_2 & -\text{Re } f_2 \end{pmatrix}$$

With coeffs

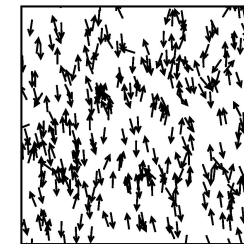
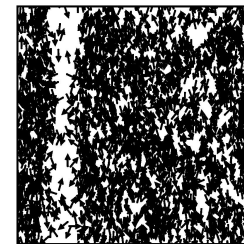
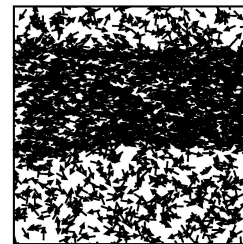
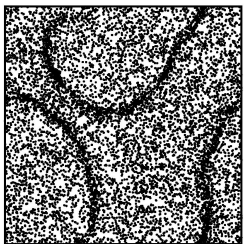
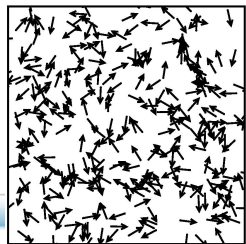
$$\begin{aligned}\nu &= \left[\frac{136}{35\pi} \rho + 1 - \hat{P}_3 \right]^{-1} & \omega &= \frac{8}{\pi} \left[\frac{1}{6} - \frac{\sqrt{2}-1}{2} \hat{P}_2 \right] \\ \mu &= \frac{8}{\pi} \left[\frac{2\sqrt{2}-1}{3} \hat{P}_2 - \frac{8}{5} \right] \rho - 1 + \hat{P}_2 & \varepsilon &= \frac{8}{5\pi} \\ \alpha &= \frac{8}{\pi} \left[\frac{1}{3} - \frac{1}{4} \hat{P}_1 \right] \rho + 1 - \hat{P}_1 & \chi &= \nu \frac{2}{\pi} \left[\frac{4}{5} + \hat{P}_3 \right] \\ \kappa &= \nu \frac{8}{15} \left[\frac{19}{7} - \frac{\sqrt{2}+1}{\pi} \hat{P}_2 \right] & \gamma &= \nu \frac{4}{3\pi} \left[\frac{2}{7} - \hat{P}_1 \right] \\ \tau &= \chi \frac{8}{15} \left[\frac{19}{7} - \frac{\sqrt{2}+1}{\pi} \hat{P}_2 \right] & \beta &= \gamma \frac{2}{\pi} \left[\frac{4}{5} + \hat{P}_3 \right] \\ \xi &= \frac{32}{35\pi} \left[\frac{1}{15} + \hat{P}_4 \right] \left[\frac{13}{9} - \frac{6\sqrt{2}+1}{\pi} \hat{P}_2 \right] \left[\frac{8}{3\pi} \left(\frac{31}{21} + \frac{\hat{P}_4}{5} \right) \rho + 1 - \hat{P}_4 \right]^{-1}\end{aligned}$$

- All coefficients have explicit dependence on *local* density and Fourier coefficients of noise distribution
- $\alpha > 0$
- Key density-dependence of μ

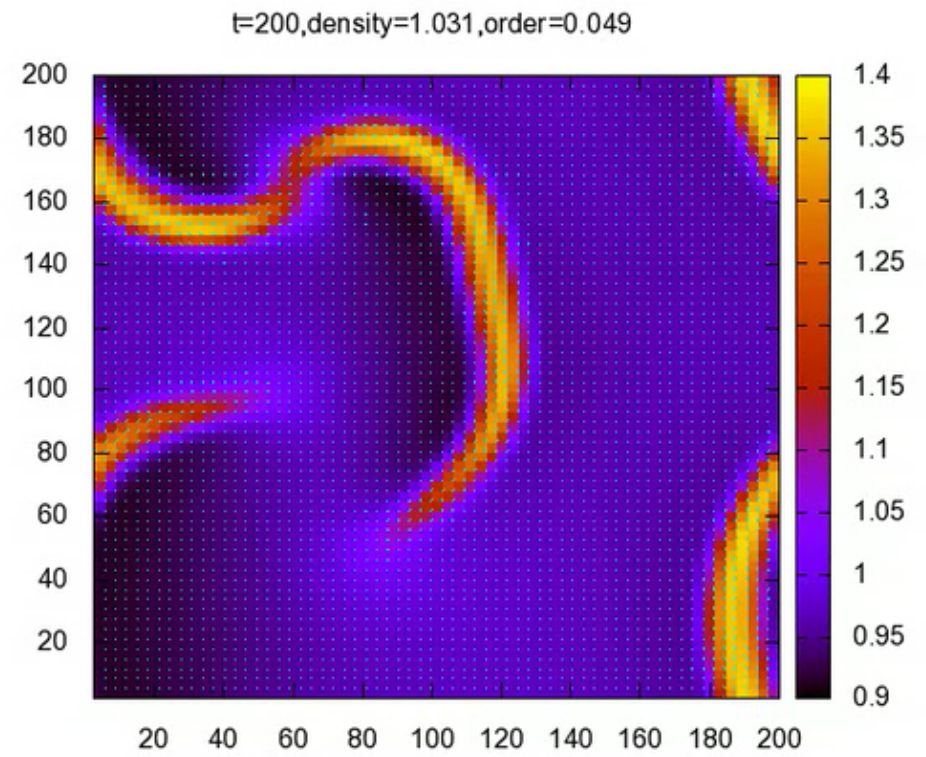
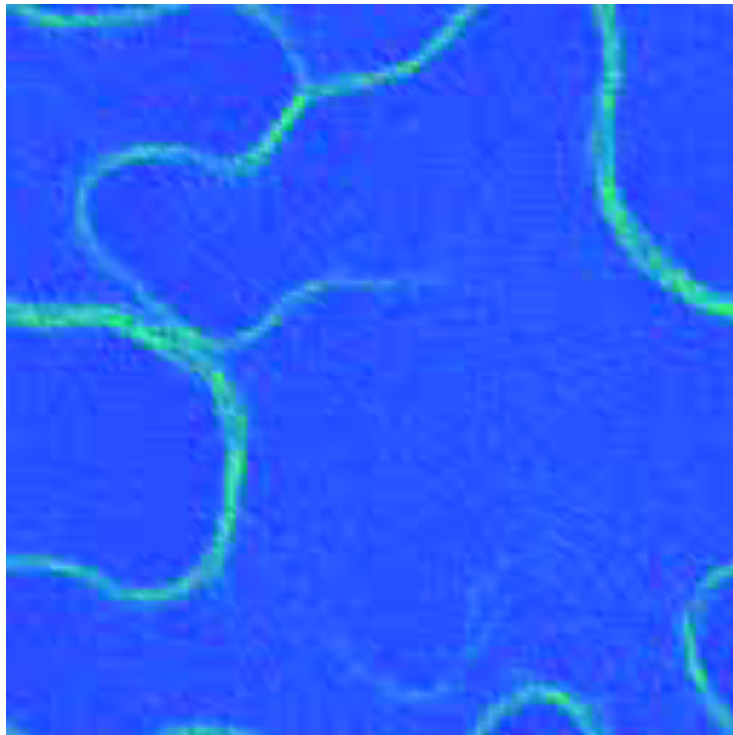
Overall excellent qualitative agreement with microscopic simulations



Mesoscopic simulation
(pseudospectral method)



Microscopic simulations
(molecular dynamics)



Slow and not-so-slow fields: the polar order parameter

At threshold, polar order parameter is trivially enslaved

$$\text{if } f_2 \sim \varepsilon \quad (\text{since } \alpha \gg \beta |f_2|^2)$$
$$\Rightarrow f_1 \approx -\frac{1}{2\alpha} (\nabla \rho + \bar{\nabla} f_2) \sim \varepsilon^2$$

And gives active nematic equations

$$\frac{\partial}{\partial t} \rho = \frac{1}{2\alpha} (\Delta \rho + \text{Re}[\bar{\nabla} \bar{\nabla} f_2])$$

\Rightarrow

$$\frac{\partial}{\partial t} f_2 = \left(\mu(\rho) - \beta |f_2|^2 \right) f_2 + \nu' \Delta f_2 + \frac{1}{4\alpha} \nabla \bar{\nabla} \rho$$

Slow and not-so-slow fields: the polar order parameter

But, at finite distance from threshold, time scales are more complicated. E.g.:

$$\frac{\partial f_1}{\partial t} = -\frac{1}{2}\nabla\rho - \frac{1}{2}\bar{\nabla}f_2 + \frac{\gamma}{2}\bar{f}_2\nabla f_2 - \left(\alpha - \beta|f_2|^2\right)f_1 - \epsilon\bar{f}_1f_2$$

f_2 reduces damping

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THANK YOU...



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