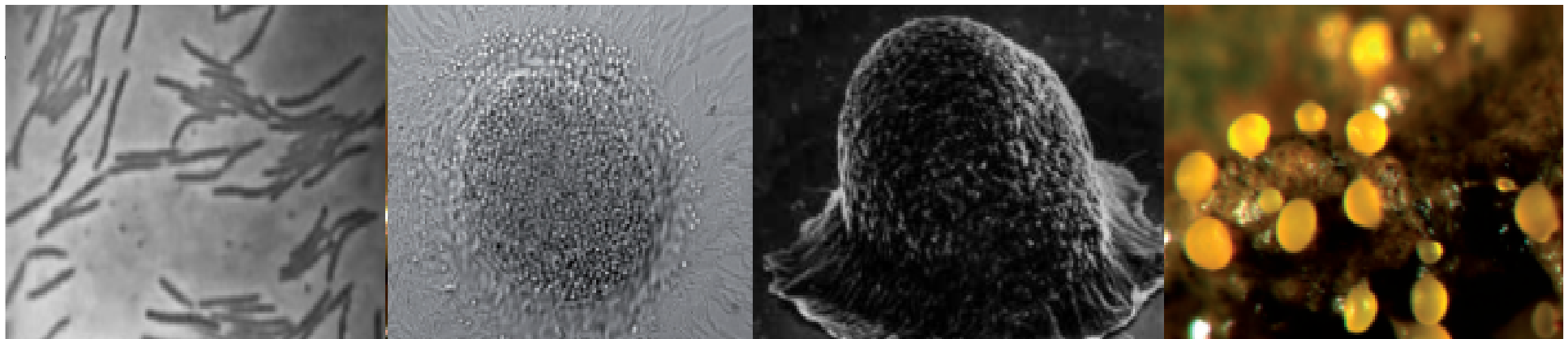


Active soft-matter: modeling living matter and mimicking it.

Fernando Peruani

BIOMAT – La Falda – 08.2014





outline

P1

- 1. Definition of active soft-matter**
- 2. Examples in biology and non-living systems**
- 3. Minimal models of active particles**
 - a. non-interacting**
 - b. interacting**
- 4. Symmetries and boundary conditions**
- 5. Gas-liquid-like transitions**

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P2

Active soft-matter?

What is active soft-matter?

It is a novel area of research at the interface between biology, mathematics, and soft-matter physics that is being developed to understand the physics behind non-equilibrium systems such as bacterial colonies, tissue formation, cancer growth, and more generally, embryogenesis.

Active soft-matter (ASM) has recently witnessed the emergence of a promising new direction: the design and construction of biomimetic, active materials, which are essentially ensembles of artificial active particles.

Specifically, ASM deals with **ensembles of active particles** and their macroscopic properties.

Active soft-matter?

What is an active particle?

What is the difference between a passive and an active particle?

Are there examples of such kind of particles?

Active soft-matter?

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What is an active particle?

**It is a particle able to convert energy into work
in order to self-propel in a dissipative medium.**

(for instance, it could be a particle equipped with a propelling engine.)

What is the difference between a passive and an active particle?

Are there examples of such kind of particles?

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There is energy consumption, energy dissipation, while the FDT does not necessary apply, and in general, momentum (neither linear nor angular) is not conserved.

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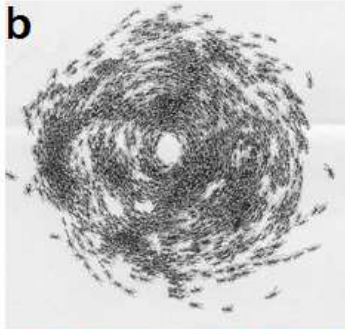
Are there examples of such kind of particles?

Plenty!

Active matter systems: examples

Pattern formation and active matter

Order motion



Vortexes

density waves



Various
"collective motion" patterns
in **animals and insects**

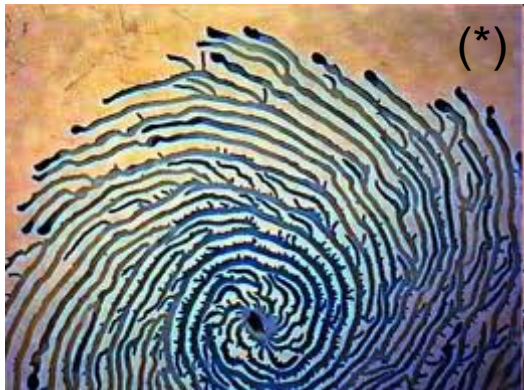
Self-organized motion
at high density



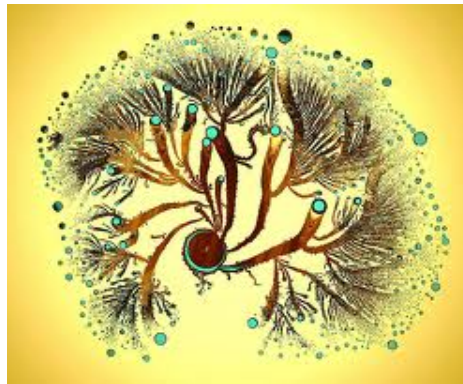
See movies!

From Vicsek's review

Pattern formation and active matter



(*)

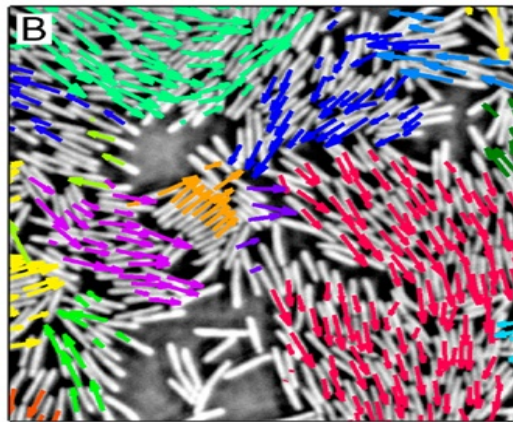
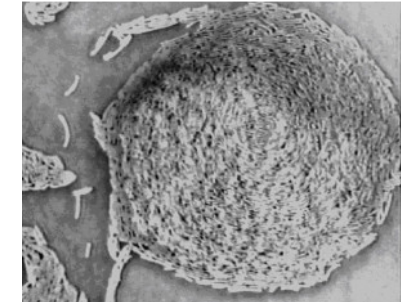


Various CM patterns in **bacteria**

(*) Vortex in bacteria!

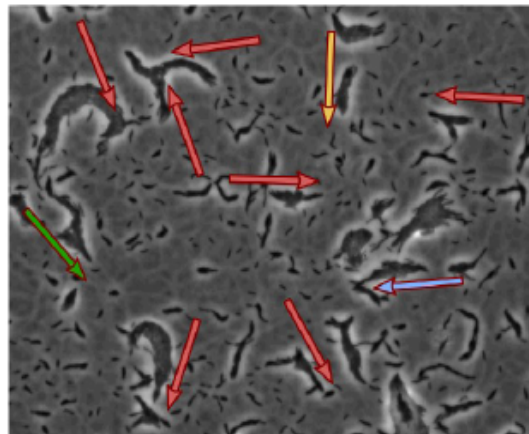
Paenibacillus

Ben-Jacob's group



Zhang et al. (2010)

B. subtilis



Peruani et al. (2011)

Myxobacteria

Order motion and clustering
In bacteria

Myxobacteria



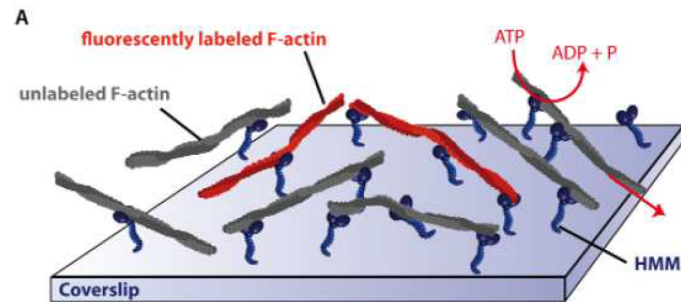
Strassmann and Queller (2011)

Super complex coordinated motion in bacteria:
They pile up and form complex 3D structures!

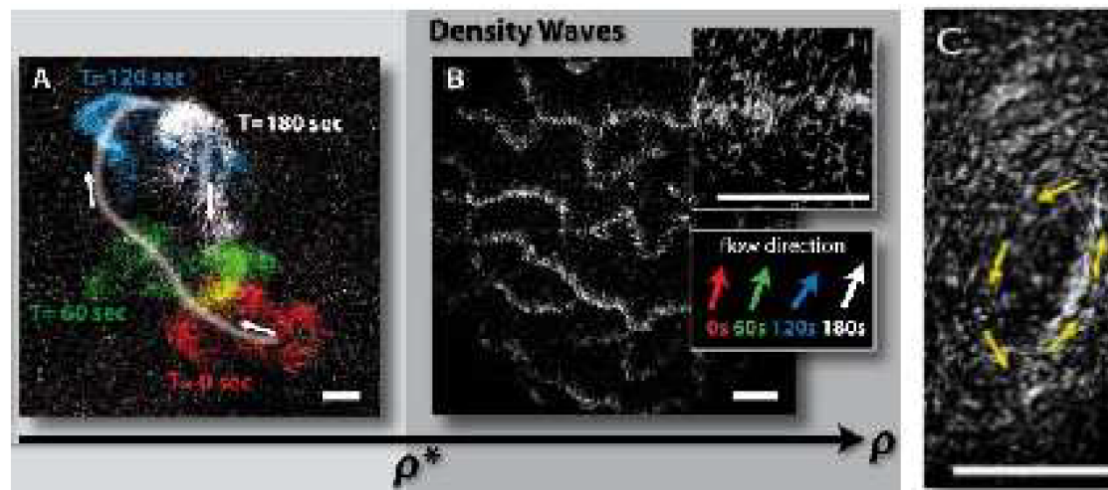


[See movie from Reichenbach (1965) and others]

Pattern formation and active matter

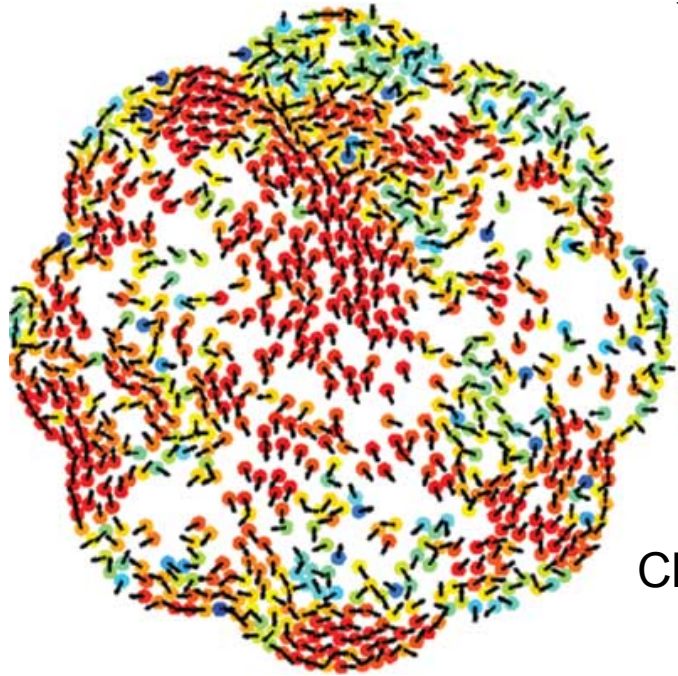


Various CM patterns at **intracellular scale**



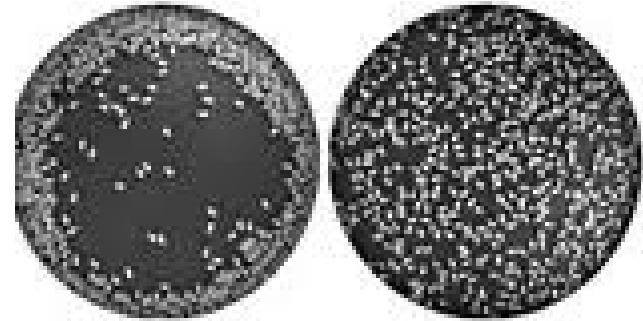
Schaller et al. (2010)

Non-living active matter systems



Chaté et al.

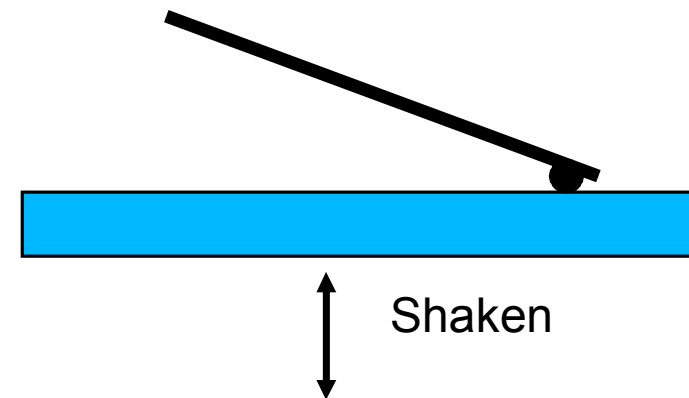
Driven granular media



Kudrolli et al.



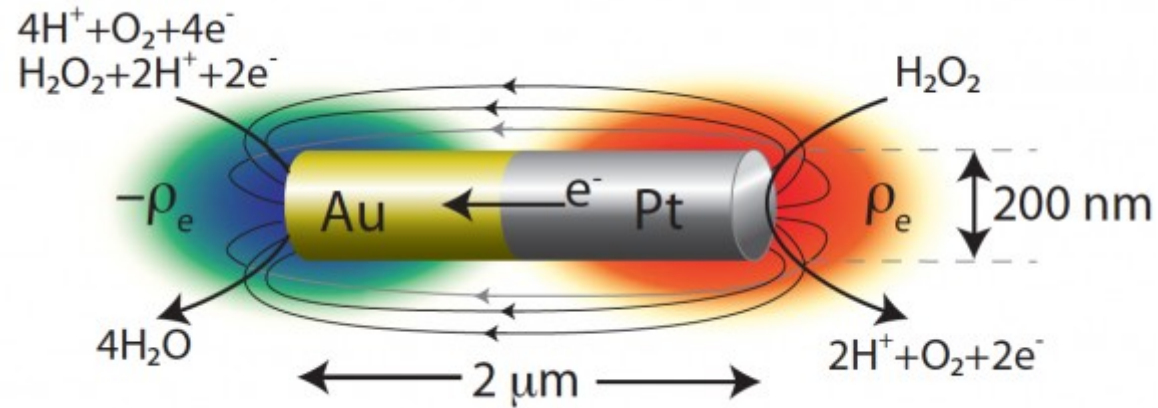
Blair et al.



SP particles with fixed asymmetry

Non-living active matter systems

Chemically driven particles



Posner et al.

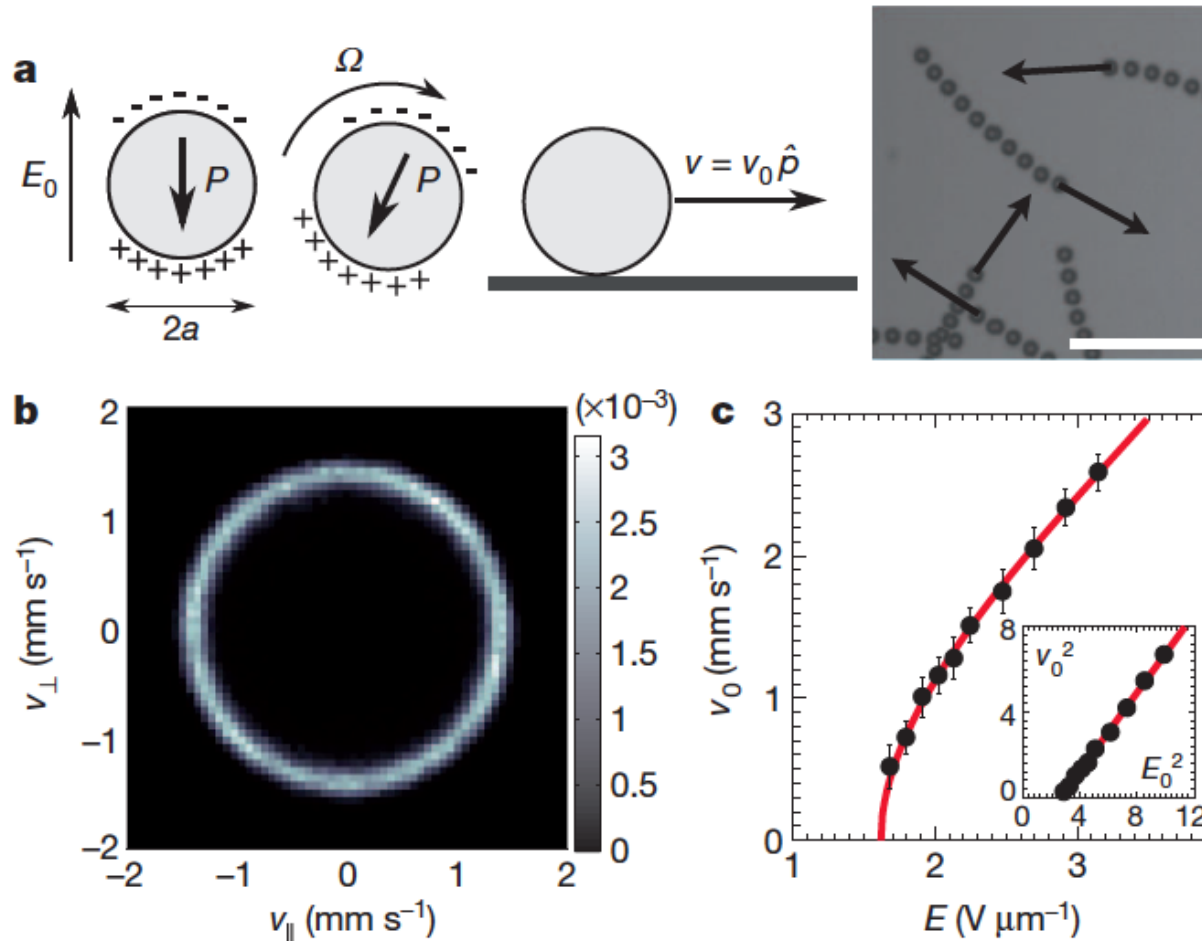


Freemantle et al.

SP particles with fixed asymmetry

Non-living active matter systems

Experimental example that exhibits the claimed symmetry: Quincke rollers!



SP particles that undergo a spontaneous symmetry breaking

Bricard, Caussin, Desreumaux, Dauchot, Bartolo, Nature (2013)

**Active matter systems:
theoretical challenges & minimal models**

Theoretical challenges

Active systems are intrinsically non-equilibrium systems

- Energy consumption → Often particles have an energy depot (e.g., ATP in cells)

- Energy dissipation →
- Is there a balance?

It depends on the time scale we look at.
In several experiments the answer is no!
[we look at a long transient]

- Often active systems (if we forget about the medium where they move) do not conserve momentum!
- Anomalous fluctuations are found everywhere: density, speed, etc, etc

Theoretical challenges

active systems - classification

- Non-interacting active particles
- Interacting active particles

- long-range interactions
- short-range interactions
- homogeneous populations of particles
- inhomogeneous populations of particles (e.g., with leaders)



We will focus (mainly) on identical active particles with short-range interactions

Theoretical challenges

Active systems - classification

- Interaction “forces”:

- **Attraction**
- **Repulsion**
- **Alignment (velocity-velocity interactions!)**

Minimal models -- non-interacting active particles

- A minimal model for non-interacting active particles:

Equations of motion:

$$\begin{aligned}\dot{\mathbf{x}}_i &= v_i(t) \mathbf{V}(\theta_i) \\ \dot{\theta}_i &= \eta \xi_i(t)\end{aligned}$$

where $\mathbf{V}(\theta) \equiv (\cos(\theta), \sin(\theta))$

Minimal models -- non-interacting active particles

Fluctuations in the direction of motion and in the propelling engine!

Random direction of motion + constant speed:



If you drive a car at constant speed while randomly turning the direction wheel, you perform a well-known type of motion called persistent Brownian motion.

Random direction of motion + fluctuations in the speed:



+



If now instead of keeping the speed constant, you randomly press the gas and break pedals while still randomly turning the direction wheel, the resulting movement is no longer well described by a plain persistent Brownian motion.

Fluctuations in the direction of motion + fluctuations in the speed
=
Anomalous (Brownian) motion

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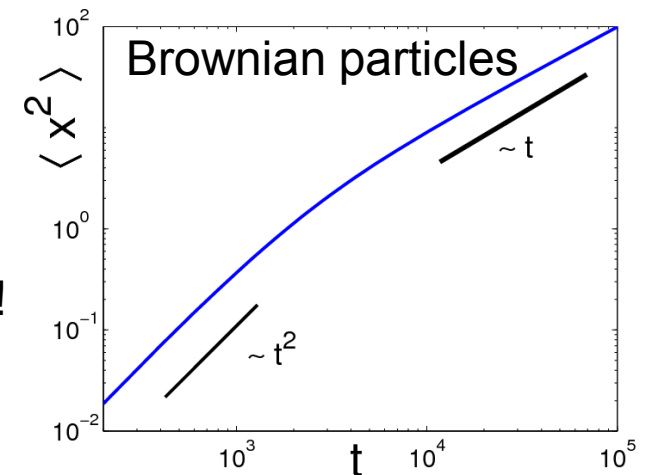
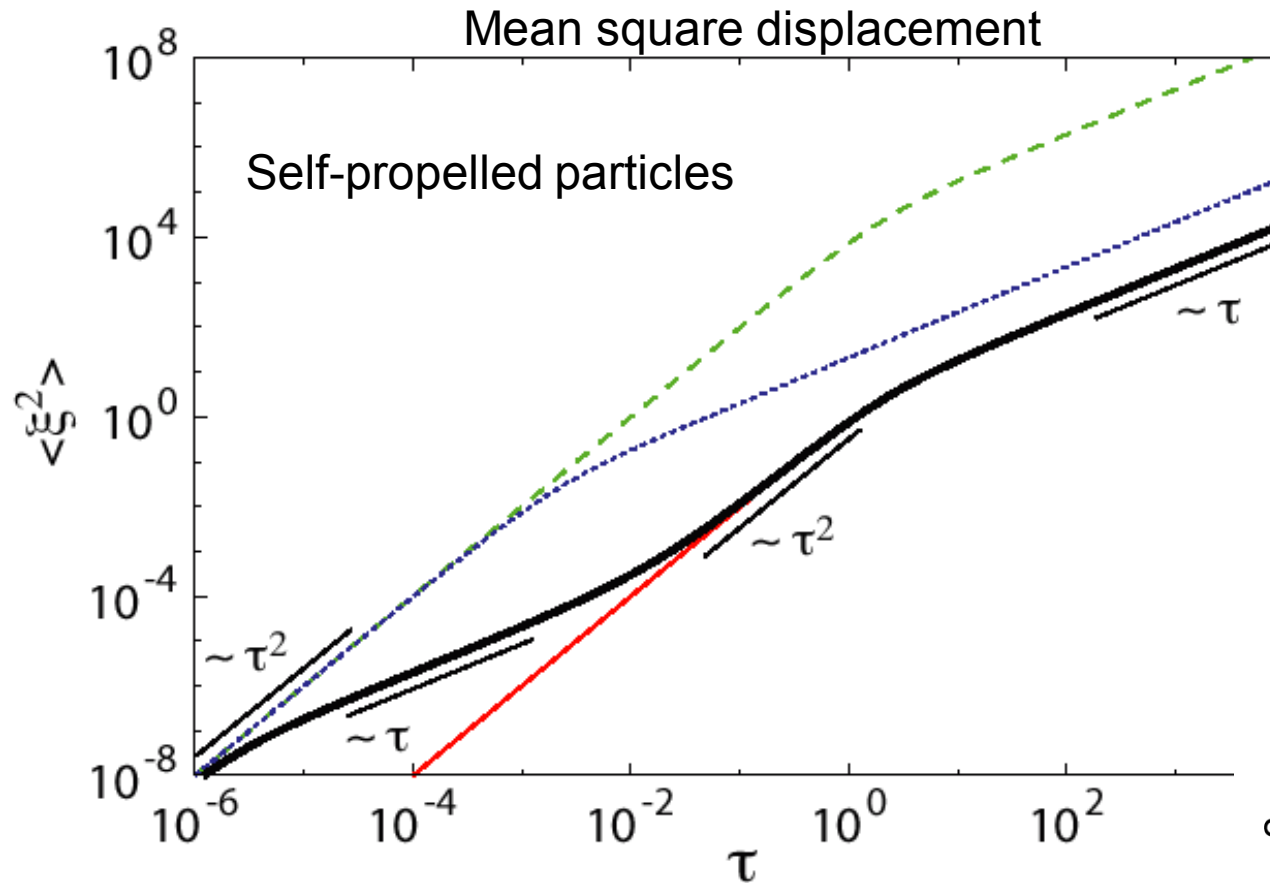


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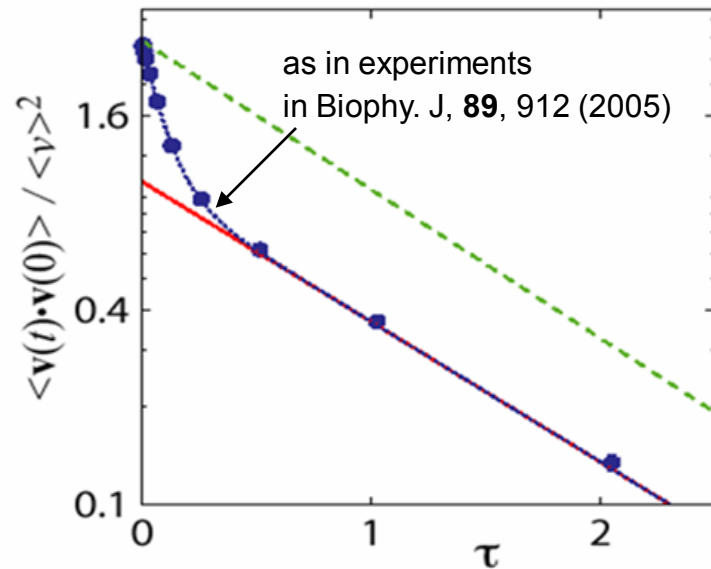


We are going to see how to generalize the Fierth formula!

Peruani, Morelli, PRL (2007)

Minimal models -- non-interacting active particles

Active fluctuations and the anomalous transient can be observed in cell motility experiments



$$\begin{aligned} \langle \mathbf{x}^2(t) \rangle &= 2 \frac{\langle v \rangle^2}{\kappa^2} (\kappa t - 1 + e^{-\kappa t}) \\ &+ 2 \frac{\langle v^2 \rangle - \langle v \rangle^2}{(\kappa + \beta)^2} ((\kappa + \beta)t - 1 + e^{-(\kappa + \beta)t}). \end{aligned}$$

$$D = D_{\text{Thermal}} + D_{\text{Active}} + D_{\text{Active Fluct}}$$

Minimal models -- non-interacting active particles

• A simple model of active particles in heterogeneous media:

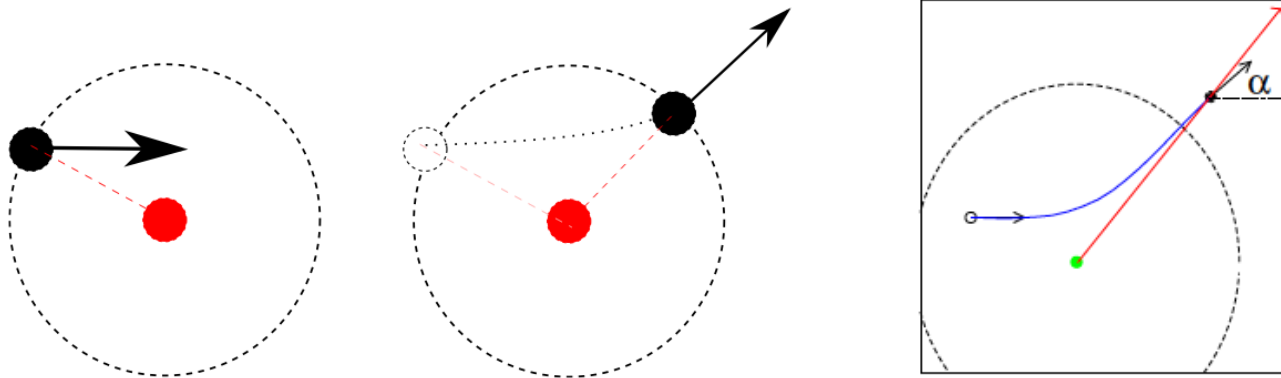
Equations of motion:

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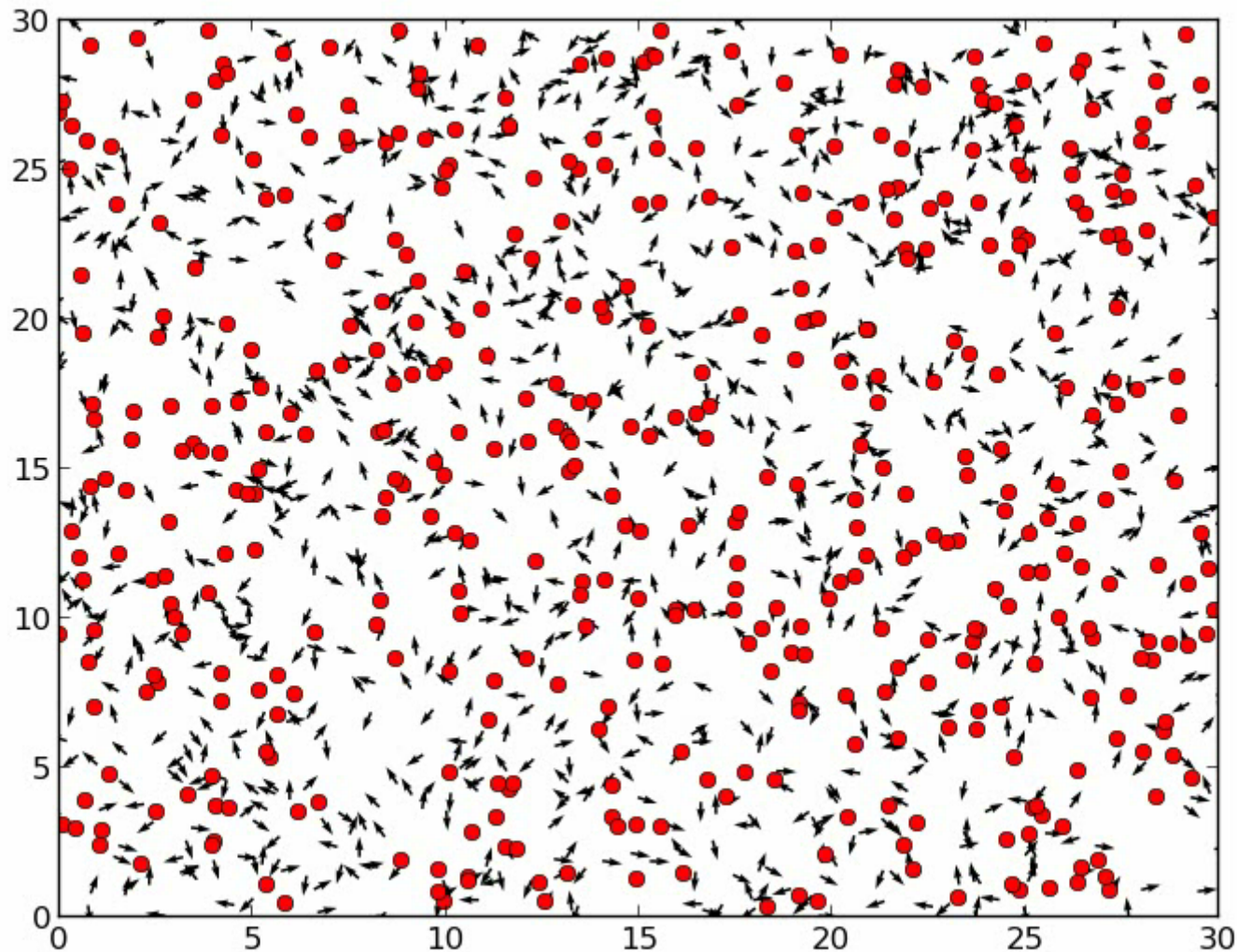
where $\mathbf{V}(\theta) \equiv (\cos(\theta), \sin(\theta))$

Interaction with “obstacles”:

$$h(\mathbf{x}_i) = \begin{cases} \frac{\gamma}{n(\mathbf{x}_i)} \sum_{\Omega_i} \sin(\alpha_{k,i} - \theta_i) & \text{if } n(\mathbf{x}_i) > 0 \\ 0 & \text{if } n(\mathbf{x}_i) = 0 \end{cases}$$

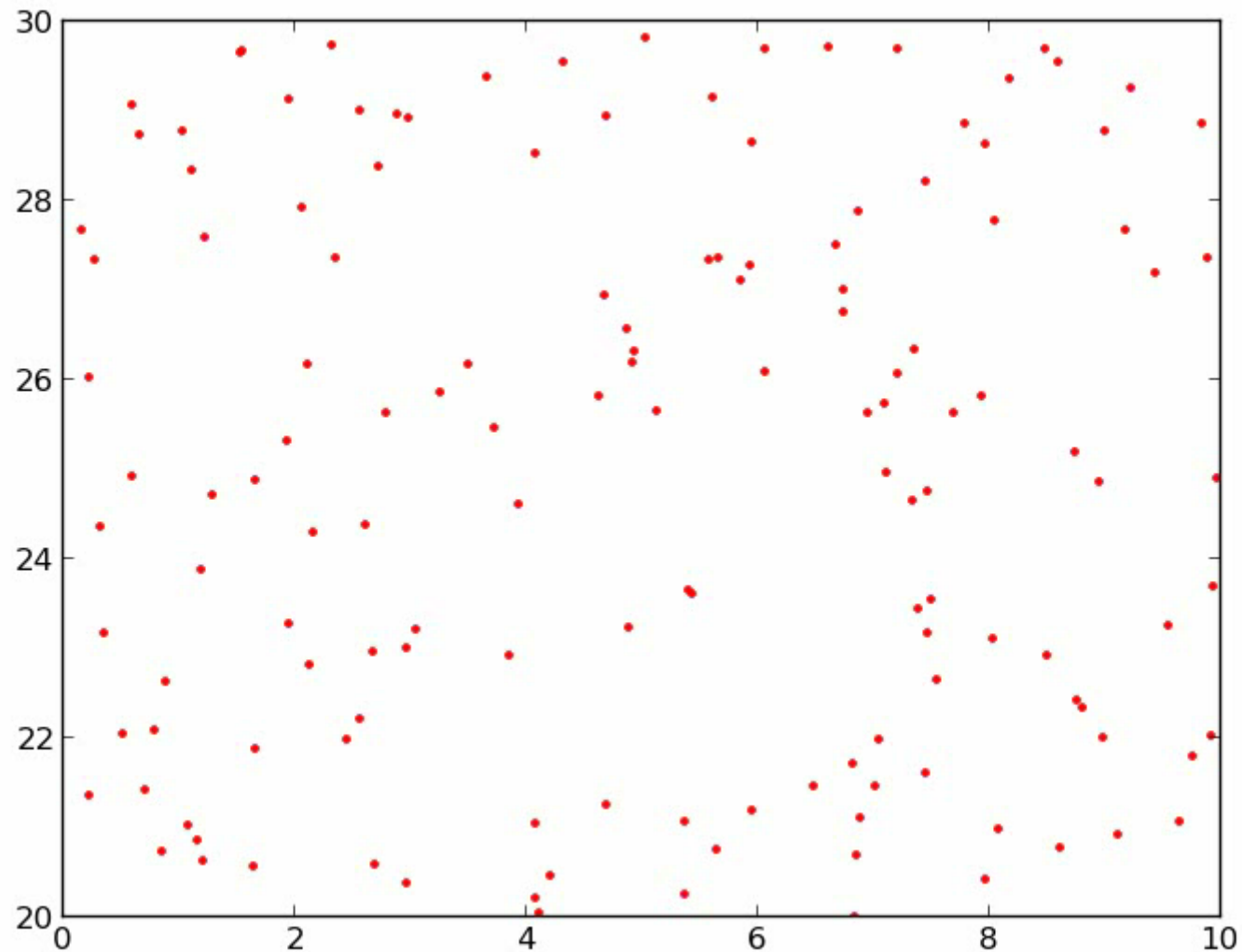


Minimal models -- non-interacting active particles



Starting from a random initial condition, traps emerge. The time that particles spend in a particular trap depends on the particular configuration of obstacles.

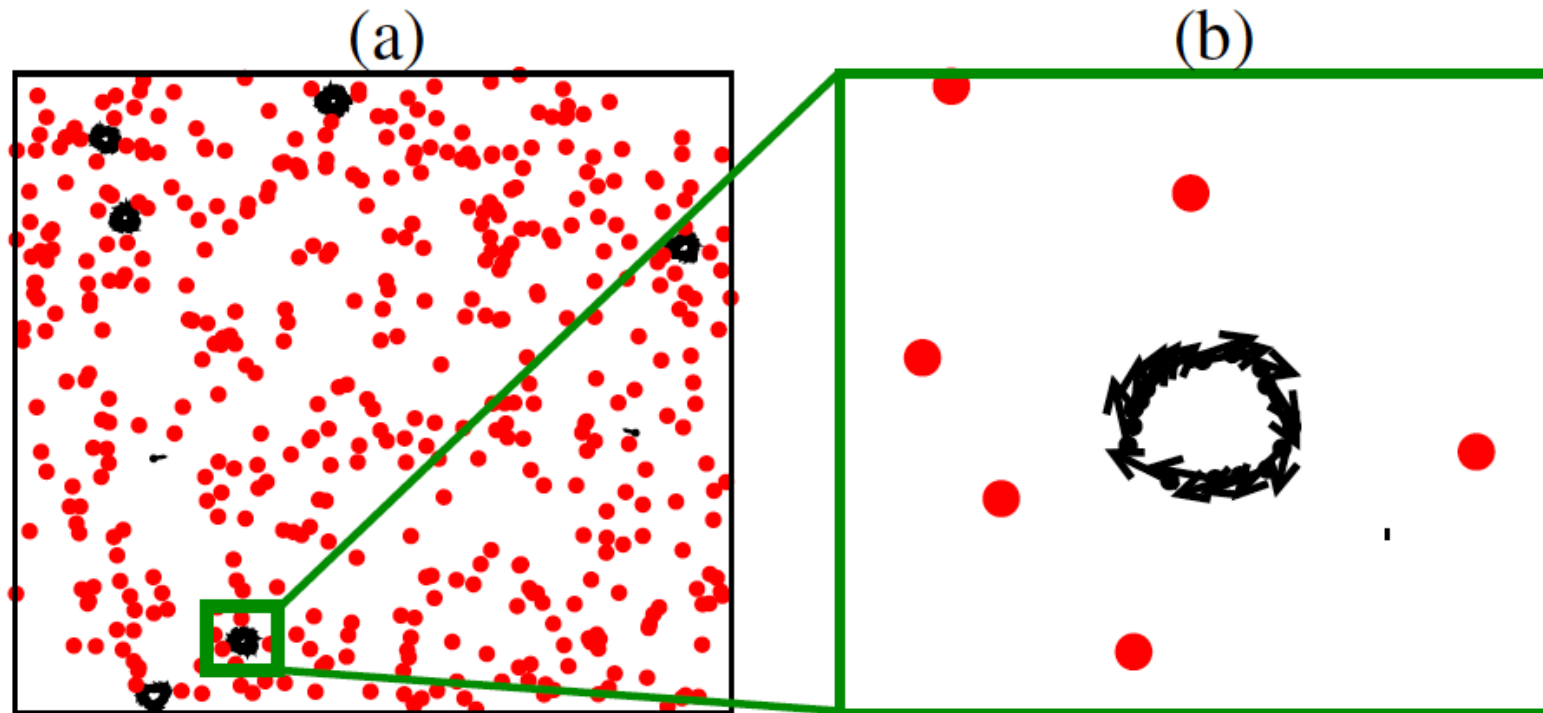
Minimal models -- non-interacting active particles



Looking at a small part of a large system at real time

Minimal models -- non-interacting active particles

- How is possible to trapped particles moving at constant speed?



These traps are closed stable orbits that are found by the active particles in the landscape of obstacles.

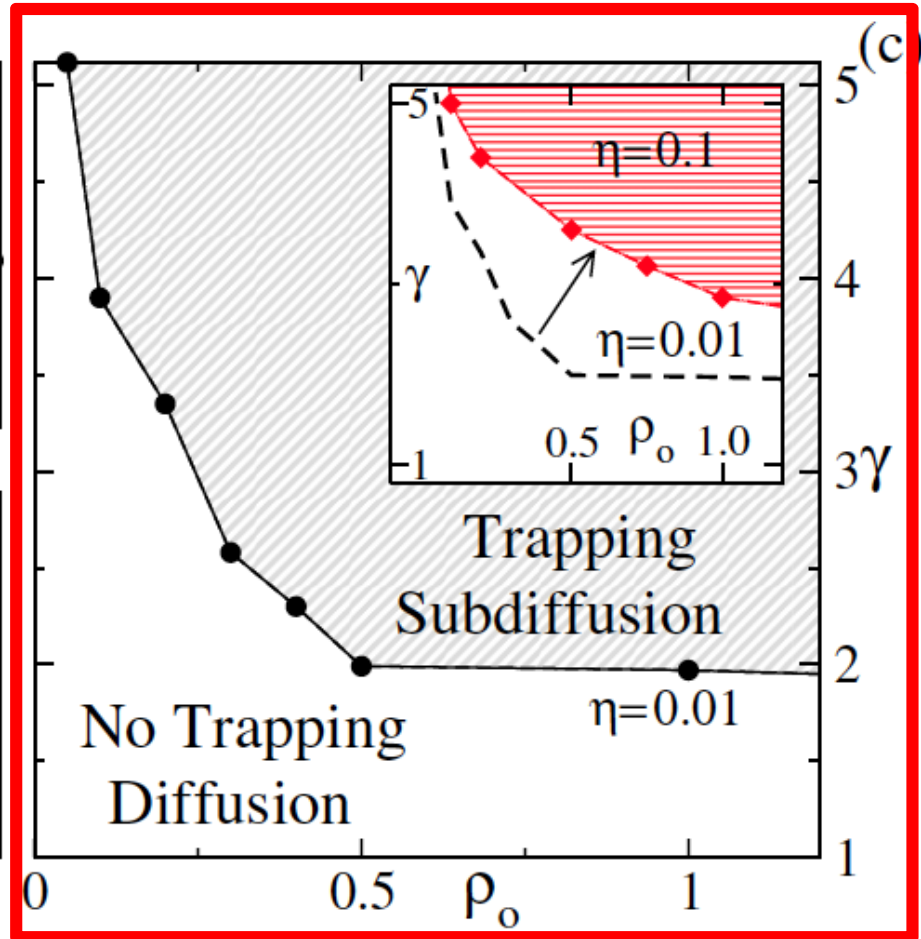
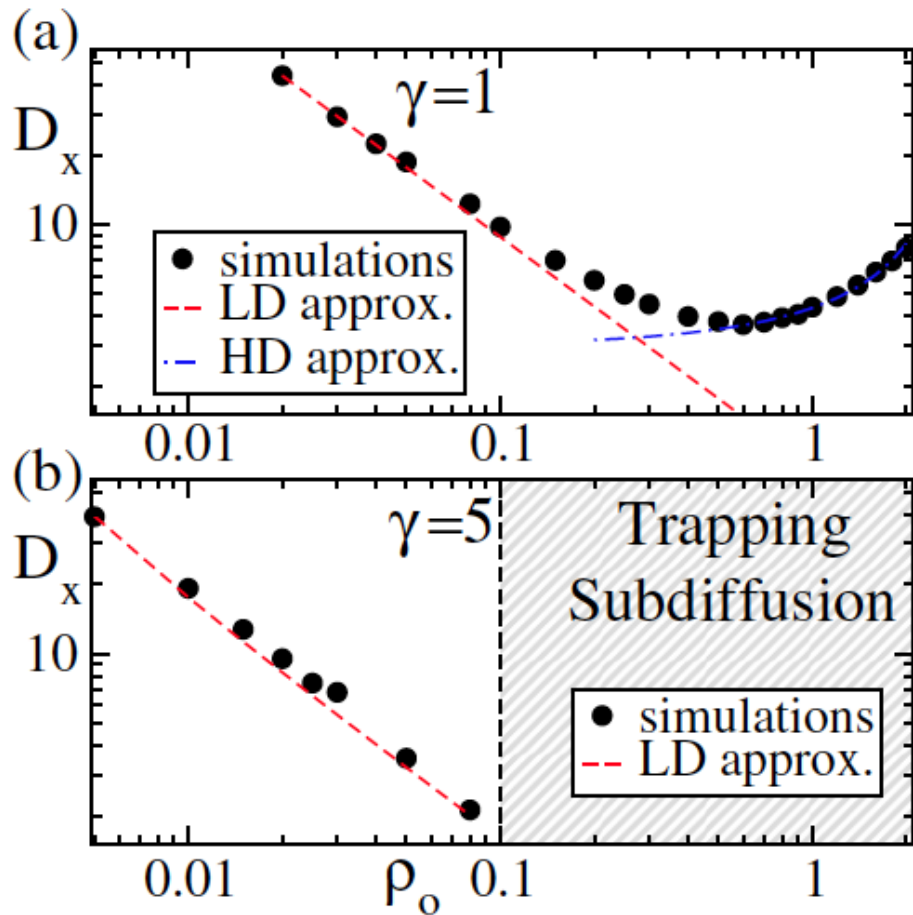
Remember that noise is present. These orbits are not absorbing, and particle can escape.

Minimal models -- non-interacting active particles

- The transport properties – dependency with γ and ρ_o

$$\dot{\mathbf{x}}_i = v_0 \mathbf{V}(\theta_i)$$

$$\dot{\theta}_i = \frac{\gamma}{n(\mathbf{x}_i)} \sum_{|\mathbf{x}_i - \mathbf{y}_k| < R} \sin(\alpha_{k,i} - \theta_i) + \eta \xi_i(t)$$



Diffusion and subdiffusion are observed!

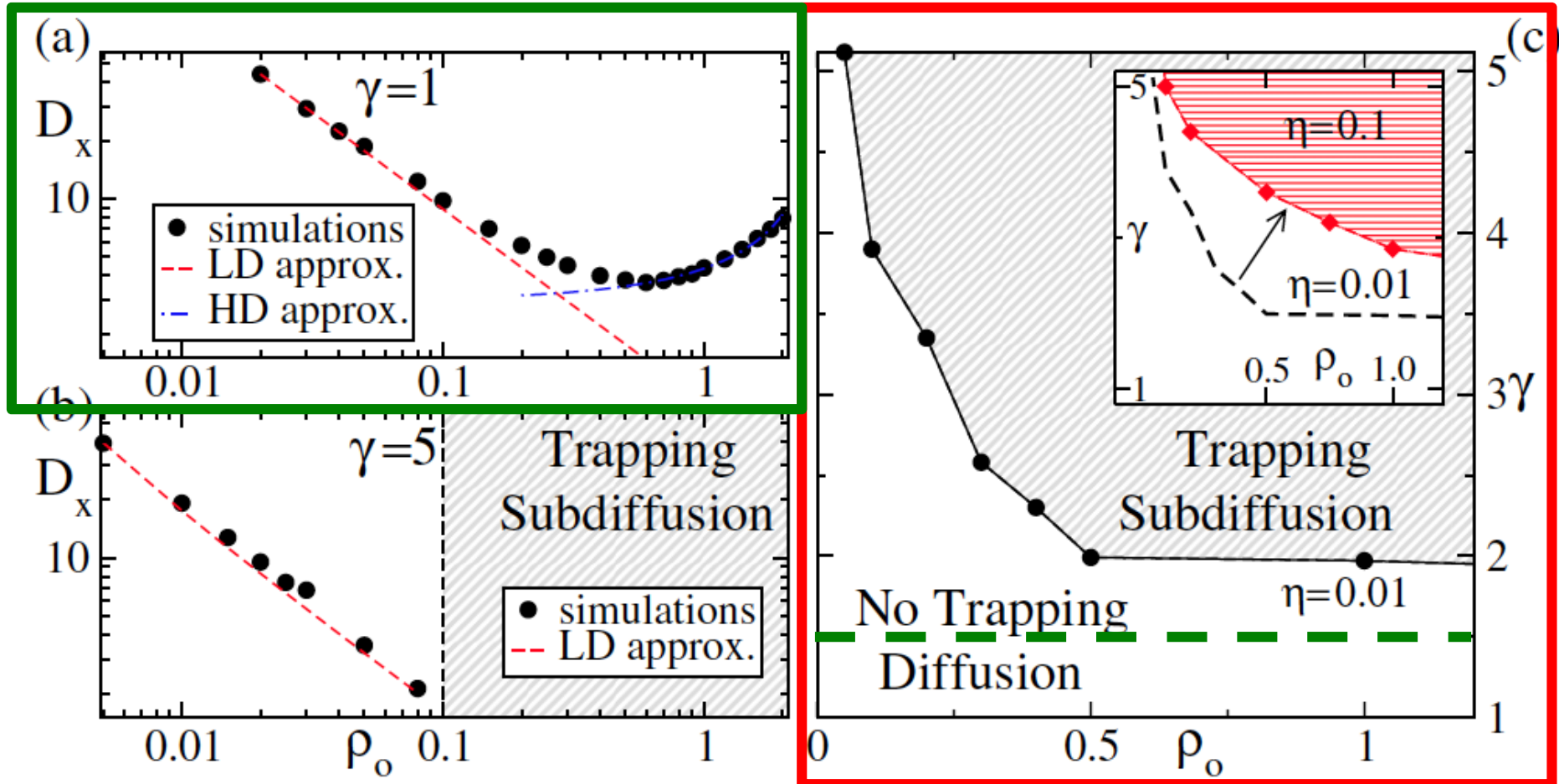
Subdiffusion is related to the emergence of trapping!

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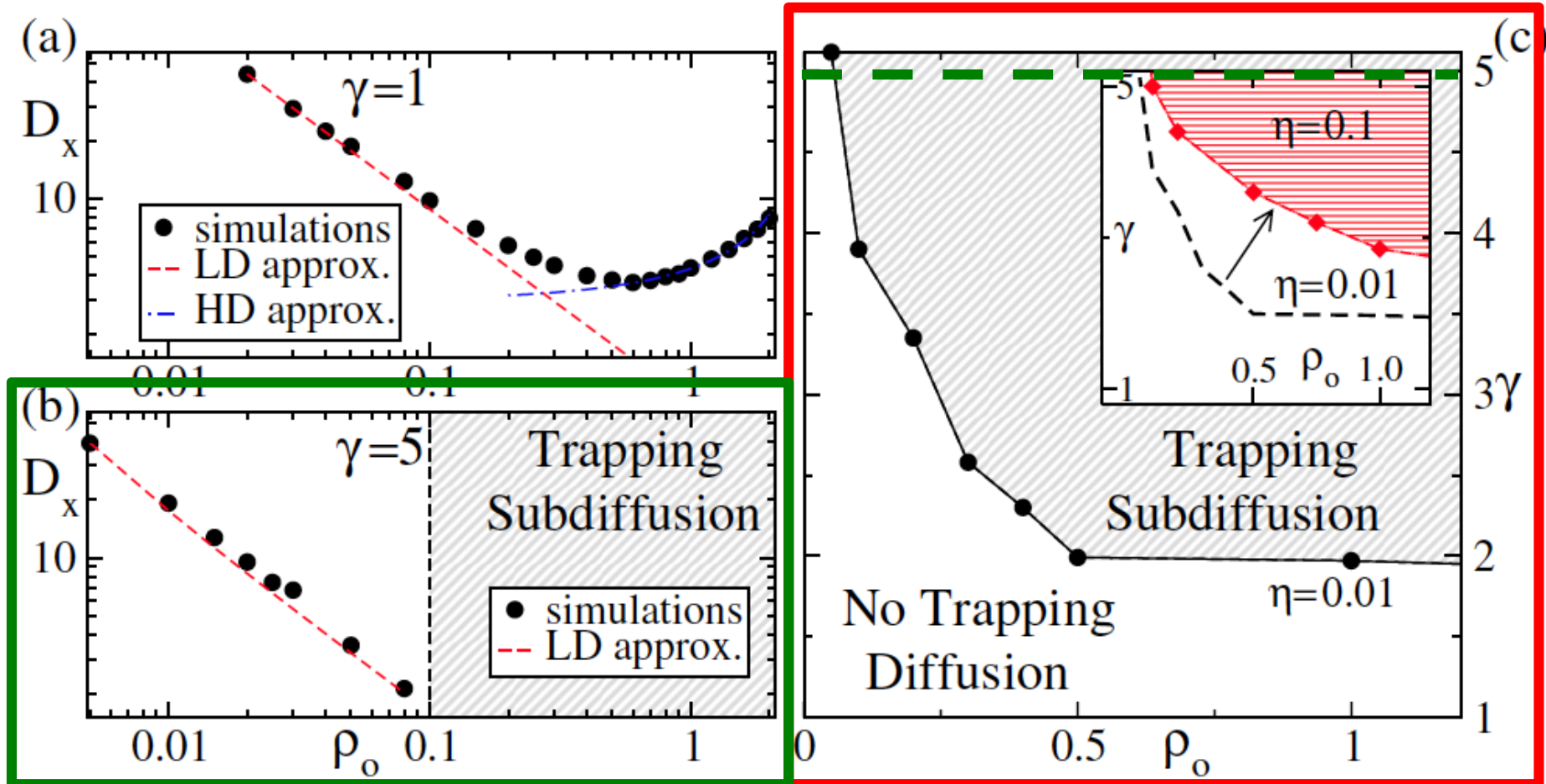
(These findings can be understood theoretically!)

Minimal models -- non-interacting active particles

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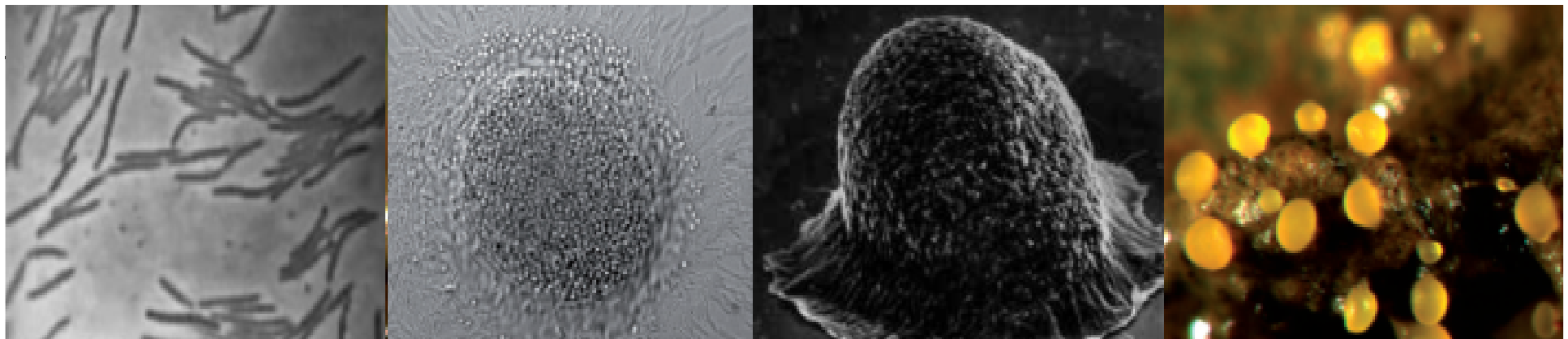
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Active soft-matter: modeling living matter and mimicking it.

-- second part --

Fernando Peruani

BIOMAT – La Falda – 08.2014



outline

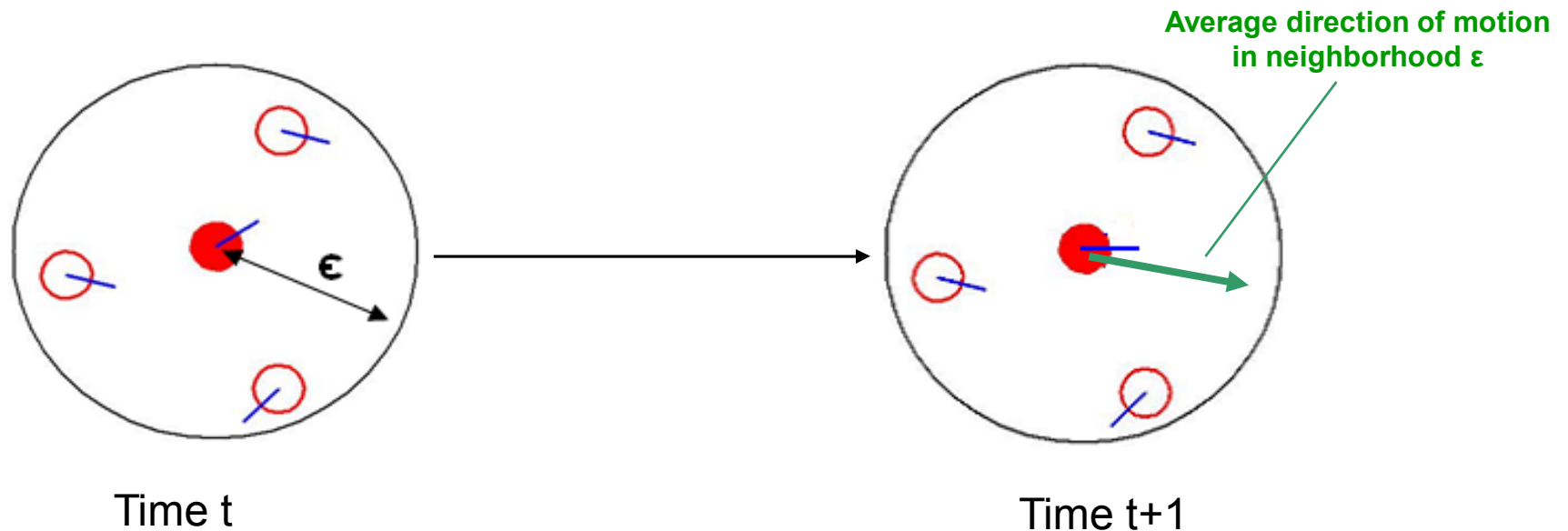
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P2

Minimal models -- interacting active particles

The Vicsek model – moving spins

[T. Vicsek *et al.*, Phys. Rev. Lett. 75, 1226 (1995)]



Motion in space

$$\mathbf{x}_i(t + 1) = \mathbf{x}_i(t) + \mathbf{v}_i(t)\Delta t$$

Change of the direction of motion

$$\theta(t + 1) = \langle \theta(t) \rangle_r + \Delta\theta$$

Average direction of motion at time t

Angular noise !!!

Minimal models -- interacting active particles

A more general, better defined active particle models

$$\dot{\mathbf{x}}_i = v_0 e^{i\theta_i}$$

$$\dot{\theta}_i = -\gamma \frac{\partial U}{\partial \theta_i}(\mathbf{x}_i, \theta_i) + \tilde{\eta}_i(t)$$

Ferromagnetic alignment $\rightarrow U(\theta, \theta') = -\cos(\theta - \theta')$

Polar order parameters:

$$\phi = \left\langle \left| \frac{1}{N} \sum_{k=1}^N \exp(i\theta_k^t) \right| \right\rangle \rightarrow \text{[global] average velocity}$$

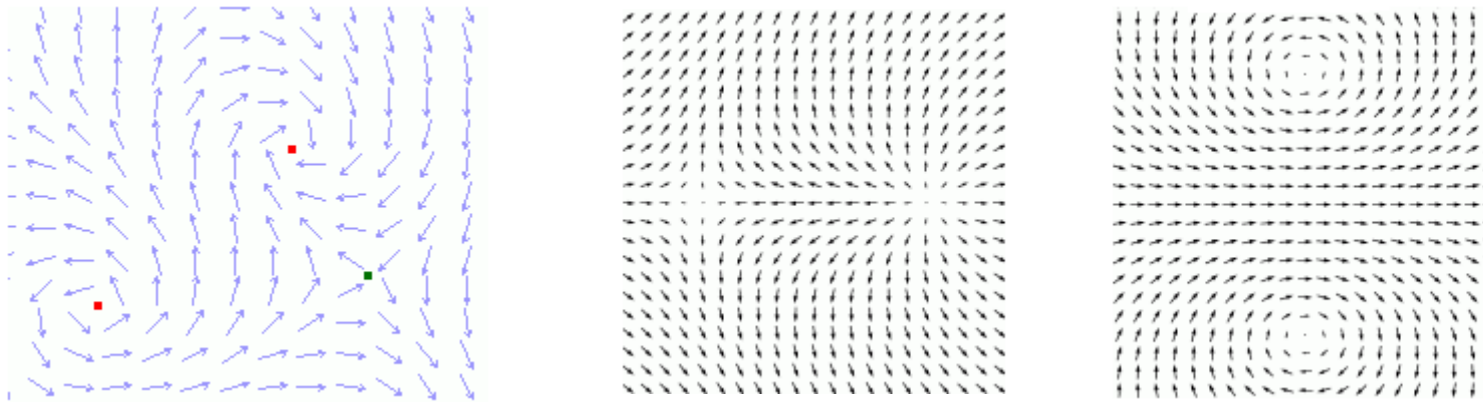
(or average magnetization if we treat the velocity vector as spins).

Minimal models -- interacting active particles

Imperfect flow of information leads to defects, and defects set the limit to the size/scale of the patterns we can observe

Some classical results from statistical mechanics:

- The Kosterlitz-Thouless transition: $E_{ij} = -J (\mathbf{s}_i \mathbf{s}_j) = -J \cos(\varphi_i - \varphi_j)$



- The Mermin-Wagner theorem:

In equilibrium systems with SU2 symmetry, long-range order out of short-range interactions cannot emerge in 1D or 2D!



What is short- and long-range order? And how to measure it?

Minimal models -- interacting active particles

Imperfect flow of information leads to defects, and defects set the limit to the size/scale of the patterns we can observe

- The Mermin-Wagner theorem:

In equilibrium systems with SU2 symmetry, long-range order out of short-range interactions cannot emerge in 1D or 2D!

- Long-range order is not possible in equilibrium systems (spin waves and vortices)
- MW theorem also works in several non-equilibrium systems
- Random motion (of diffusive type) of the spins is not enough to get long-range order in the thermodynamical limit (though it is for finite systems)

Minimal models -- interacting active particles

Properties of the Vicsek model – when the spins move!

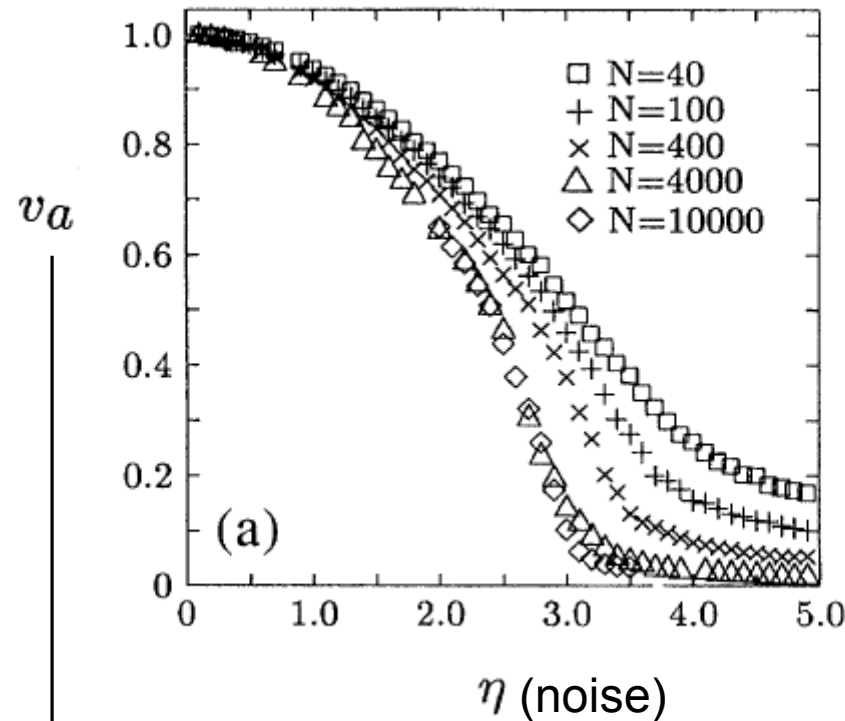


Decreasing noise values

[Vicsek et al. PRL (1995)]

Minimal models -- interacting active particles

The phase transition and long-range order



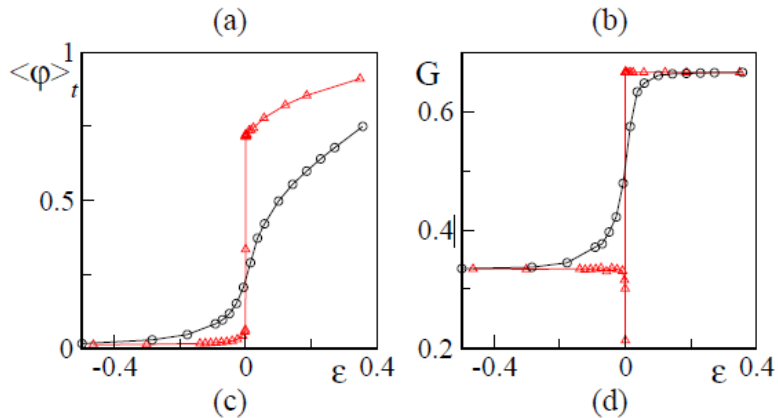
[Vicsek et al. PRL (1995)]

$$v_a = \frac{1}{Nv} \left| \sum_{i=1}^N \mathbf{v}_i \right|$$

[explain LRO, QLRO, and Short RO for finite size systems]

Minimal models -- interacting active particles

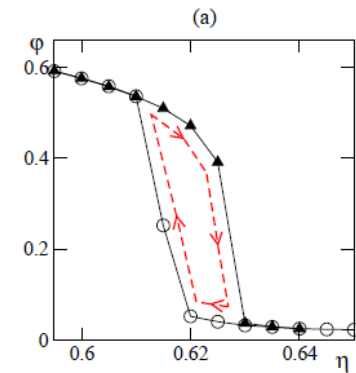
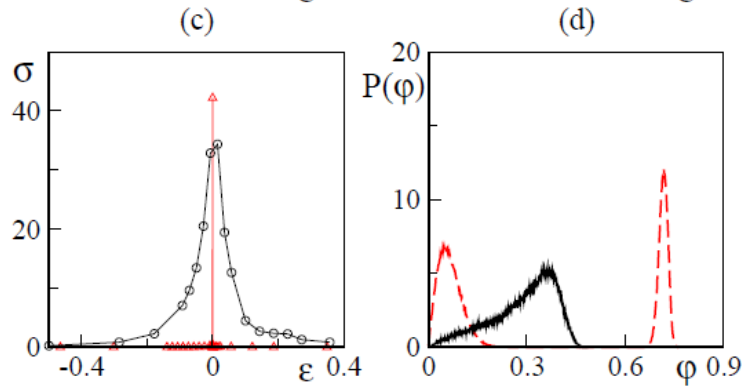
First vs second order transition



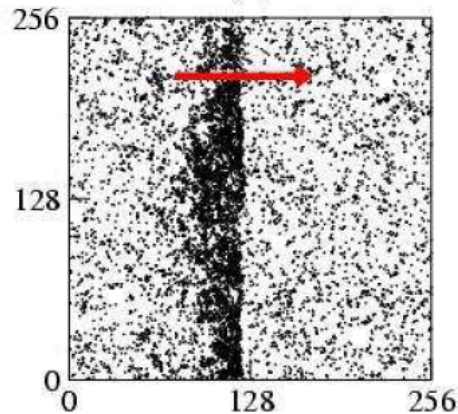
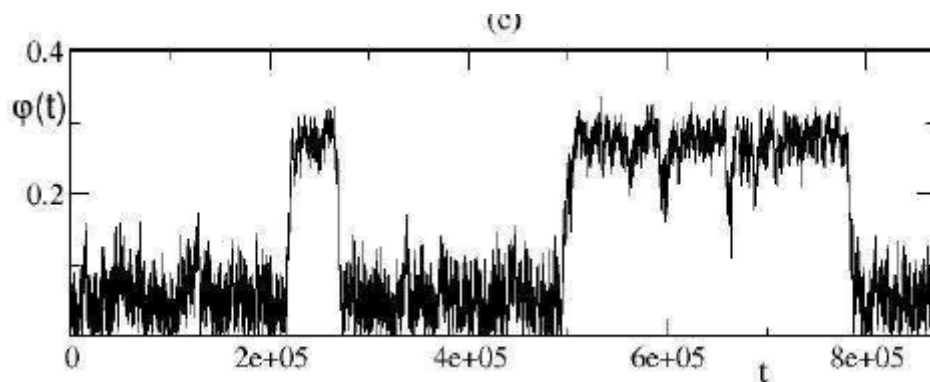
$$\vec{\varphi}(t) = \frac{1}{v_0} \langle \vec{v}_i(t) \rangle_i$$

$$\sigma(\eta, L) = L^d (\langle \varphi^2 \rangle_t - \langle \varphi \rangle_t^2)$$

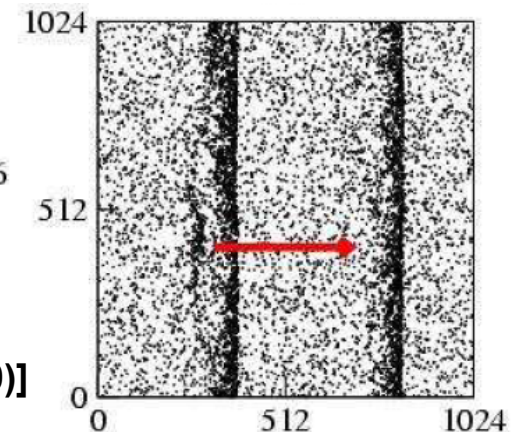
$$G(\eta, L) = 1 - \frac{\langle \varphi^4 \rangle_t}{3 \langle \varphi^2 \rangle_t^2}$$



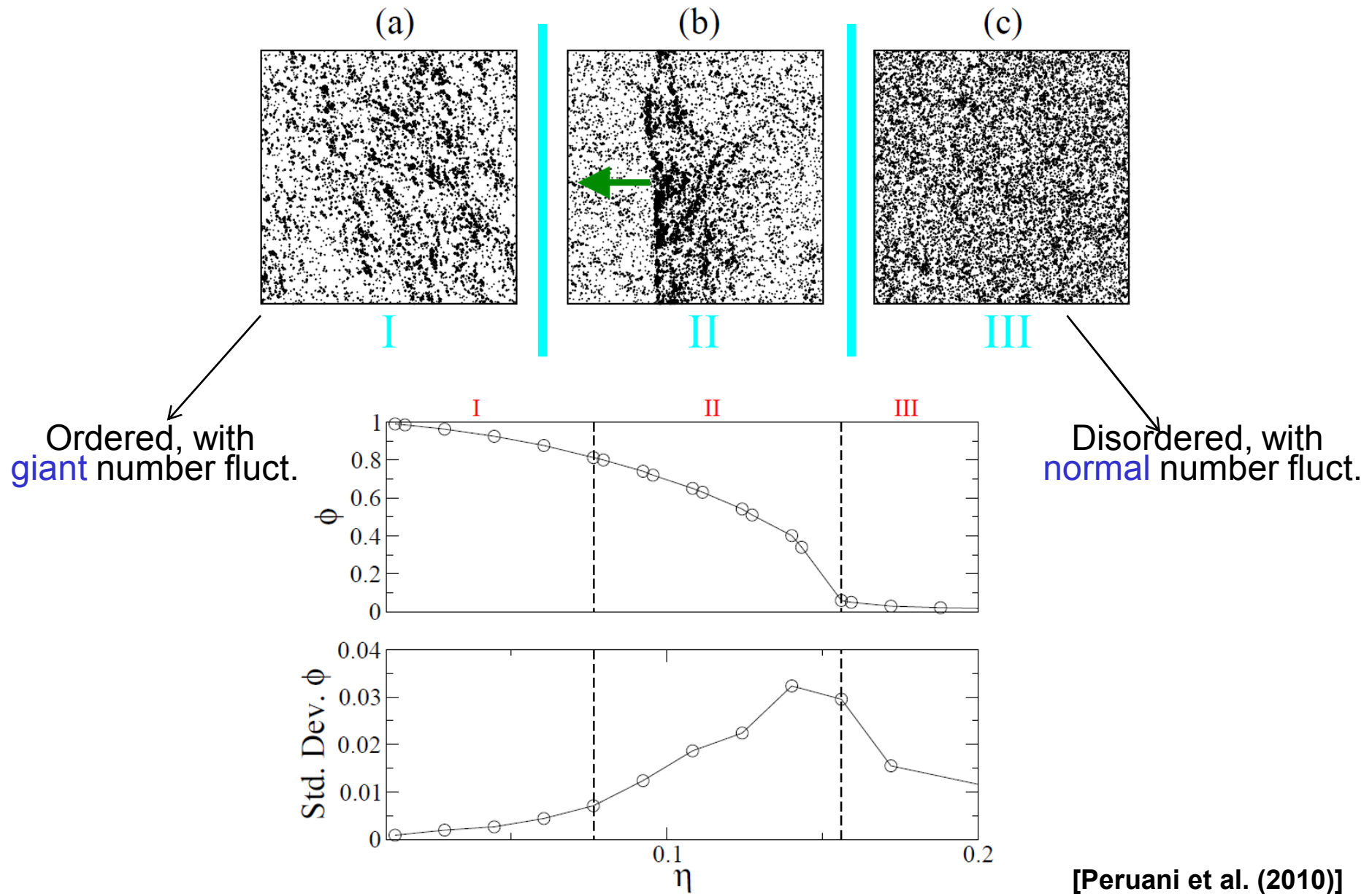
Bands!



[Chaté et al. PRE (2010)]



Minimal models -- interacting active particles



Minimal models -- interacting active particles

Number fluctuations

[at low cell densities]

Average number:

$$\langle n(L) \rangle = \rho L^2$$

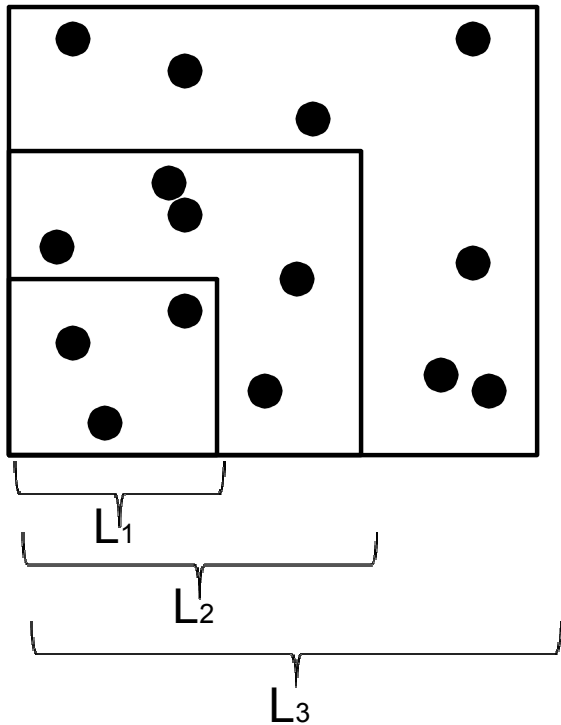
Average square number:

$$\Delta n^2 = \langle [n(L) - \langle n(L) \rangle]^2 \rangle$$

$$\Delta n = (\langle [n(L) - \langle n(L) \rangle]^2 \rangle)^{1/2} = \langle n(L) \rangle^{1/2}$$

Normal number fluctuations

$$\Delta n = \langle n(L) \rangle^{1/2} !$$



$n(L)$ = number of particles
in box of size L

Minimal models -- interacting active particles

Number fluctuations

[at low cell densities]

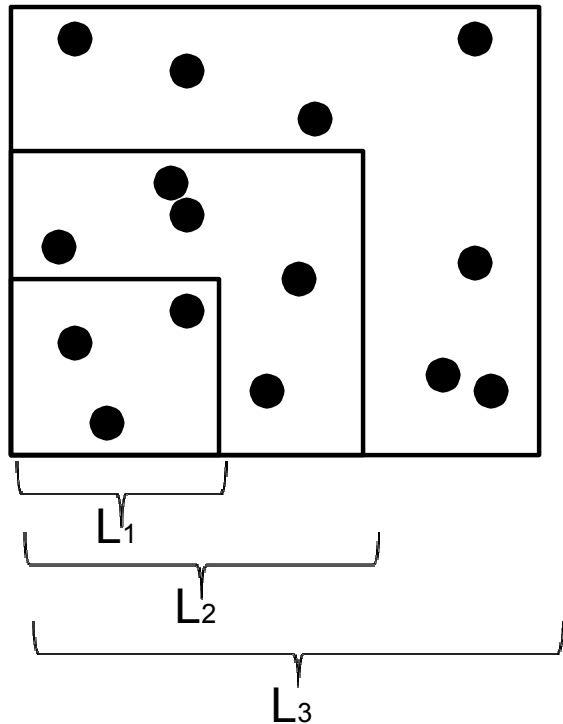
Average number:

$$\langle n(L) \rangle = \rho L^2$$

Average square number:

$$\Delta n^2 = \langle [n(L) - \langle n(L) \rangle]^2 \rangle$$

$$\Delta n = (\langle [n(L) - \langle n(L) \rangle]^2 \rangle)^{1/2} = \langle n(L) \rangle^{\beta}$$



$n(L)$ = number of particles
in box of size L

Giant number fluctuations

$$\Delta n = \langle n(L) \rangle^{\mu} \quad \mu > 1/2 !$$

Minimal models -- interacting active particles

- A minimal continuum time SPP model with obstacles:

$$\dot{\mathbf{x}}_i = v_0 \mathbf{V}(\theta_i)$$

$$\dot{\theta}_i = g(\mathbf{x}_i) \left[\frac{\gamma_b}{n_b(\mathbf{x}_i)} \sum_{|\mathbf{x}_i - \mathbf{x}_j| < R_b} \sin(\theta_j - \theta_i) \right] + h(\mathbf{x}_i) + \eta \xi_i(t),$$

$$h(\mathbf{x}_i) = \begin{cases} \frac{\gamma_o}{n_o(\mathbf{x}_i)} \sum_{|\mathbf{x}_i - \mathbf{y}_k| < R_o} \sin(\alpha_{k,i} - \theta_i) & \text{if } n_o(\mathbf{x}_i) > 0 \\ 0 & \text{if } n_o(\mathbf{x}_i) = 0 \end{cases},$$

Minimal models -- interacting active particles

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$$+ h(\mathbf{x}_i) + \eta \xi_i(t),$$

Continuum time version of Vicsek model (1995), i.e. a self-propelled XY model as introduced in Peruani, Deutch, Baer, Eur. J-ST (2008)

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Minimal models -- interacting active particles

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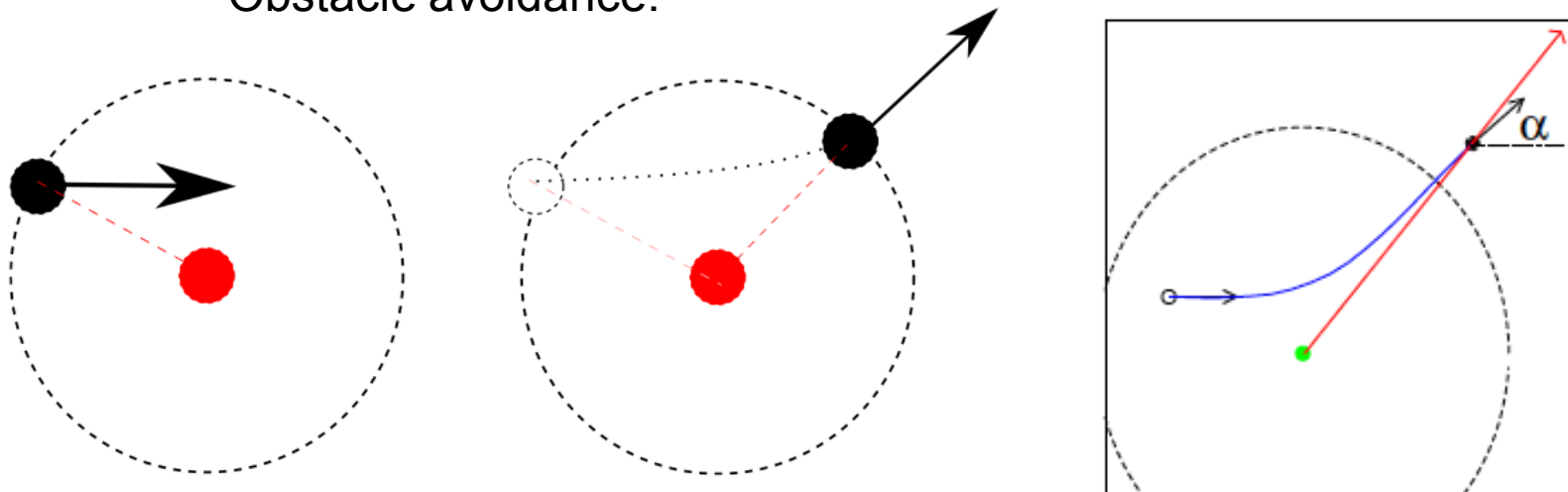
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$$\dot{\theta}_i = g(\mathbf{x}_i) \left[\frac{\gamma_b}{n_b(\mathbf{x}_i)} \sum_{|\mathbf{x}_i - \mathbf{x}_j| < R_b} \sin(\theta_j - \theta_i) \right]$$

$$+ h(\mathbf{x}_i) + \eta \xi_i(t),$$

$$h(\mathbf{x}_i) = \begin{cases} \frac{\gamma_o}{n_o(\mathbf{x}_i)} \sum_{|\mathbf{x}_i - \mathbf{y}_k| < R_o} \sin(\alpha_{k,i} - \theta_i) & \text{if } n_o(\mathbf{x}_i) > 0 \\ 0 & \text{if } n_o(\mathbf{x}_i) = 0 \end{cases},$$

Obstacle avoidance:



Minimal models -- interacting active particles

- A minimal continuum time SPP model with obstacles:

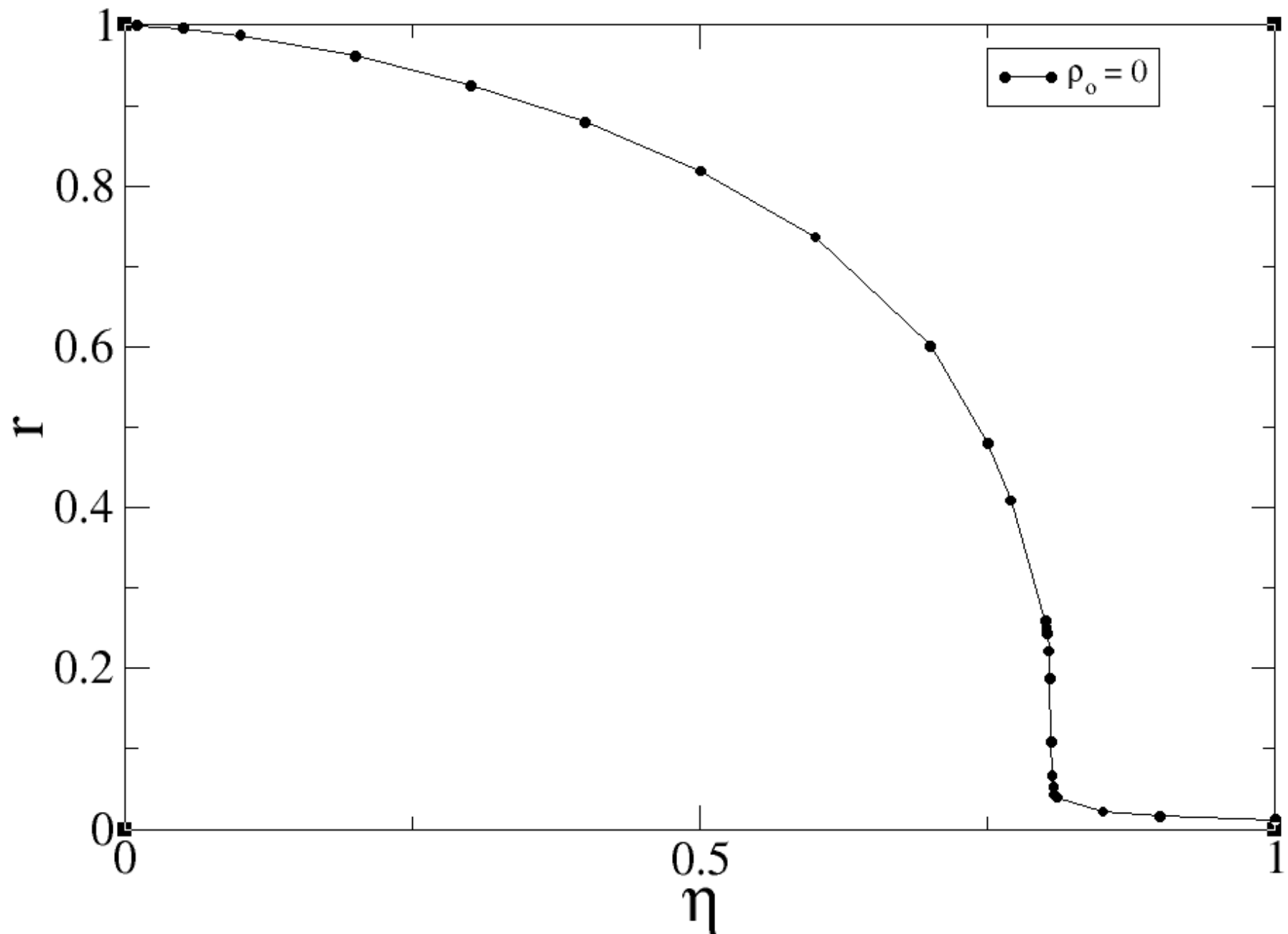
$$\begin{aligned}\dot{\mathbf{x}}_i &= v_0 \mathbf{V}(\theta_i) \\ \dot{\theta}_i &= g(\mathbf{x}_i) \left[\frac{\gamma_b}{n_b(\mathbf{x}_i)} \sum_{|\mathbf{x}_i - \mathbf{x}_j| < R_b} \sin(\theta_j - \theta_i) \right] \\ &\quad + h(\mathbf{x}_i) + \eta \xi_i(t),\end{aligned}$$

Order parameter $\longrightarrow r = \langle r \rangle_t = \left\langle \left| \frac{1}{N_b} \sum_{i=1}^{N_b} e^{i\theta_i(t)} \right| \right\rangle_t$ [equiv. to the magnetization]

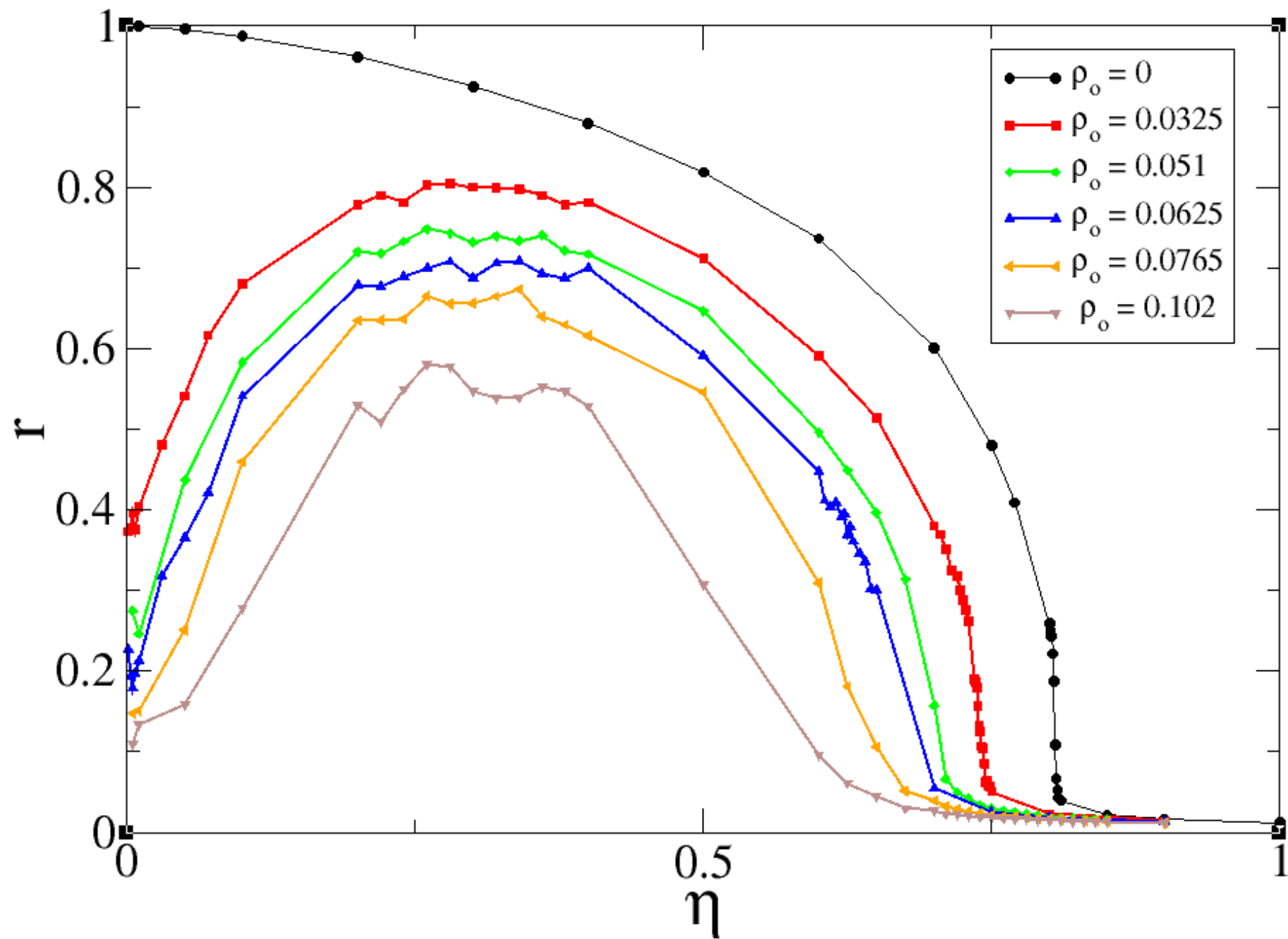
Susceptibility $\longrightarrow \chi = \langle (r(t) - r)^2 \rangle_t$

Binder cumulant $\longrightarrow G = 1 - \frac{\langle r^4 \rangle_t}{3 \langle r^2 \rangle_t^2}$

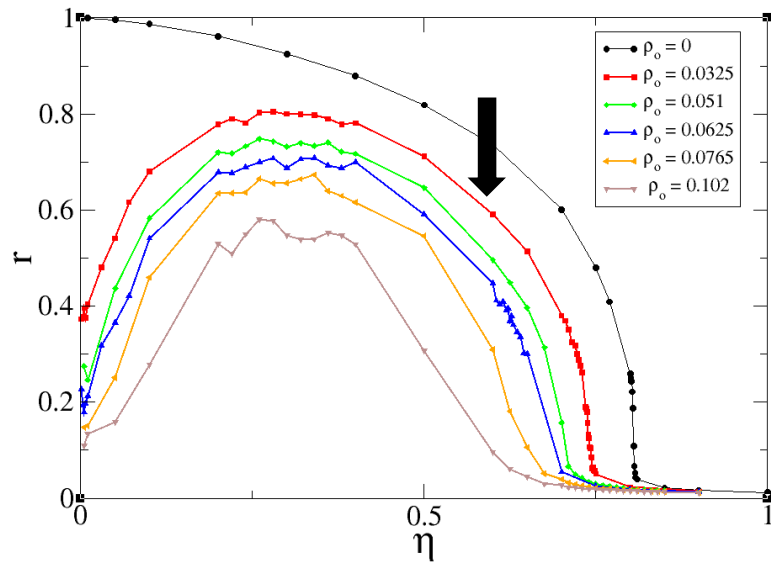
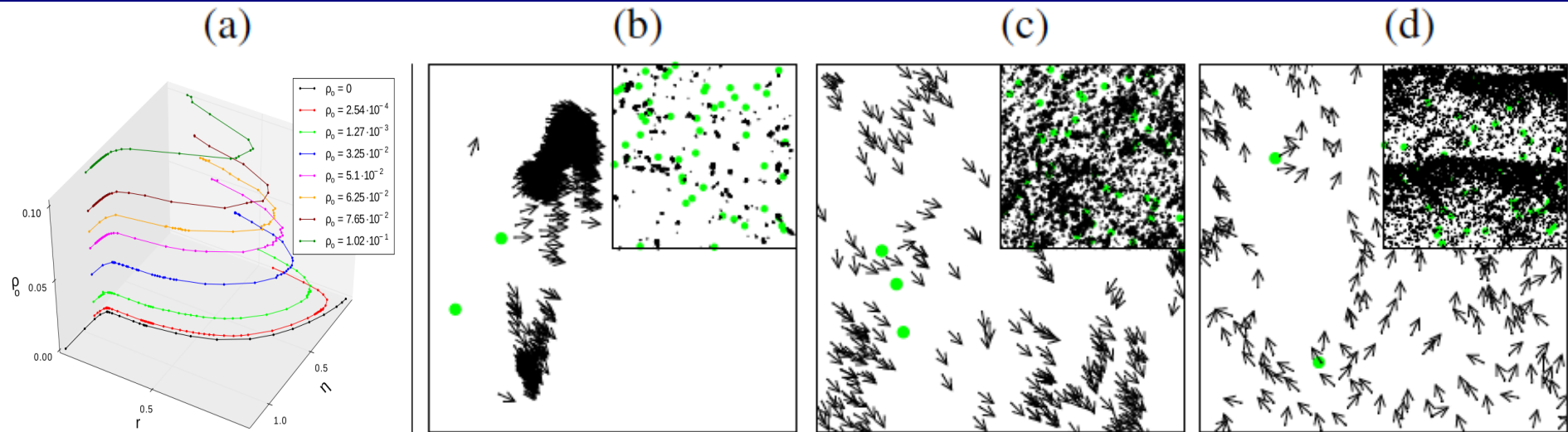
Minimal models -- interacting active particles



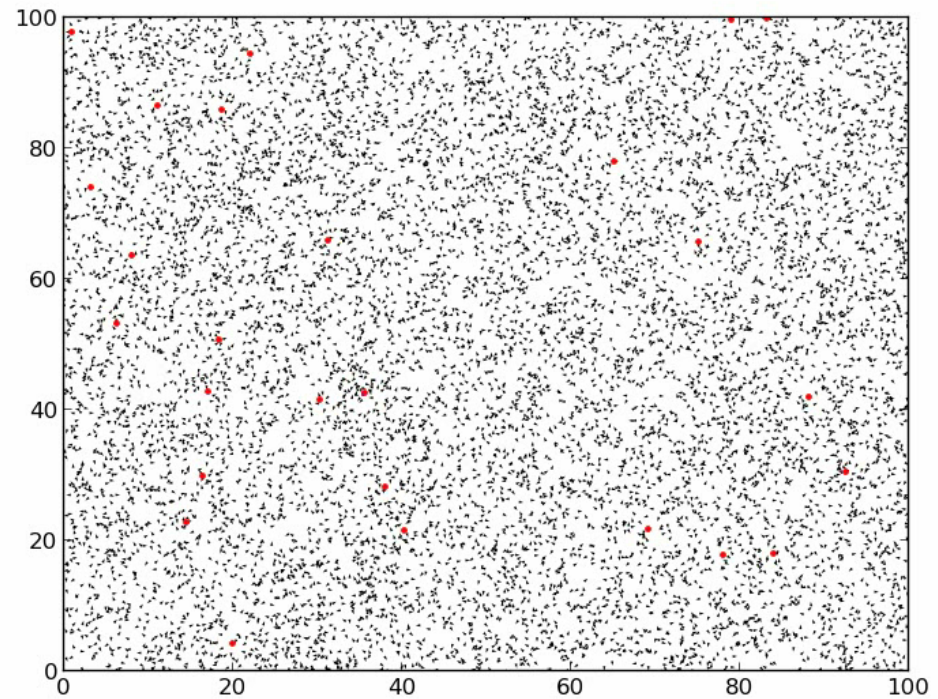
Minimal models -- interacting active particles



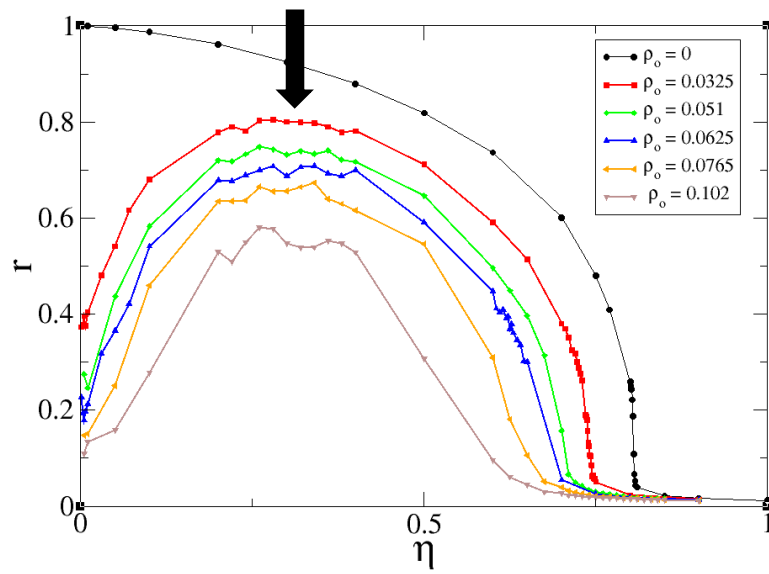
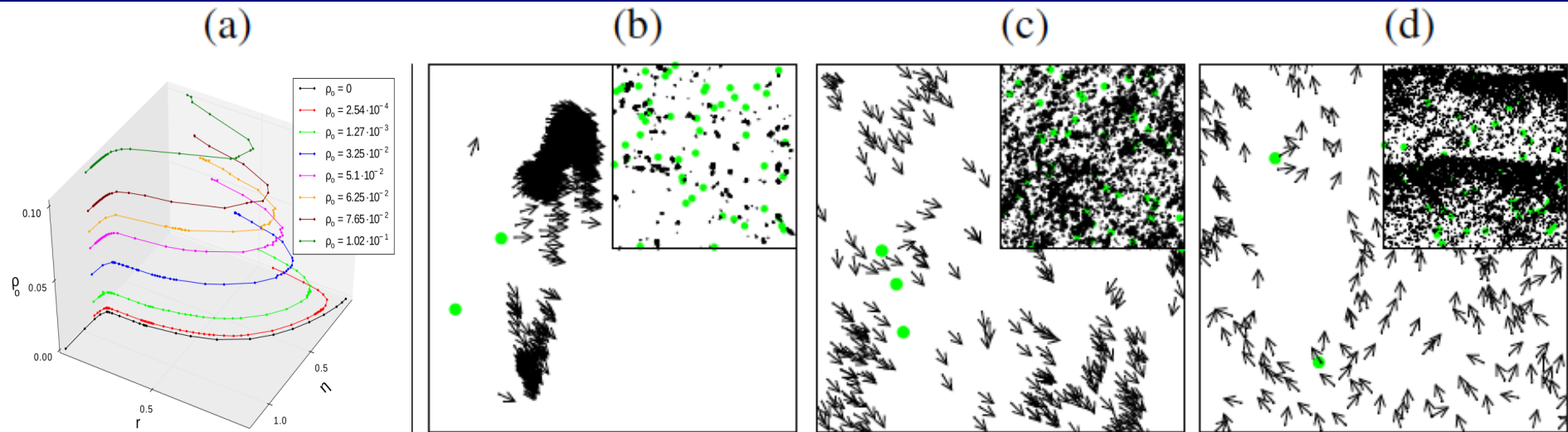
Minimal models -- interacting active particles



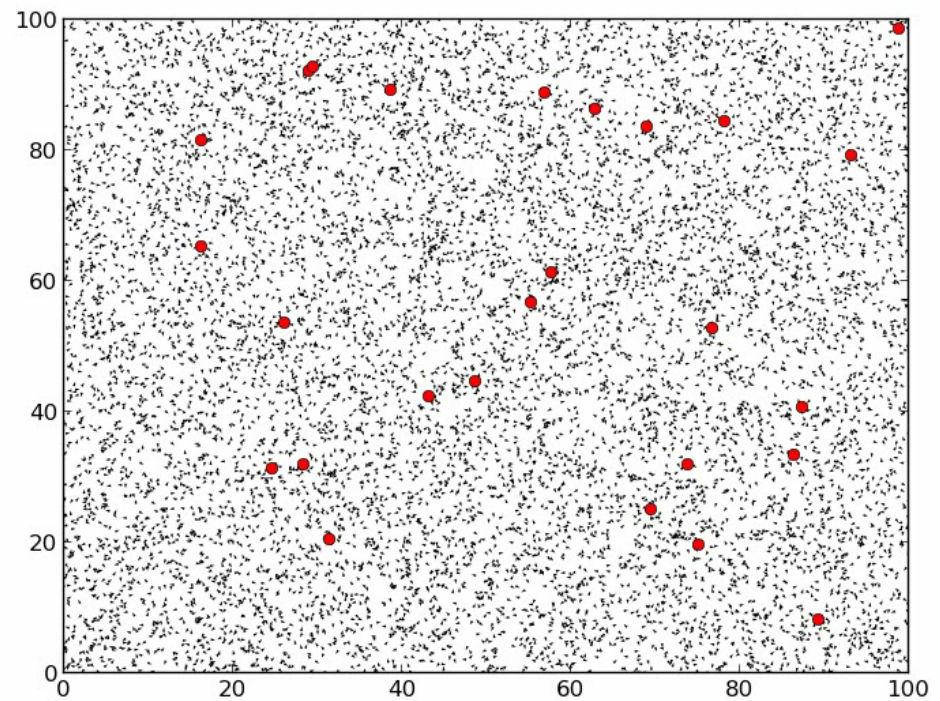
$N=10000$



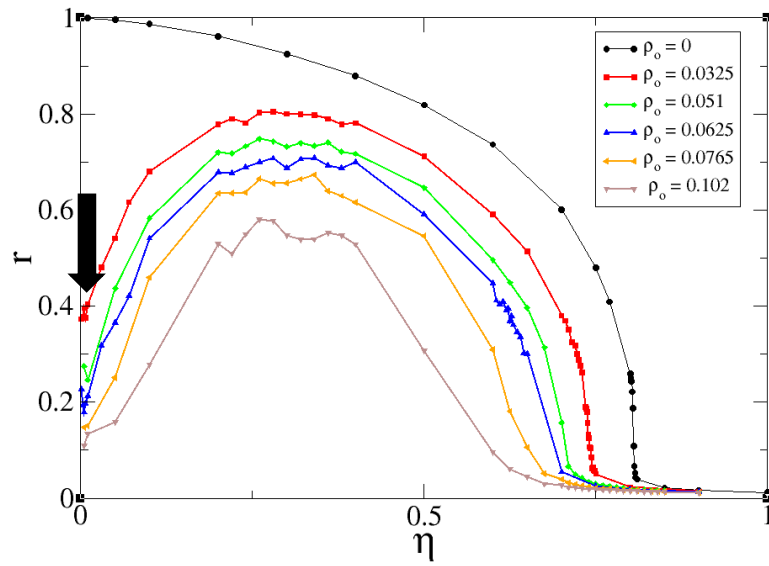
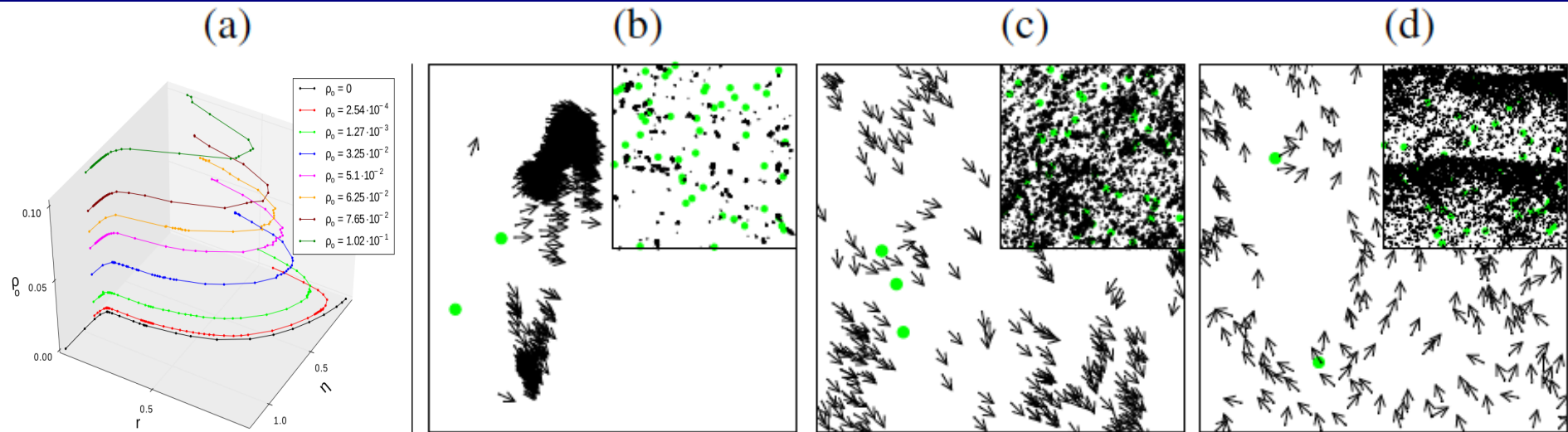
Minimal models -- interacting active particles



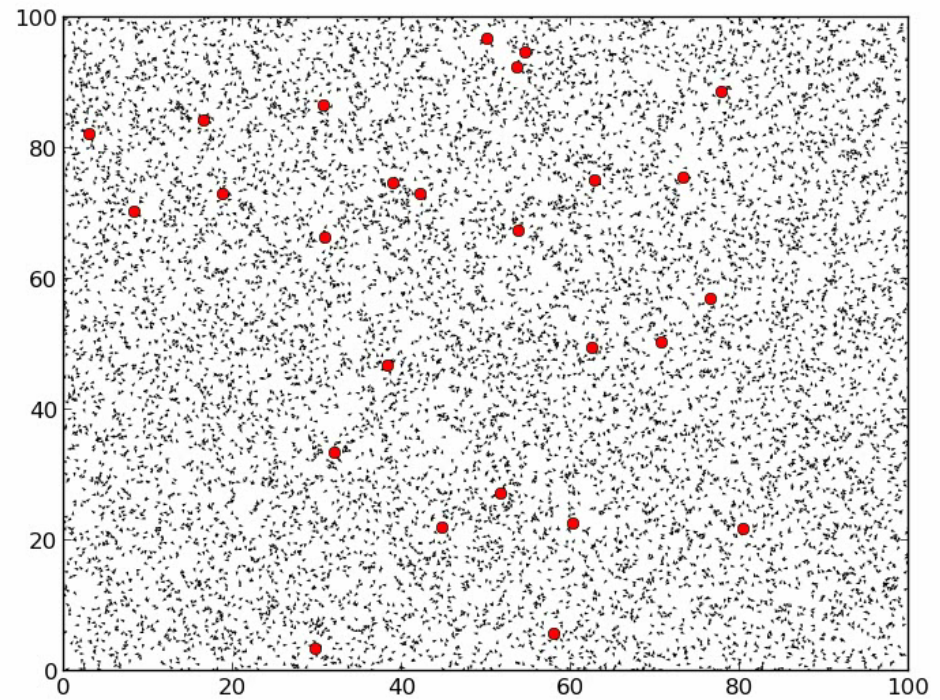
N=10000



Minimal models -- interacting active particles



$N=10000$



Minimal models -- interacting active particles

All this would have been impossible without the help of Sasha!



Oleksandr (Sasha) Chepizhko

Chepizkho, Peruani, PRL (2013)

Chepizkho, Altmann, Peruani, PRL (2013)

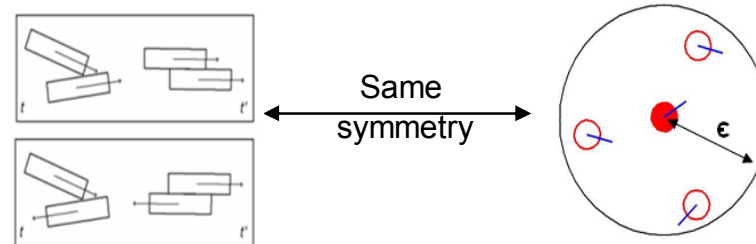
And many more to come in 2014!

Symmetries in active matter systems

Symmetries!

A simple model for (“point-like”) self-propelled rods (e.g., bacteria)

[F. Peruani, A. Deutsch, and M. Bär, Eur. Phys. J. Special Topics 157, 111 (2008)]



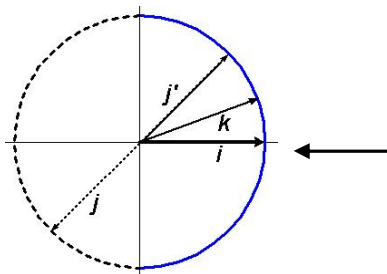
$$\mathbf{x}_i^{t+\Delta t} = \mathbf{x}_i^t + v_0 \mathbf{v}(\theta_i^t) \Delta t$$

Particles move in the direction given by:
 $\mathbf{v}(\theta_i) = (\cos(\theta_i), \sin(\theta_i))$

$$\theta_i^{t+\Delta t} = \arg \left(\sum_{|\mathbf{x}_i^t - \mathbf{x}_j^t| \leq \epsilon} \mathbf{f}(\mathbf{v}(\theta_j^t), \mathbf{v}(\theta_i^t)) \right) + \eta_i^t$$

Update of the moving direction

Alignment Additive noise



$$f(\mathbf{v}_j, \mathbf{v}_i) = \begin{cases} \mathbf{v}_j & \text{if } \mathbf{v}_i \cdot \mathbf{v}_j \geq 0 \\ -\mathbf{v}_j & \text{if } \mathbf{v}_i \cdot \mathbf{v}_j < 0 \end{cases}$$

Minimal models -- interacting active particles

A simple model for (“point-like”) self-propelled rods (e.g., bacteria)

[F. Peruani, A. Deutsch, and M. Bär, Eur. Phys. J. Special Topics 157, 111 (2008)]

$$\dot{\mathbf{x}}_i = v_0 e^{i\theta_i}$$

$$\dot{\theta}_i = -\gamma \frac{\partial U}{\partial \theta_i}(\mathbf{x}_i, \theta_i) + \tilde{\eta}_i(t)$$

Ferromagnetic alignment $\rightarrow U(\theta, \theta') = -\cos(\theta - \theta')$

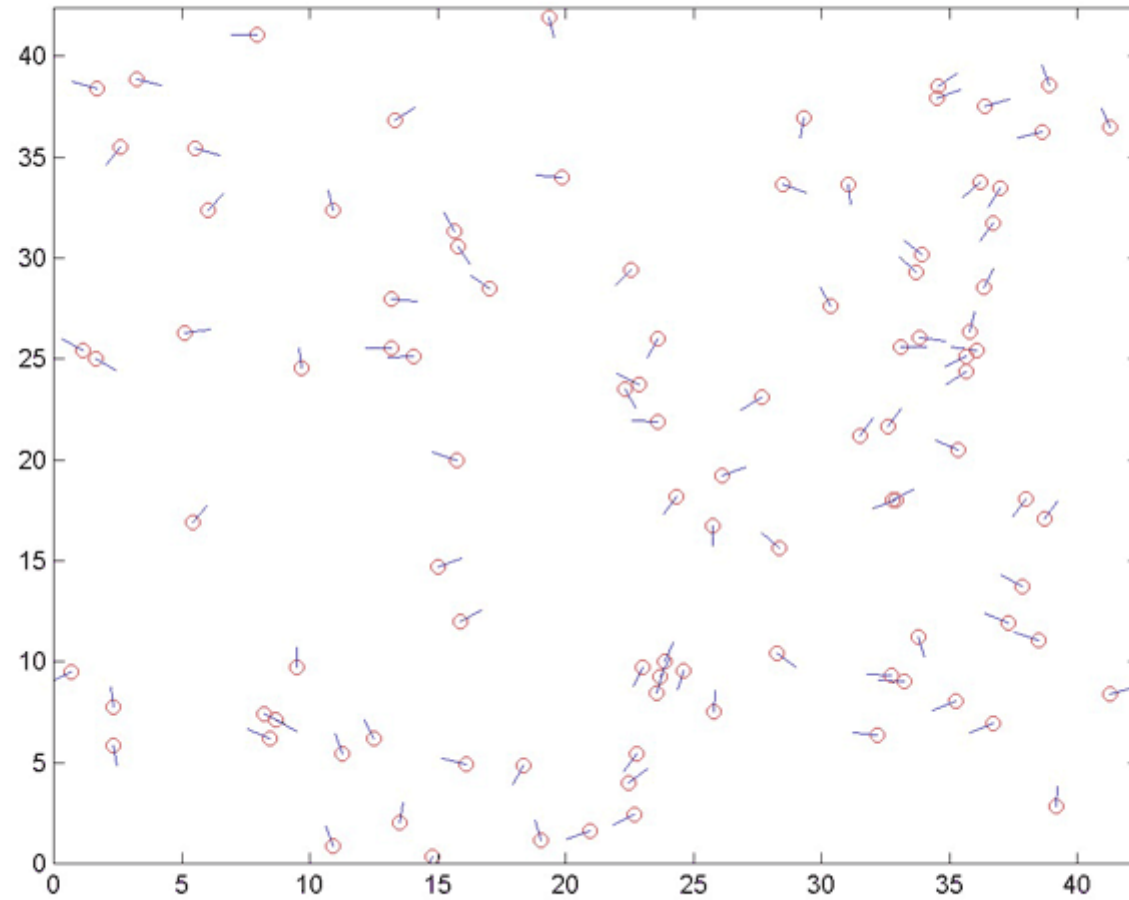
Nematic alignment $\longrightarrow U(\theta, \theta') = -\cos^2(\theta - \theta')$

Order parameters:

$$\phi = \left\langle \left| \frac{1}{N} \sum_{k=1}^N \exp(i\theta_k^t) \right| \right\rangle \quad S = \left\langle \left| \frac{1}{N} \sum_{k=1}^N \exp(i2\theta_k^t) \right| \right\rangle$$

[Peruani, Deutsch, and Bär, EPJ ST 157, 111 (2008)]

Symmetries!

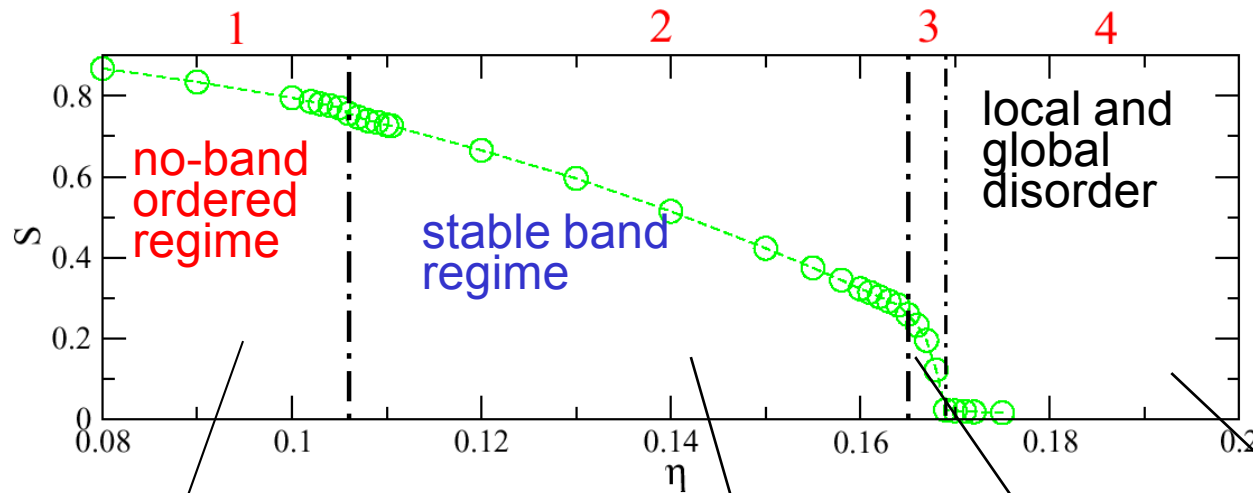


[F. Peruani et al., EJP-ST (2008)]

Symmetries!

The symmetry of the alignment plays a crucial role in pattern formation

[F. Ginelli, F. Peruani, M. Bär, and H. Chaté, Phys. Rev. Lett. 104, 184502 (2010)]

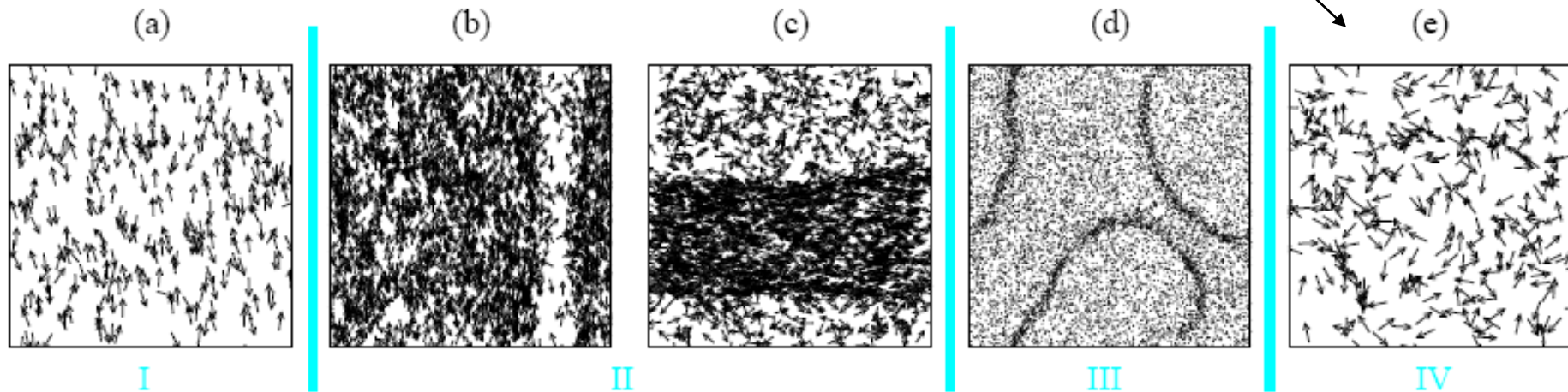


Nematic OP:

$$\langle S \rangle = \left\langle \left| \frac{1}{N} \sum_{k=1}^N e^{i2\theta_k} \right| \right\rangle_t$$

Ferromagnetic OP:

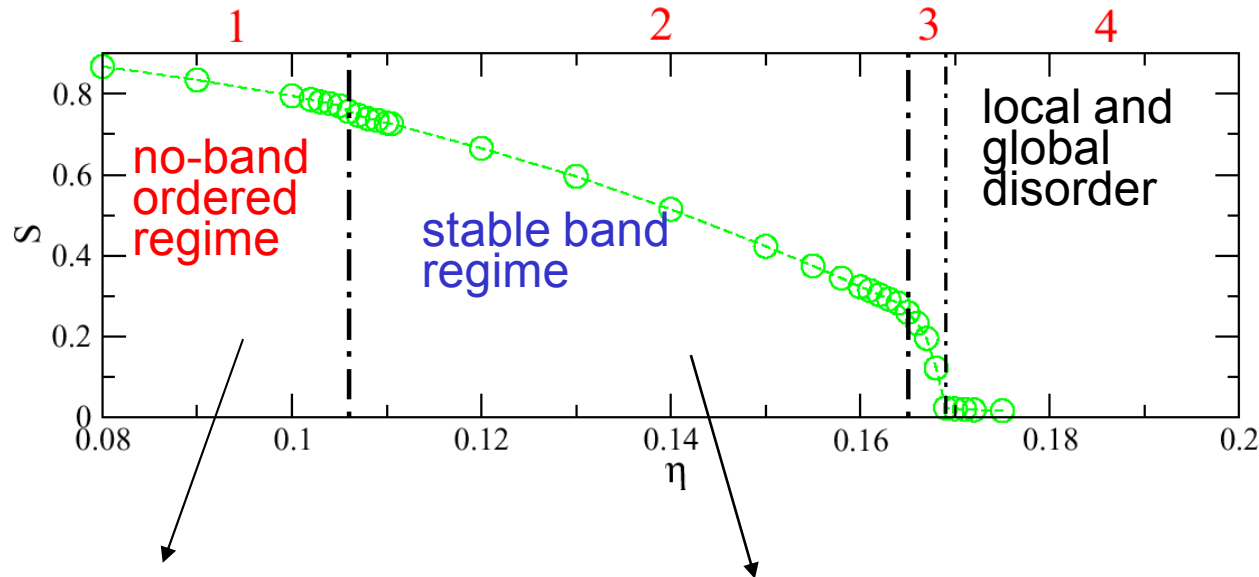
$$\langle \phi \rangle = \left\langle \left| \frac{1}{N} \sum_{k=1}^N e^{i\theta_k} \right| \right\rangle_t$$



Symmetries!

The symmetry of the alignment plays a crucial role in pattern formation

[F. Ginelli, F. Peruani, M. Bär, and H. Chaté, Phys. Rev. Lett. 104, 184502 (2010)]

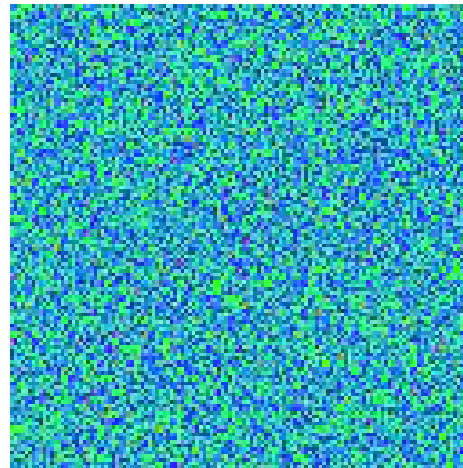
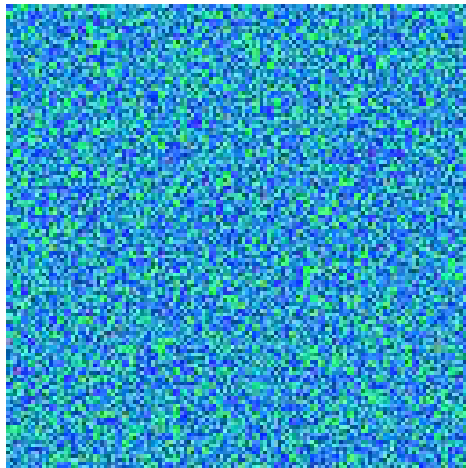


Nematic OP:

$$\langle S \rangle = \left\langle \left| \frac{1}{N} \sum_{k=1}^N e^{i2\theta_k} \right| \right\rangle_t$$

Ferromagnetic OP:

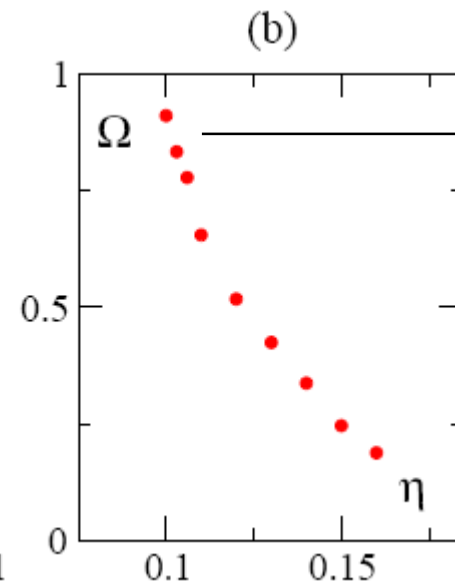
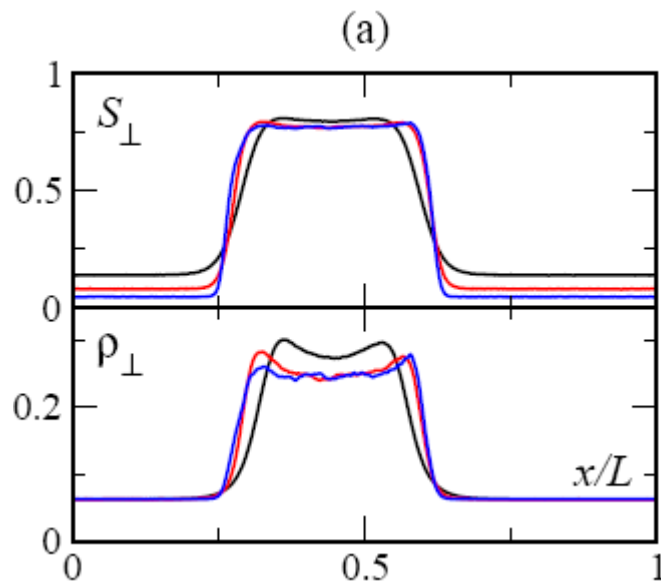
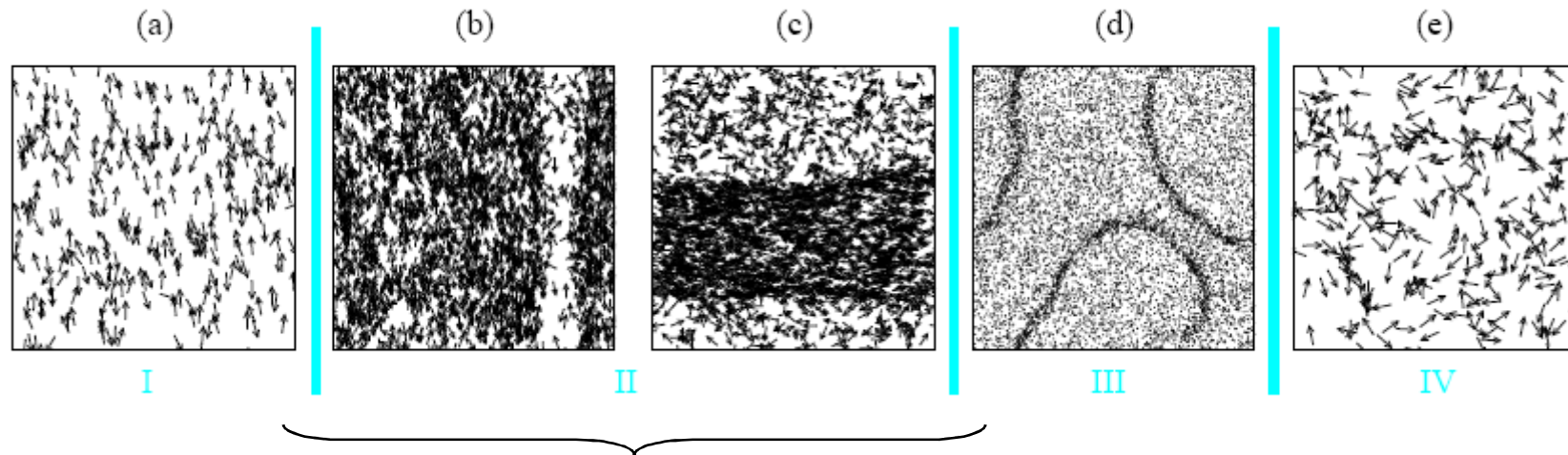
$$\langle \phi \rangle = \left\langle \left| \frac{1}{N} \sum_{k=1}^N e^{i\theta_k} \right| \right\rangle_t$$



[watch them using VLC!]

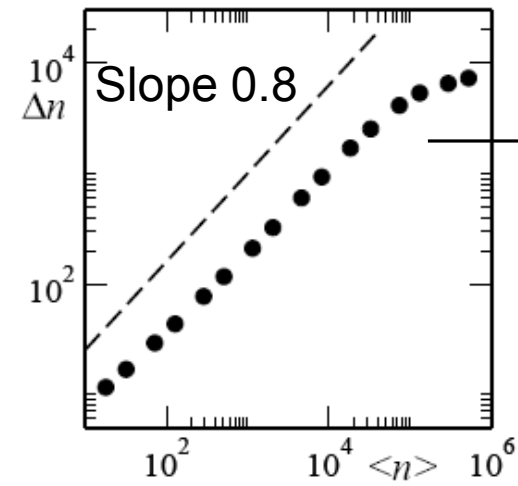
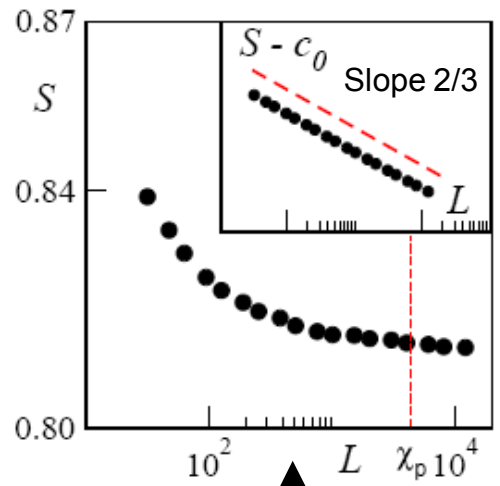
Symmetries!

The symmetry of the alignment plays a crucial role in pattern formation



Fraction of the area occupied by the band

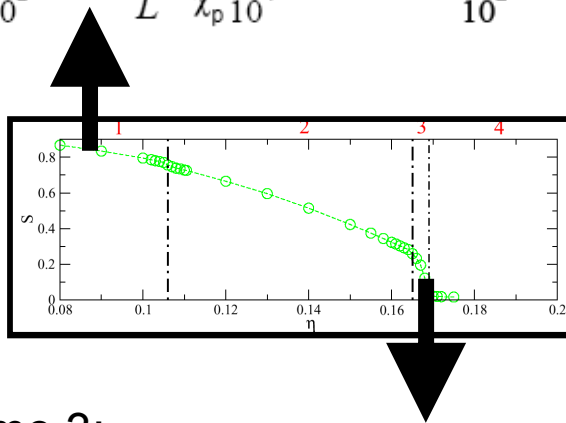
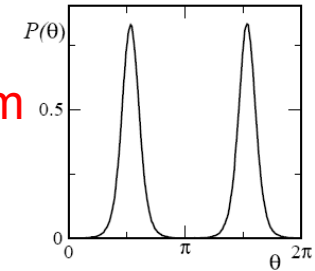
Symmetries!



In regime 1:

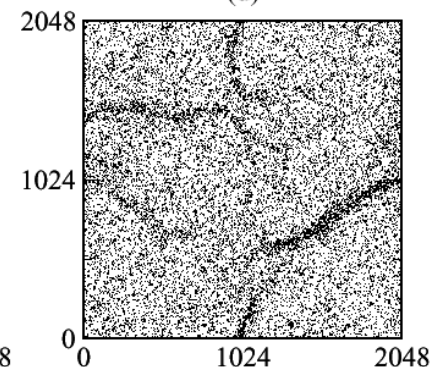
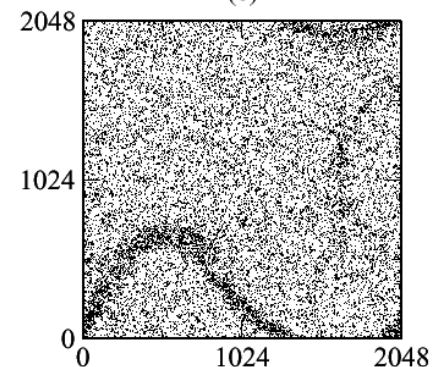
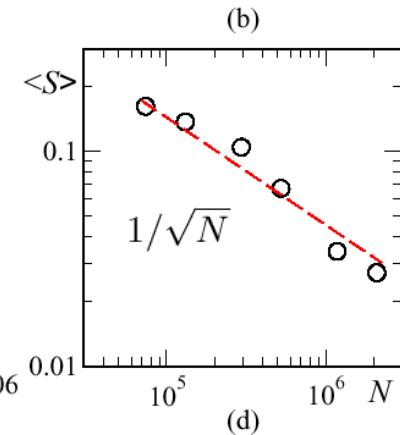
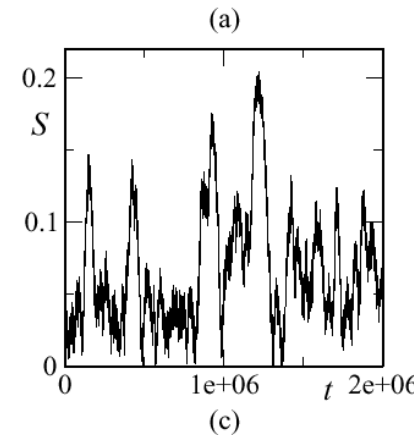
- True Long-Range Order (LRO)
- Giant fluctuations

Mermin Wagner Theorem
(for equilibrium syst.)
does not allow for LRO!



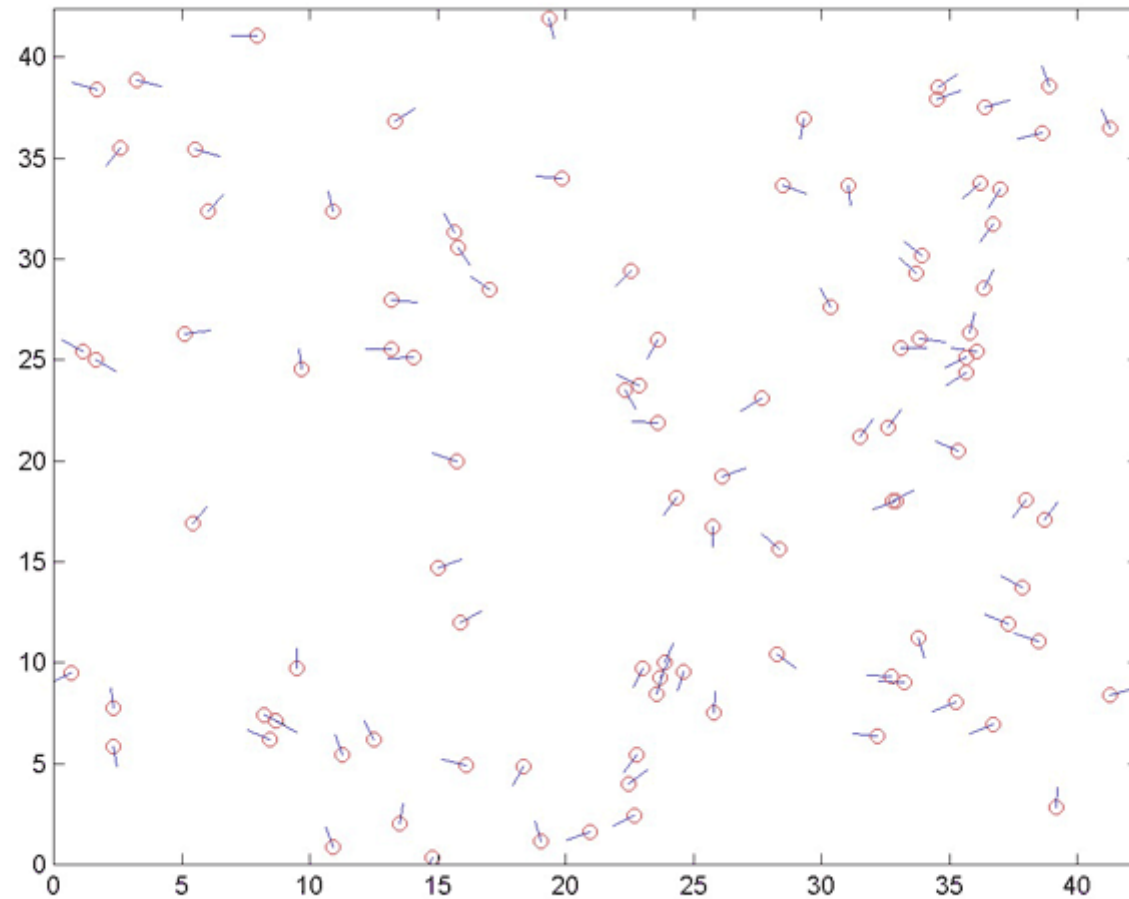
In regime 3:

- There is no LRO
- Unstable macroscopic structures (bands!)



Symmetries!

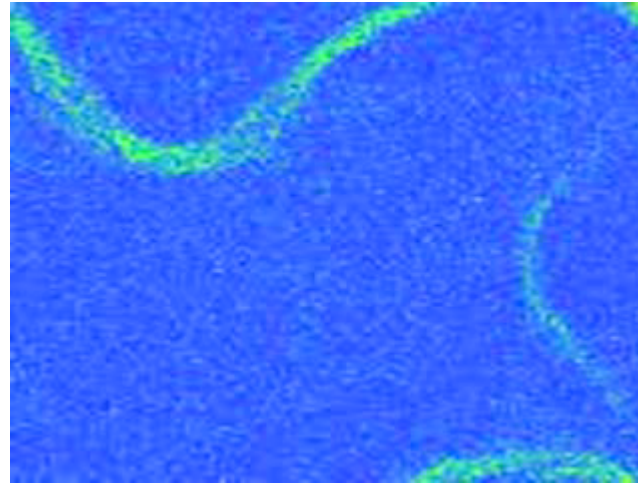
The symmetry of the alignment plays a crucial role in pattern formation



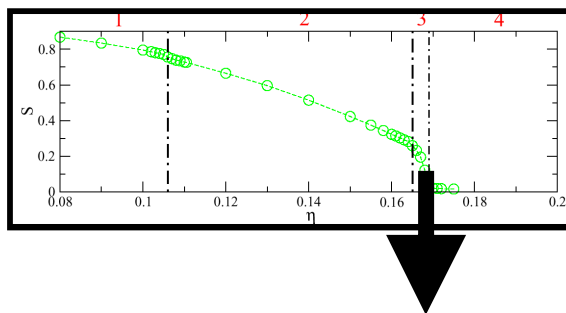
If we observe a very small system size or using a small box in a large system, particles behaves as shown in the movie

Symmetries!

The symmetry of the alignment plays a crucial role in pattern formation



Green areas correspond to high density of particles, while blue means very low density



We are looking at the behavior of the system for this noise amplitude

Symmetries!

The symmetry of the alignment determines the type of macroscopic order

- A mean-field approach to understand collective motion

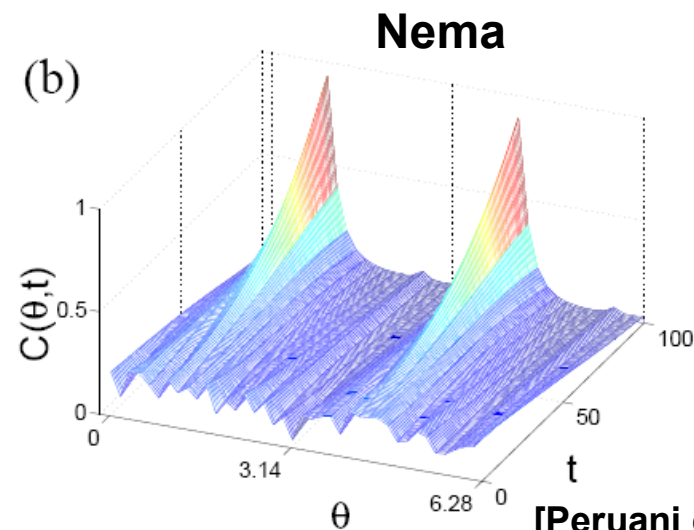
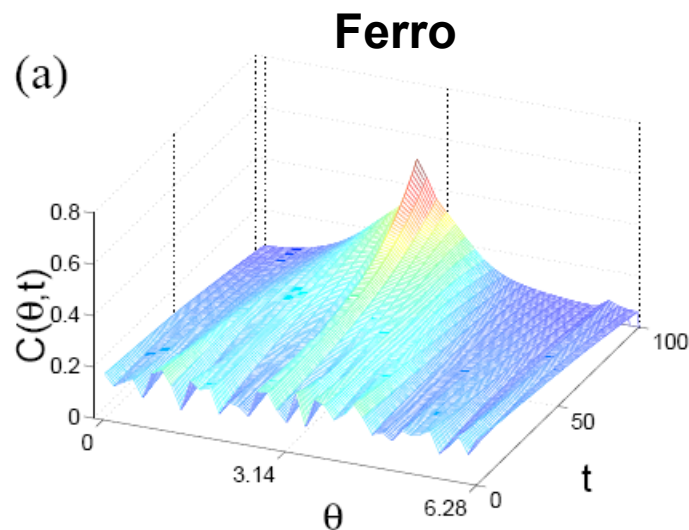
$$\partial_t C = \underbrace{D_\theta \partial_{\theta\theta} C}_{\text{noise}} + \gamma(\rho) \partial_\theta \left[\underbrace{\partial_\theta \left(\int_0^{2\pi} d\theta' C(\theta', t) U(\theta, \theta') \right)}_{\text{alignment}} C(\theta, t) \right]$$

noise

alignment

Ferromagnetic alignment $\rightarrow U(\theta, \theta') = -\cos(\theta - \theta')$

Nematic alignment $\rightarrow U(\theta, \theta') = -\cos^2(\theta - \theta')$



[Peruani et al., 2008]

Symmetries!

The symmetry of the alignment determines the type of macroscopic order

- A mean-field approach to understand collective motion

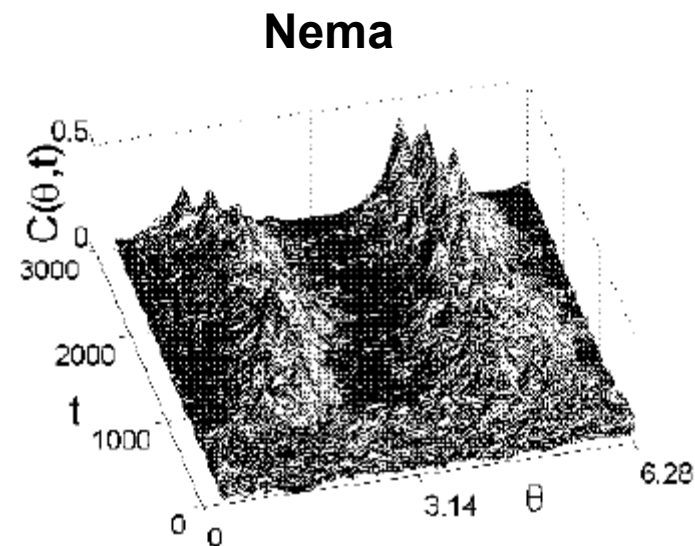
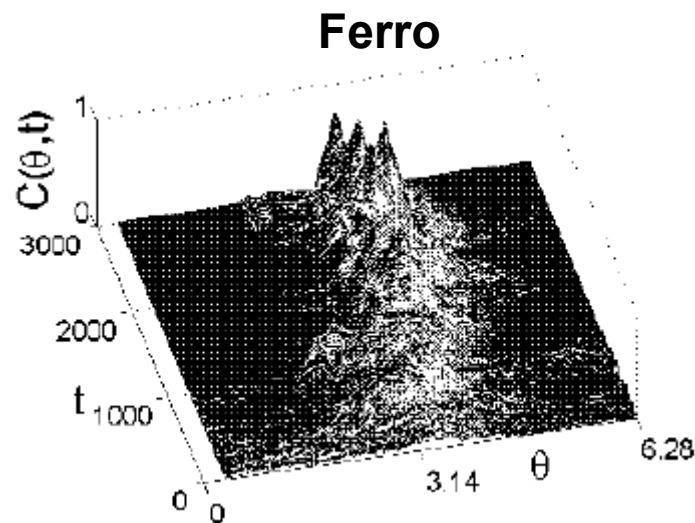
$$\partial_t C = \underbrace{D_\theta \partial_{\theta\theta} C}_{\text{noise}} + \gamma(\rho) \partial_\theta \left[\underbrace{\partial_\theta \left(\int_0^{2\pi} d\theta' C(\theta', t) U(\theta, \theta') \right) C(\theta, t)}_{\text{alignment}} \right]$$

noise

alignment

Ferromagnetic alignment $\rightarrow U(\theta, \theta') = -\cos(\theta - \theta')$

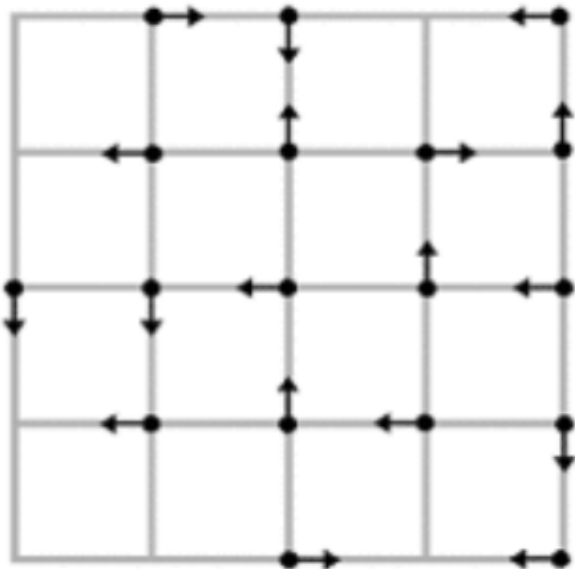
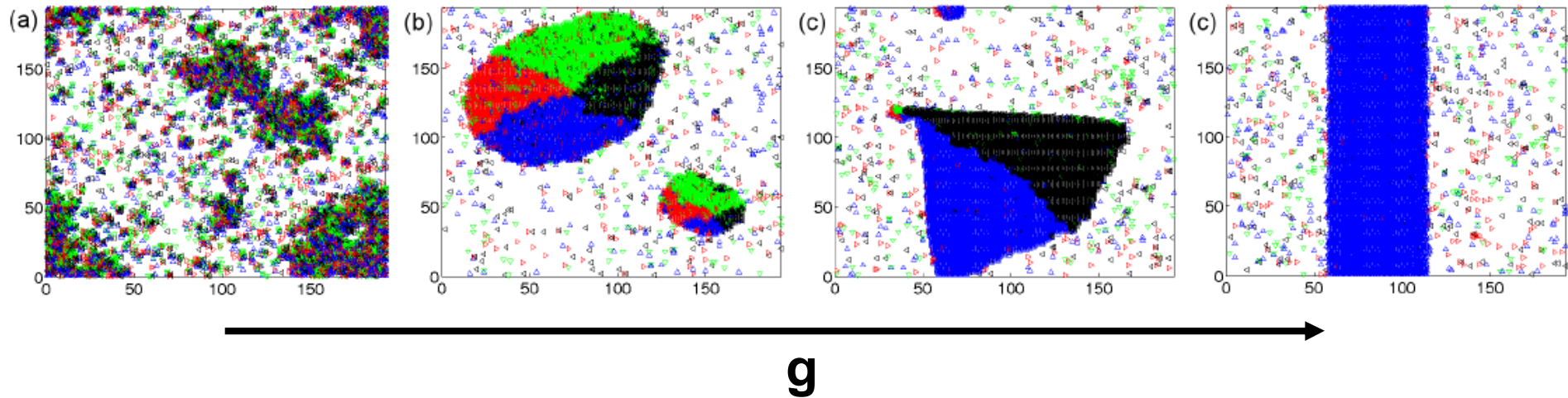
Nematic alignment $\rightarrow U(\theta, \theta') = -\cos^2(\theta - \theta')$



Gas-liquid-like transitions in active matter systems

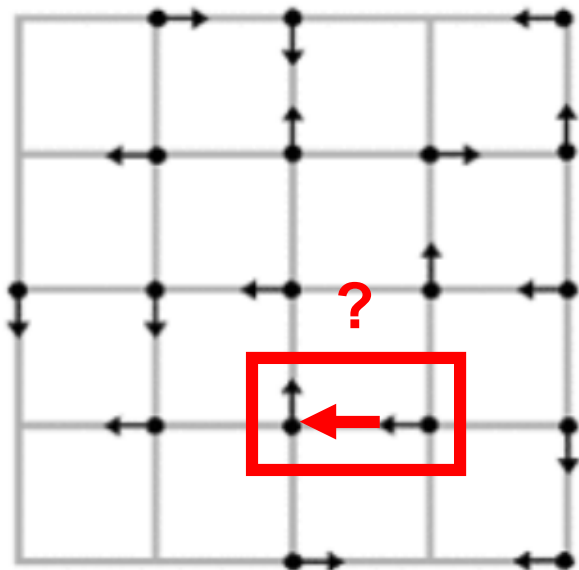
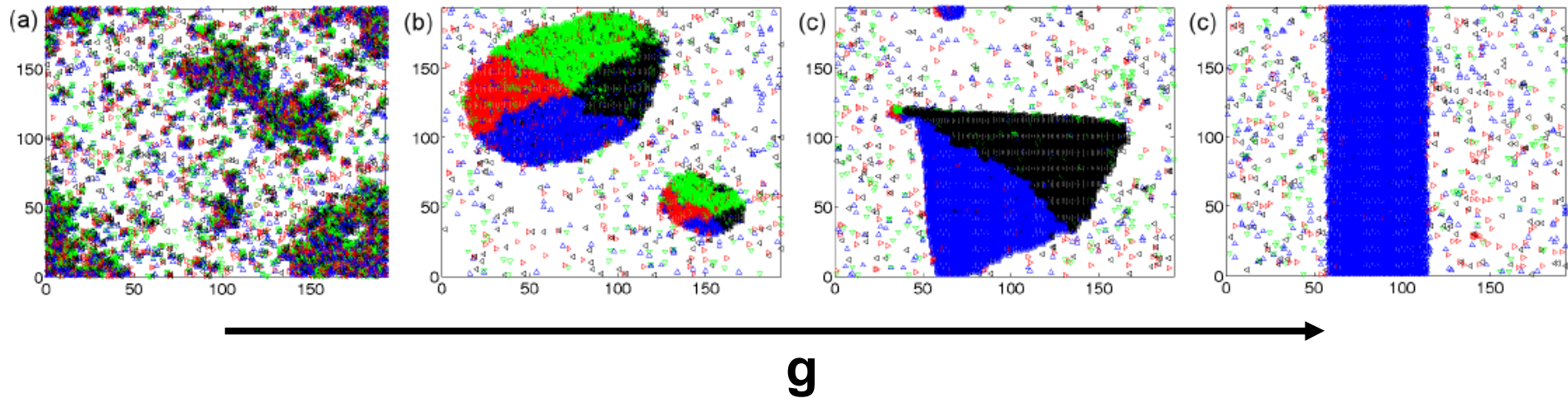
Gas-liquid-like transitions in active matter

Coupling between local orientation, density and **local particle speed!**



- Each particle can perform two actions:
- 1) **Migrate according to its velocity direction**
 - 2) **Reorient its velocity direction**

Gas-liquid-like transitions in active matter

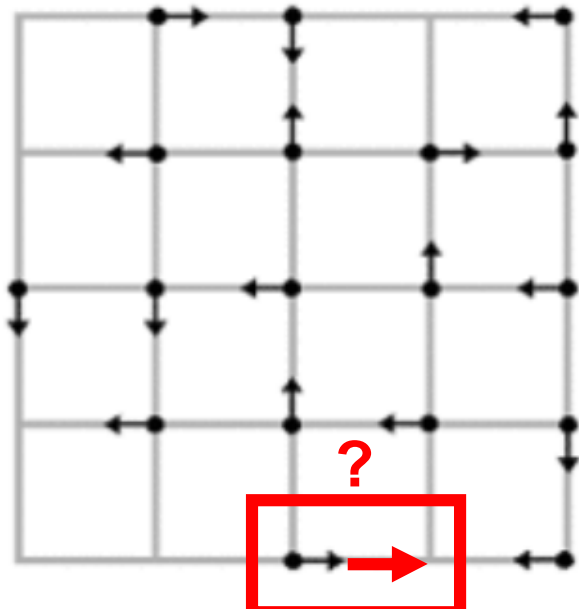
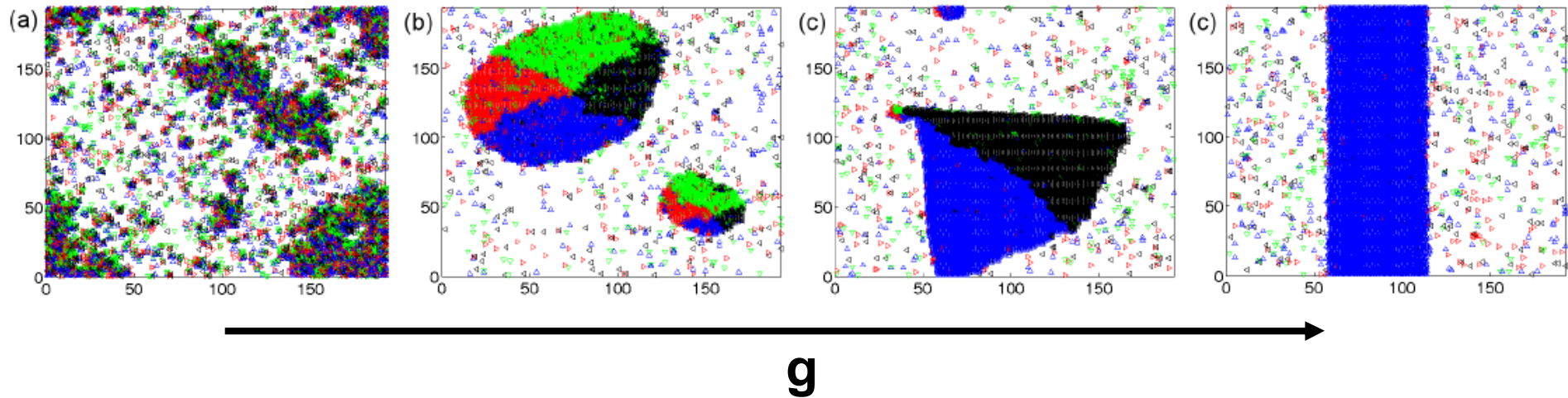


1) Migration according to its velocity direction

$$T_M((\mathbf{x}, \mathbf{v}) \rightarrow (\mathbf{y} = \mathbf{x} + \mathbf{v}, \mathbf{v})) = \begin{cases} m & \text{if node } \mathbf{y} \text{ is empty} \\ 0 & \text{if node } \mathbf{y} \text{ is occupied} \end{cases}$$

Peruani, Klauss, Deutsch, Voss-Boehme, PRL (2011)

Gas-liquid-like transitions in active matter

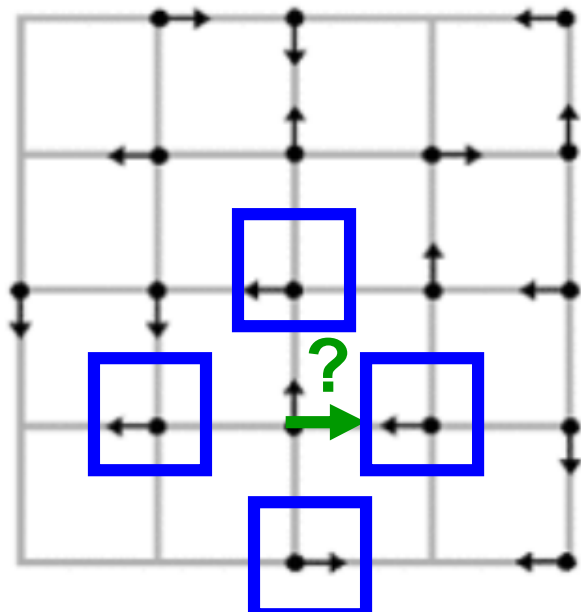
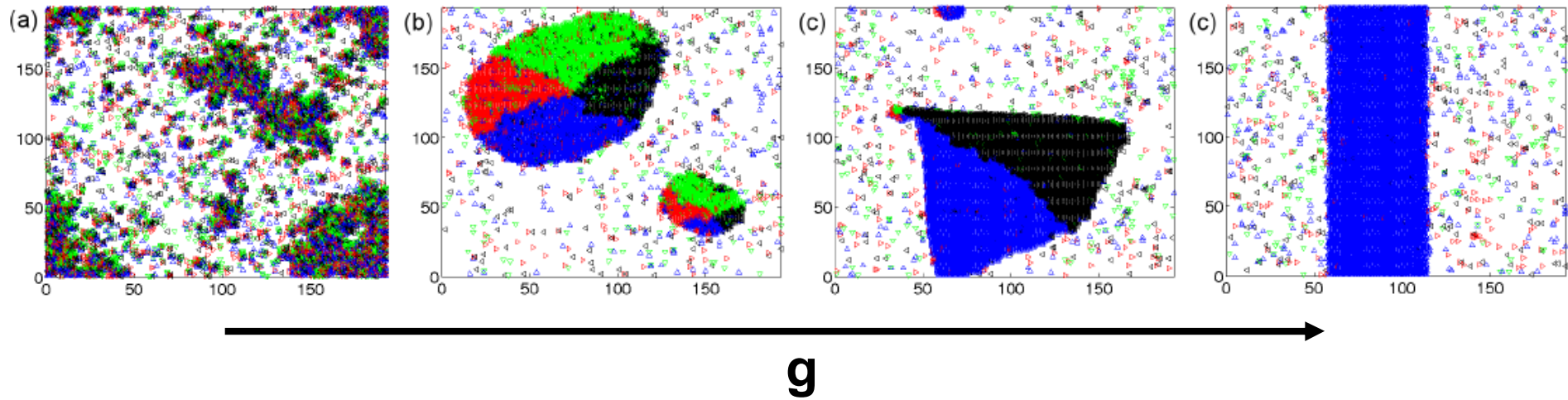


1) Migration according to its velocity direction

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Peruani, Klauss, Deutsch, Voss-Boehme, PRL (2011)

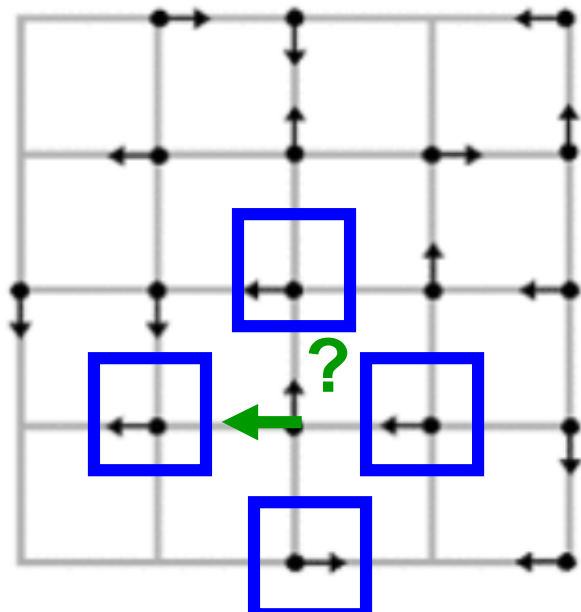
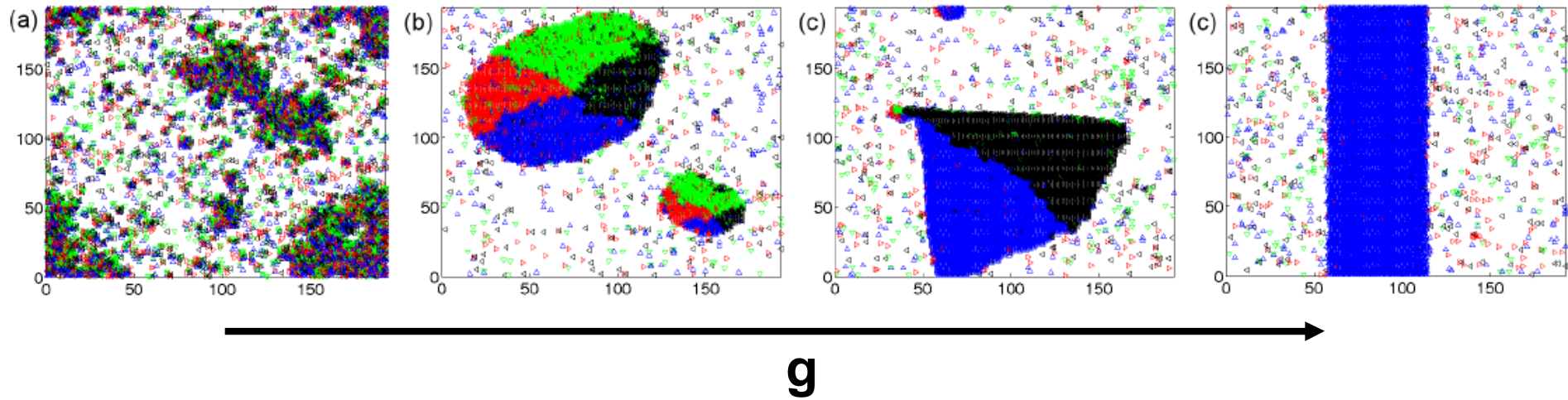
Gas-liquid-like transitions in active matter



2) Reorient its velocity direction

$$T_R((\mathbf{x}, \mathbf{v}) \rightarrow (\mathbf{x}, \mathbf{w})) = \exp\left(g \sum_{\mathbf{y} \in A(\mathbf{x})} \langle \mathbf{w} | \mathbf{V}(\mathbf{y}) \rangle\right)$$

Gas-liquid-like transitions in active matter

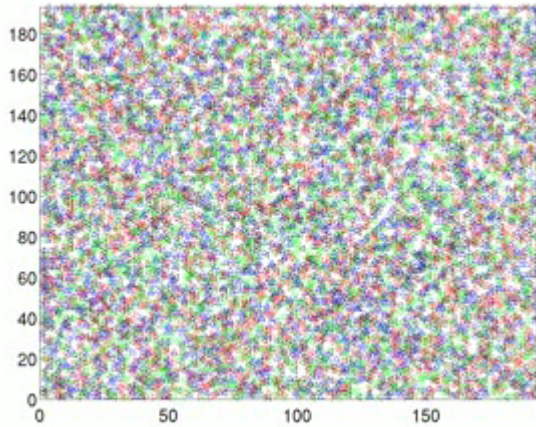


2) Reorient its velocity direction

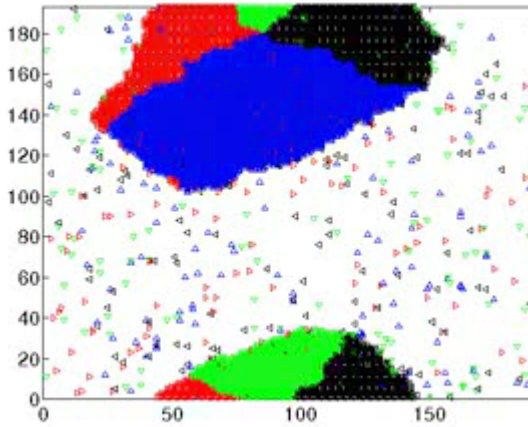
$$T_R((\mathbf{x}, \mathbf{v}) \rightarrow (\mathbf{x}, \mathbf{w})) = \exp\left(g \sum_{\mathbf{y} \in A(\mathbf{x})} \langle \mathbf{w} | \mathbf{V}(\mathbf{y}) \rangle\right)$$

Gas-liquid-like transitions in active matter

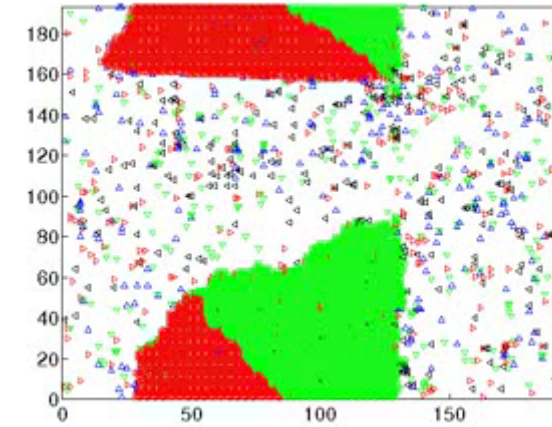
$g=1.4$



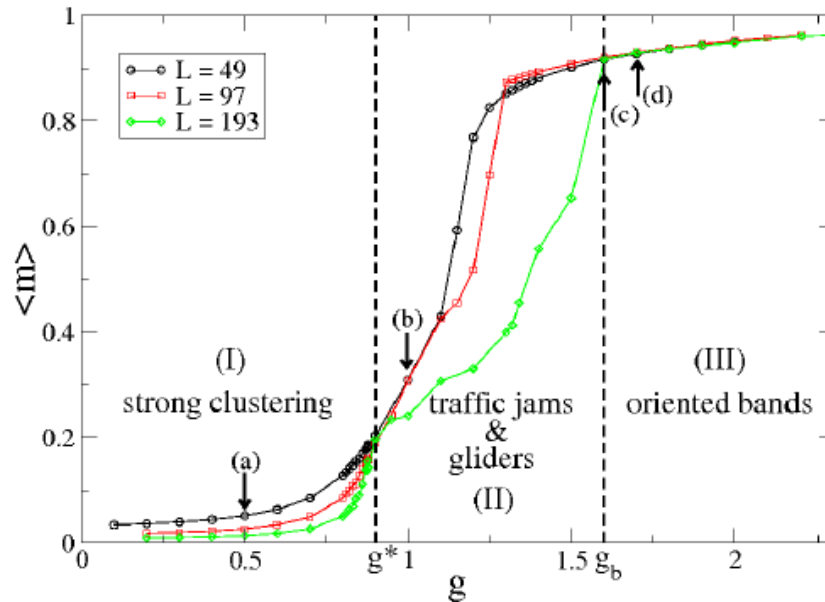
$g=1.5$



$g=1.6$



g



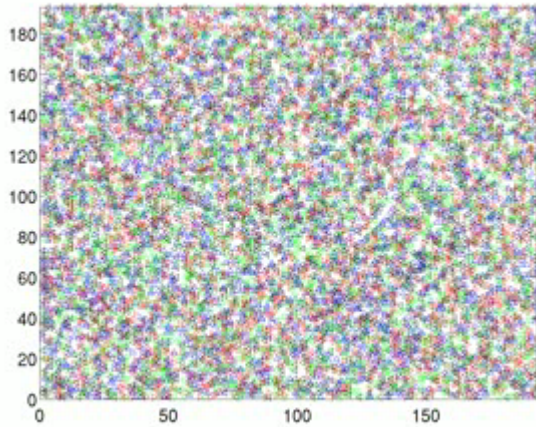
As g is increased, we observe:

- jamming
- moving jams
- bands

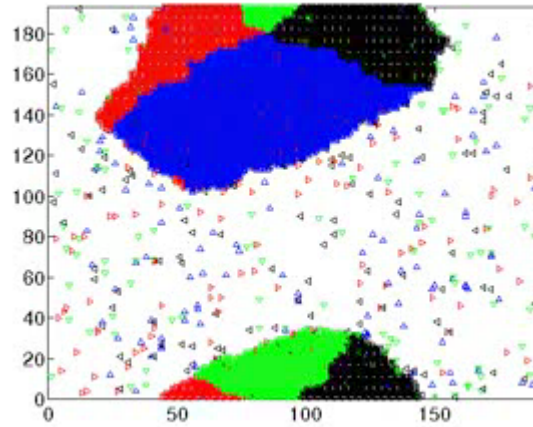
and a transition to orientational order!

Gas-liquid-like transitions in active matter

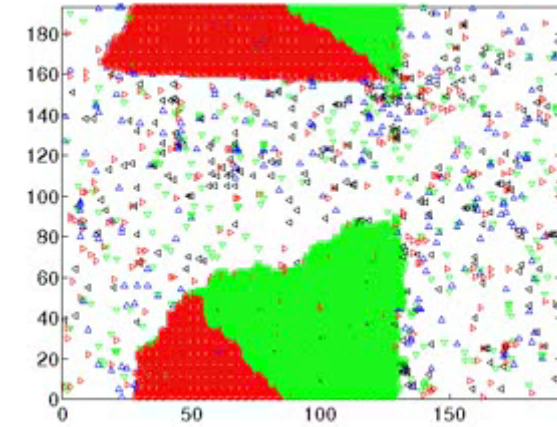
$g=1.4$



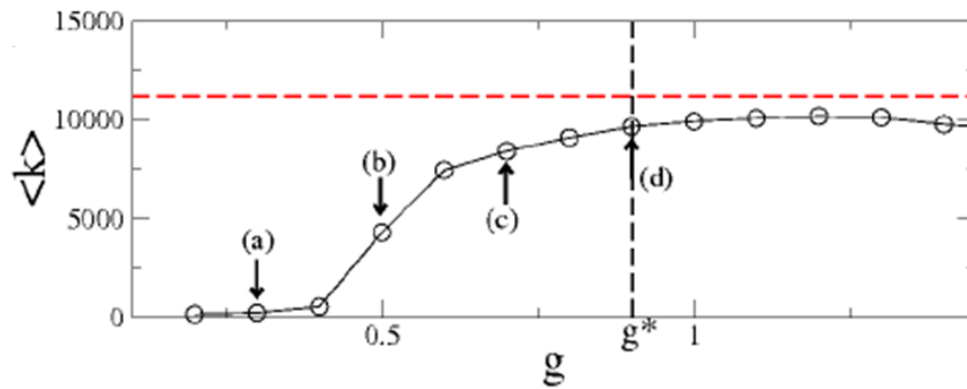
$g=1.5$



$g=1.6$



g



- Gas-liquid-like transition
- Second orientational order

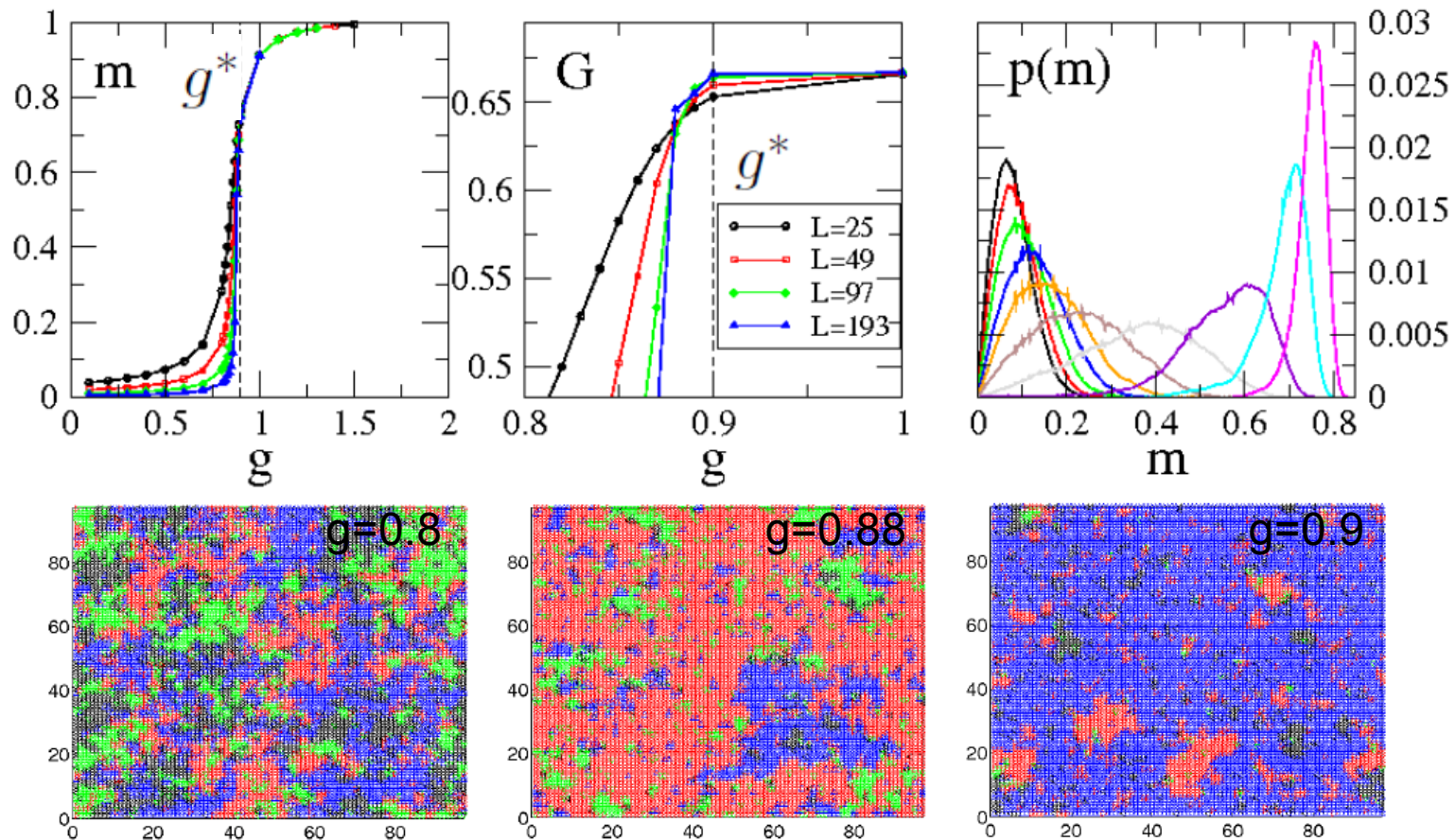
Different behavior
at low and high densities
(particularly evident at full occupancy)

Gas-liquid-like transitions in active matter

Order of the phase transition at high and low density

Results at “high” (=full occupancy) density

- The problem with full occupancy can be mapped onto the 4-Potts model
- The 4-Potts model exhibits a second order phase transition
- Then, our model exhibits a **second order** transition at $d=1$!



Gas-liquid-like transitions in active matter

Are these transition similar to the equilibrium gas-liquid transitions?

Can we map non-equilibrium to equilibrium?

Gas-liquid-like transitions in active matter

Equations of motion for the i -th particle:

$$\dot{\mathbf{x}}_i = v(n_i) \mathbf{u}(\theta_i) + \sqrt{2D_x} \boldsymbol{\sigma}_i(t)$$

$$\dot{\theta}_i = -\frac{\gamma}{n_i} \sum_{j=1}^N g(|\mathbf{x}_i - \mathbf{x}_j|/R) \sin(\theta_i - \theta_j) + \sqrt{2D_\theta} \eta_i(t)$$

Number of neighbors: $n_i = \sum_{j=1}^N g(|\mathbf{x}_i - \mathbf{x}_j|/R)$

Active speed:

$$v(n_i) \mathbf{u}(\theta_i)$$



$$v(\rho) = \exp(-\lambda\rho)$$

$$\mathbf{u}(\theta_i) \equiv (\cos(\theta_i), \sin(\theta_i))$$

dependency with the number of neighbors/local density

Gas-liquid-like transitions in active matter

We can write the previous equations in the following dimensionless form:

$$\begin{aligned} \frac{d\tilde{\mathbf{x}}_i}{d\tilde{t}} &= \epsilon \tilde{v}(n_i) \mathbf{u}(\theta_i) + \epsilon \sqrt{2\tilde{D}_x} \boldsymbol{\sigma}_i(\tilde{t}) \\ \frac{d\theta_i}{d\tilde{t}} &= -\frac{\bar{\gamma}}{n_i} \sum_{j=1}^N g((\tilde{\mathbf{x}}_i - \tilde{\mathbf{x}}_j)/\alpha) \sin(\theta_i - \theta_j) + \sqrt{2}\eta_i(\tilde{t}) \end{aligned}$$

$v_0/(LD_\theta)$

$\tilde{D}_x = D_x D_\theta / v_0^2$

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Evolution of the empirical density

$$\begin{aligned} \frac{\partial f_d}{\partial t} = & -\varepsilon \nabla \cdot (v(\rho(\mathbf{x}, t)) \mathbf{u}(\theta) f_d(\mathbf{x}, \theta, t)) \\ & + \frac{\bar{\gamma}}{\rho(\mathbf{x}, t)} \frac{\partial}{\partial \theta} \left(f_d(\mathbf{x}, \theta, t) \int d\theta' \sin(\theta - \theta') f_d(\mathbf{x}, \theta', t) \right) \\ & + \frac{\partial^2 f_d}{\partial \theta^2} + \varepsilon^2 D_x \nabla^2 f_d + \sqrt{\frac{2}{N}} \frac{\partial}{\partial \theta} \left(\eta(\mathbf{x}, \theta, t) \sqrt{f_d} \right) \\ & + \varepsilon \frac{\sqrt{2D_x}}{\sqrt{N}} \nabla \cdot \left(\boldsymbol{\sigma}(\mathbf{x}, \theta, t) \sqrt{f_d} \right), \end{aligned}$$

Gaussian noise delta correlated

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Instead of working with fd with can look at the evolution of the first n Fourier modes of fd:

$$\rho(\mathbf{x}, t) = \int d\theta f_d(\mathbf{x}, \theta, t)$$

→ density

$$\mathbf{P}(\mathbf{x}, t) = \int d\theta \mathbf{u}(\theta) f_d(x, y, \theta, t)$$

→ polarization

Their evolution are given by:

$$\frac{\partial \rho}{\partial t} = -\varepsilon \nabla \cdot (v \mathbf{P}) + \varepsilon^2 D_x \nabla^2 \rho + \varepsilon \frac{\sqrt{2D_x}}{\sqrt{N}} \nabla \cdot (\boldsymbol{\xi}(x, y, t))$$

$$\frac{\partial \mathbf{P}}{\partial t} = -\frac{1}{2} \varepsilon \nabla (v \rho) + \left(\frac{\bar{\gamma}}{2} - 1 \right) \mathbf{P} + \varepsilon^2 D_x \nabla^2 \mathbf{P} + \sqrt{\frac{2}{N}} \boldsymbol{\eta}(x, y, t) + O\left(\frac{\varepsilon}{\sqrt{N}}\right)$$

Gas-liquid-like transitions in active matter

The noise term are given by:

$$\begin{aligned}\eta_x(x, y, t) &= \int d\theta \sin \theta \sqrt{f_d} \eta(x, y, \theta, t) \\ \eta_y(x, y, t) &= - \int d\theta \cos \theta \sqrt{f_d} \eta(x, y, \theta, t) \\ \xi(x, y, t) &= \int d\theta \sqrt{f_d} \sigma(x, y, \theta, t) .\end{aligned}$$

With correlations:

$$\langle \eta_x(x, y, t) \eta_x(x', y', t') \rangle \simeq \delta(x - x') \delta(y - y') \delta(t - t') \frac{1}{2} \rho(x, y, t)$$

$$\langle \eta_y(x, y, t) \eta_y(x', y', t') \rangle \simeq \delta(x - x') \delta(y - y') \delta(t - t') \frac{1}{2} \rho(x, y, t)$$

$$\langle \eta_x(x, y, t) \eta_y(x', y', t') \rangle \simeq 0$$

$$\langle \xi(x, y, t) \xi(x', y', t') \rangle = \delta(x - x') \delta(y - y') \delta(t - t') \rho(x, y, t) .$$

Gas-liquid-like transitions in active matter

The evolution of \mathbf{P} is faster than the evolution of the density and asymptotically we expect $\mathbf{P}=0$, which means that at order ε we can expect:

$$\mathbf{P} = \varepsilon \frac{-1}{2 \left(1 - \frac{\bar{\gamma}}{2}\right)} \nabla(v(\rho)\rho) + \sqrt{\frac{2}{N}} \frac{1}{1 - \frac{\bar{\gamma}}{2}} \boldsymbol{\eta}$$

If we insert this expression into the equation for the density we find:

$$\begin{aligned} \frac{\partial \rho}{\partial t} = & \frac{1}{2} \nabla \cdot \left(\frac{v}{1 - \frac{\bar{\gamma}}{2}} \nabla[v(\rho)\rho] \right) + D_x \nabla^2 \rho \\ & + \frac{\sqrt{2D_x}}{\sqrt{N}} \nabla \cdot (\boldsymbol{\xi}(\mathbf{r}, t)) + \sqrt{\frac{2}{N}} \nabla \cdot \left(\frac{v}{1 - \frac{\bar{\gamma}}{2}} \boldsymbol{\eta} \right) \end{aligned}$$

Gas-liquid-like transitions in active matter

The previous equation can be rewritten as a Langevin eq. of the following form:

$$\frac{\partial \rho}{\partial t} = U[\rho](\mathbf{x}) + \frac{1}{\sqrt{N}} v(\mathbf{x}, t)$$

Where we define:

$$U[\rho](\mathbf{x}) = \frac{1}{2} \nabla \cdot \left(\frac{v(\rho)}{1 - \frac{\bar{\gamma}}{2}} \nabla [v(\rho)\rho] \right) + D_x \nabla^2 \rho$$

$$\langle v(x, y, t) v(x', y', t') \rangle = D[\rho](\mathbf{x}, \mathbf{x}') \delta(t - t')$$

and in addition:

$$b[\rho] = 2D_x \rho + \frac{\rho v^2(\rho)}{\left(1 - \frac{\bar{\gamma}}{2}\right)^2}$$

$$D[\rho](\mathbf{x}, \mathbf{x}') = \partial_x \partial_{x'} [b[\rho](\mathbf{x}) \delta(\mathbf{x} - \mathbf{x}')] + \partial_y \partial_{y'} [b[\rho](\mathbf{x}) \delta(\mathbf{x} - \mathbf{x}')]]$$

Gas-liquid-like transitions in active matter

We derive the associated FP for the previous Langevin equation:

$$\begin{aligned} \frac{\partial \mu_t}{\partial t} = & - \int d\mathbf{x} \frac{\delta}{\delta \rho(\mathbf{x})} (U[\rho](\mathbf{x}) \mu_t) \\ & + \frac{1}{2N} \int d\mathbf{x} \frac{\delta}{\delta \rho(\mathbf{x})} \left\{ \int d\mathbf{x}' D[\rho](\mathbf{x}, \mathbf{x}') \frac{\delta}{\delta \rho(\mathbf{x}')} \mu_t \right\} \end{aligned}$$

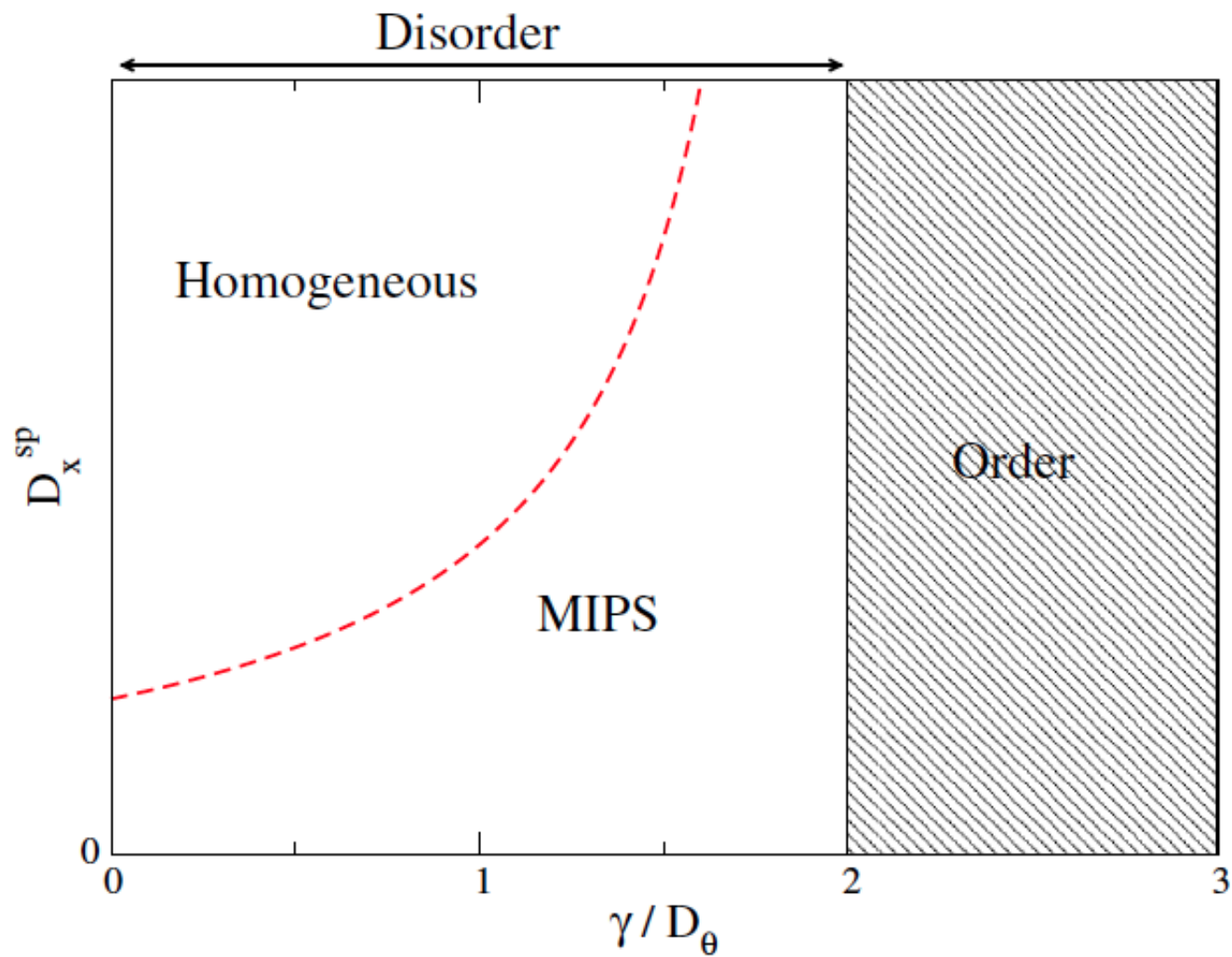
()We look for solution of the following type (formal solution of the previous eq.):

$$\mu[\rho] \sim e^{NS[\rho]} \longrightarrow S[\rho] = \int d\mathbf{x} s(\rho(\mathbf{x}))$$

After some calculations, we arrive at:

$$s''(\rho) = - \left(\frac{v^2(\rho) + \rho v(\rho) v'(\rho)}{\left(1 - \frac{\bar{v}}{2}\right) b[\rho]} + \frac{2D_x}{b[\rho]} \right)$$

Gas-liquid-like transitions in active matter



Summary

- 1. Definition of active soft-matter**
- 2. Examples in biology and non-living systems**
- 3. Minimal models of active particles**
- 4. Symmetries in active particle systems**
- 5. Gas-liquid-like transitions**



Thanks for you attention!