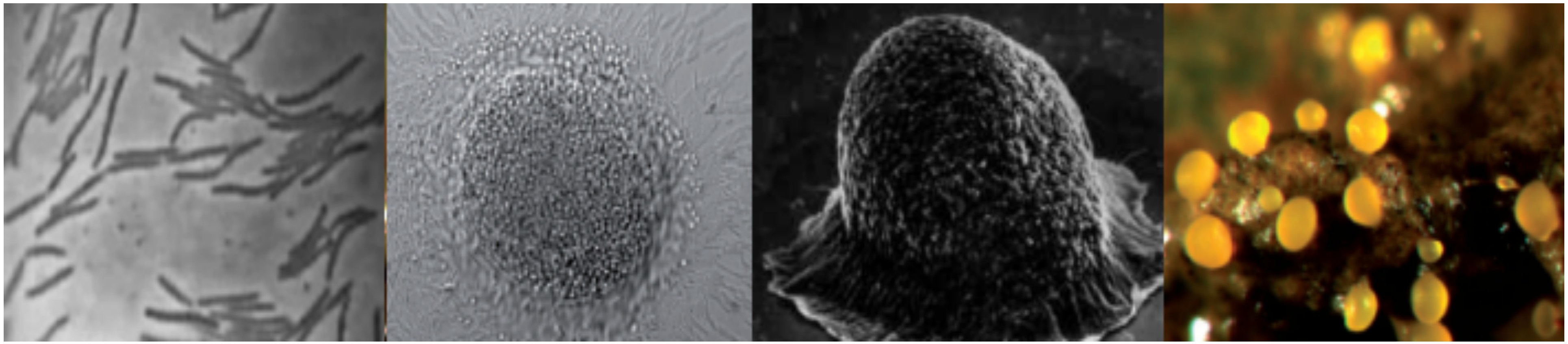
Active particles in heterogeneous media: quasi-long range order and sub-diffusion

Fernando Peruani

Bioacter14 - KITP – Santa Barbara – February 2014

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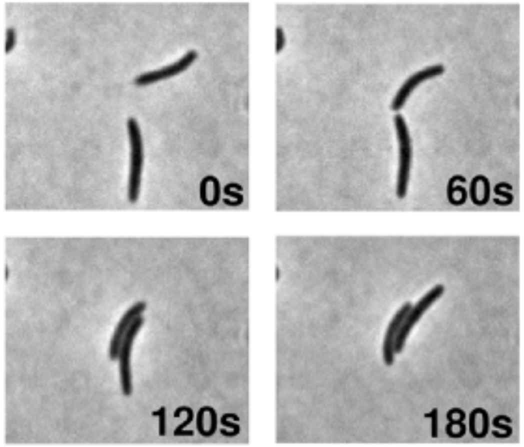
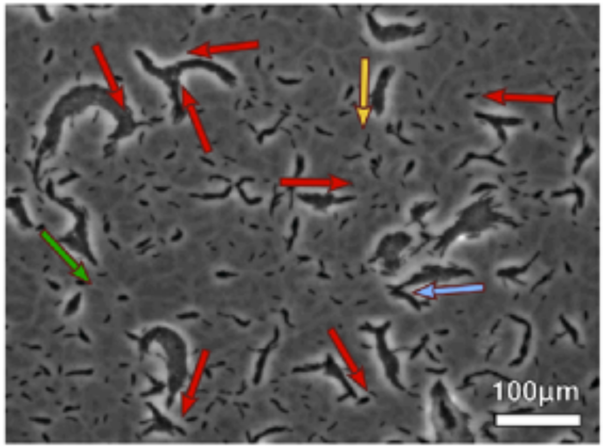
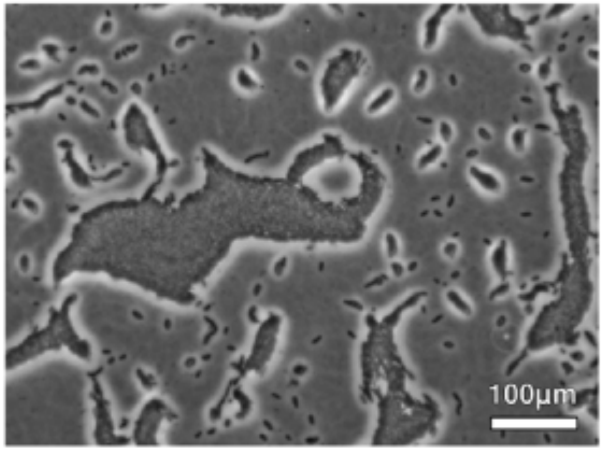
Motivation – bacteria & SP Rods

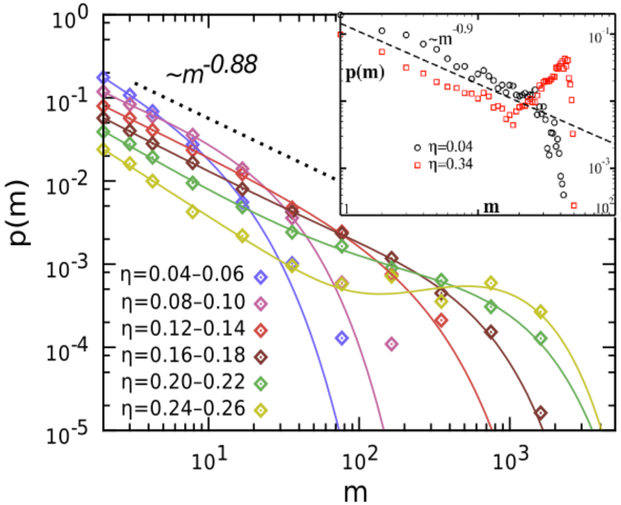
Bacteria as self-propelled liquid crystals

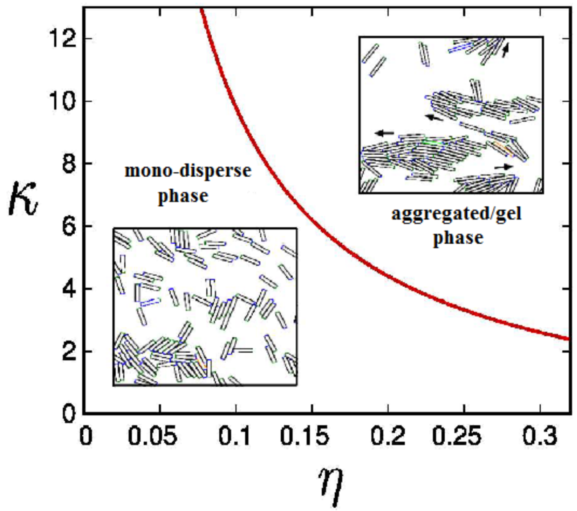
The behavior of real bacteria… (A+S-Frz- *M. xanthus* mutants)

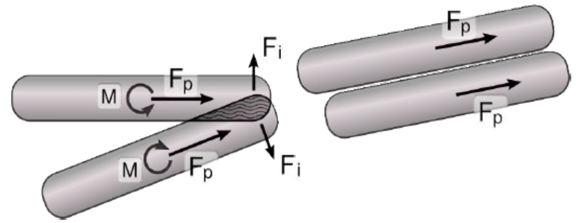












- Formation of polar clusters
- Collective movement
- Transition from an individ. to an aggregated phase

An old story that started in 2006 but that keeps on evolving…

FP et al., PRE 2006; PRL 2010; PRL 2012; NJP 2013; etc

Motivation – bacteria & SP Rods

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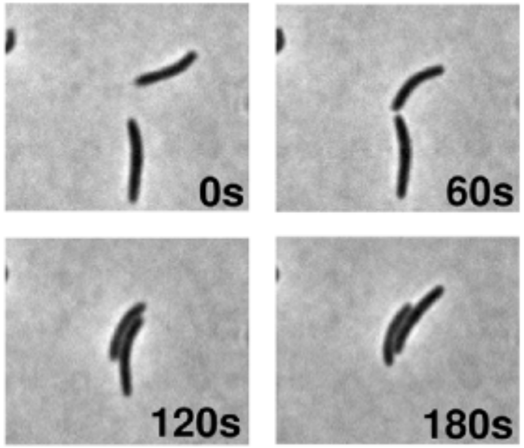
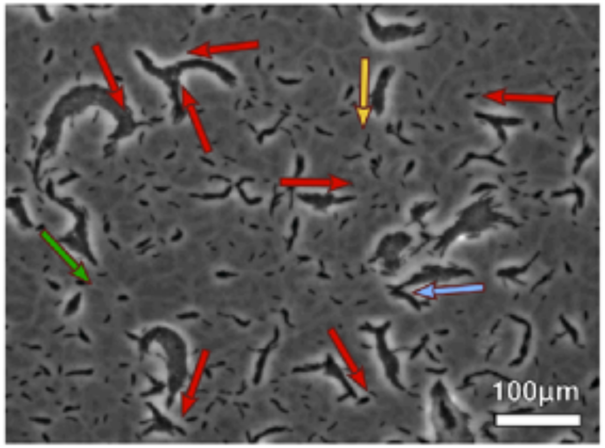
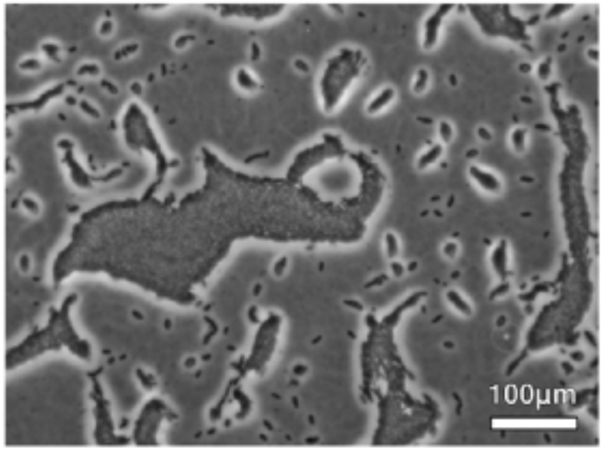
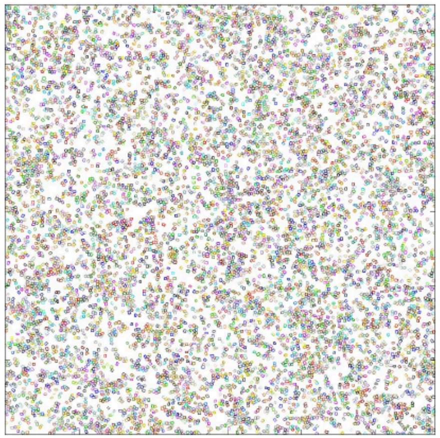
The behavior of real bacteria… (A+S-Frz- *M. xanthus* mutants)



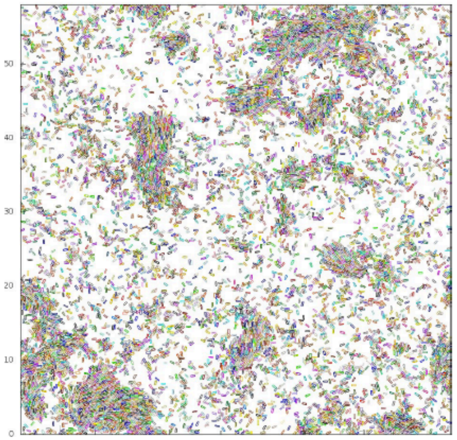




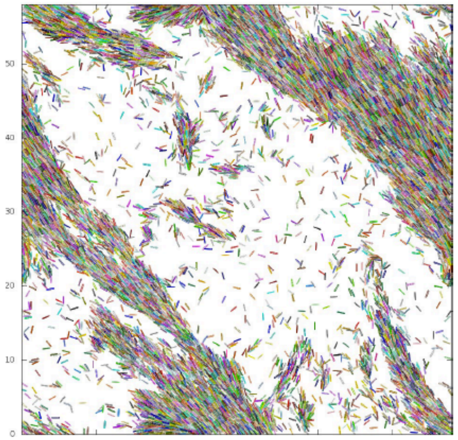
K=1



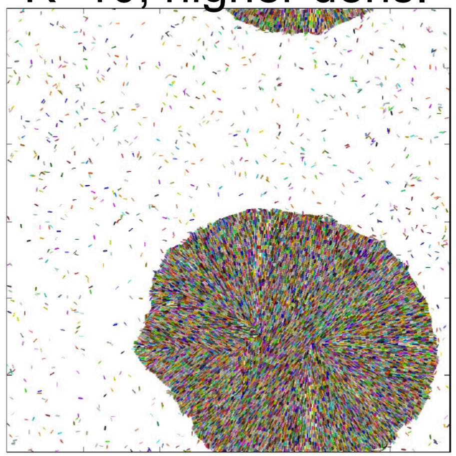
K=3



K=10



K=10, higher dens.



Results obtained in collaboration with S. Weitz

[35 min of this in Denver (Th., March 6, 11:51)]

FP et al., PRE 2006; PRL 2010; PRL 2012; NJP 2013; etc

Motivation

What is the most distinctive feature of an active particle?

The presence of some sort of engine.

Motivation

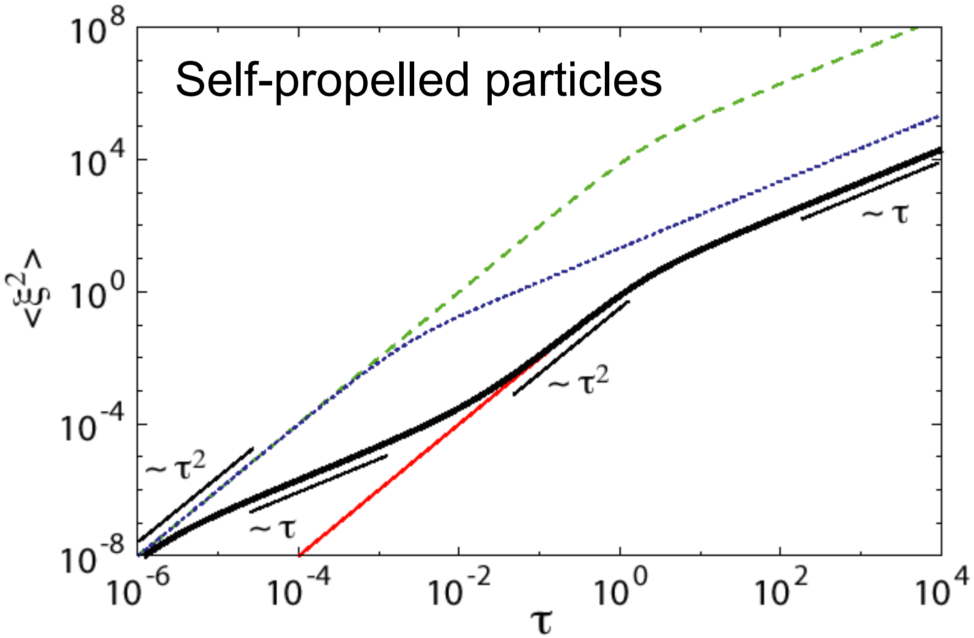
Active fluctuations

Active particles are subject to:

- **Thermal fluctuations**
- **“Active fluctuations”**

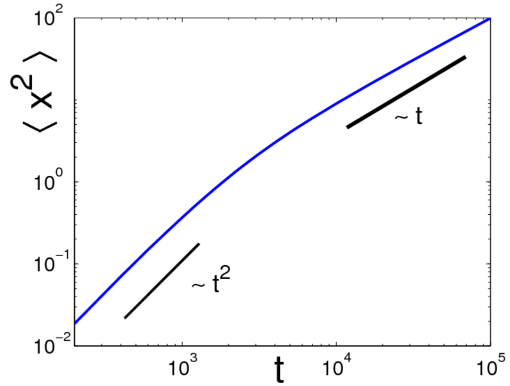
These are connected to the self-propulsion of the particles

Mean square displacement



+

Classical Brownian particles



Peruani and Morelli, PRL (2007)

Active fluctuations

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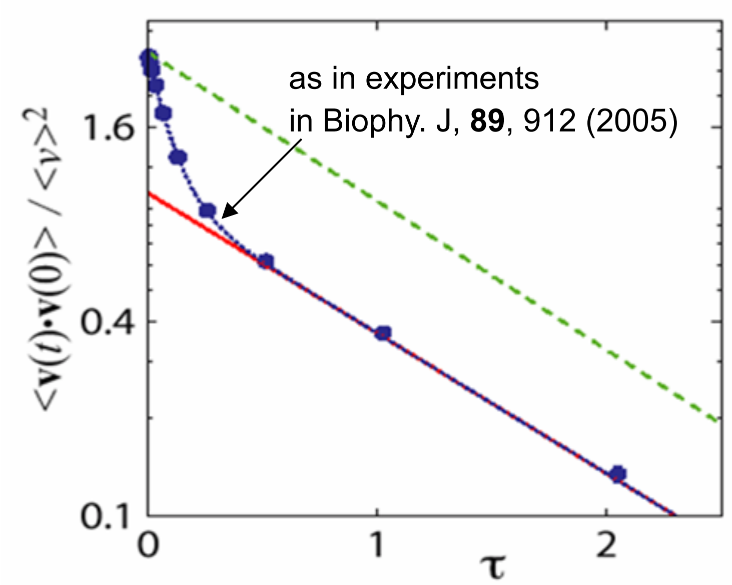


$$\langle \mathbf{x}^2(t)\rangle = 2\frac{\langle v\rangle^2}{\kappa^2}(\kappa t - 1 + e^{-\kappa t}) + 2\frac{\langle v^2\rangle - \langle v\rangle^2}{(\kappa+\beta)^2}((\kappa+\beta)t - 1 + e^{-(\kappa+\beta)t}).$$

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

Peruani and Morelli, PRL (2007)

An active “Lorentz” gas

Collective motion in heterogeneous media

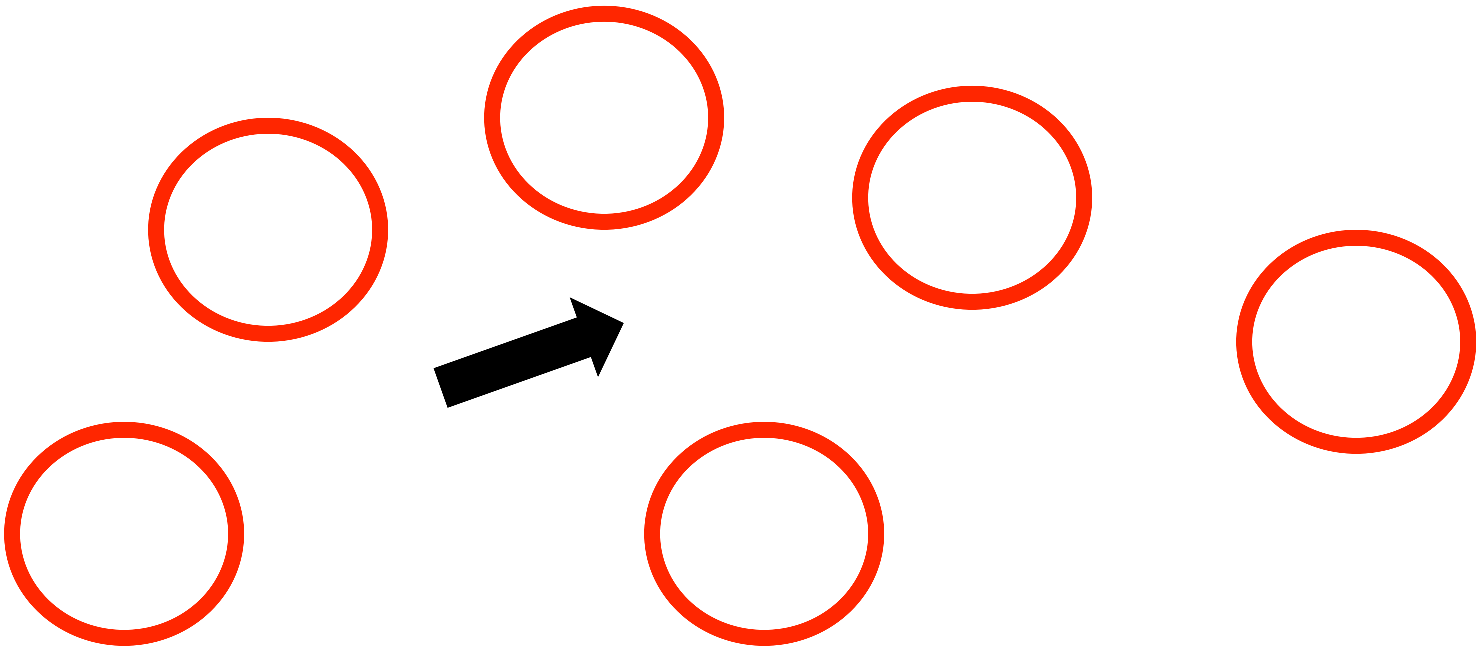
An active “Lorentz” gas

Motivation:

Bacteria as many other microorganism live in heterogeneous environments such as the soil or highly complex tissues such as in the gastrointestinal tract. But how is the behavior of an active particle in an heterogeneous environment? Should we expect something new?

Observation:

The lack of momentum conservation, plus the inherent persistence resulting from the self-propulsion of the active particles, can lead to new new interesting phenomena!



O. Chepizhko, F. Peruani, PRL (2013)

An active "Lorentz" gas

• **A simple model of active particles in heterogeneous media:**

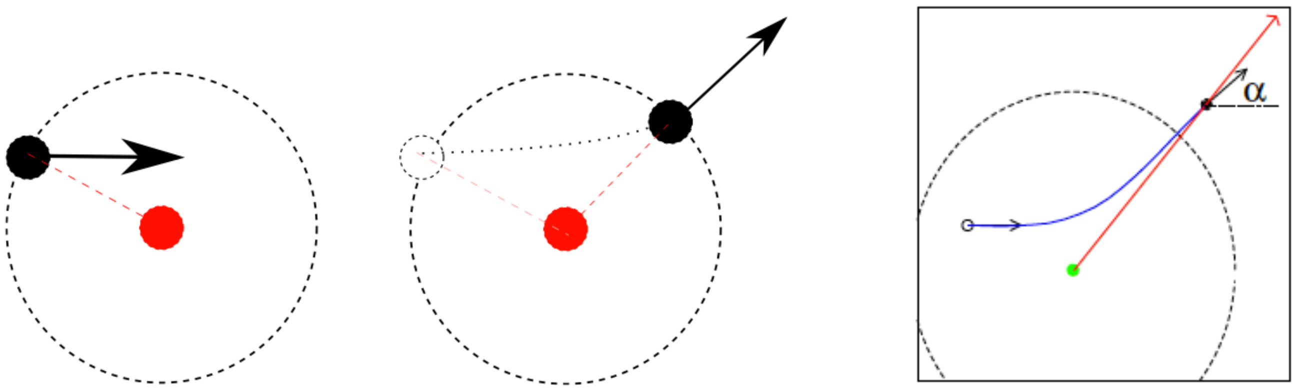
Equations of motion:

$$\begin{aligned} \dot{\mathbf{x}}_i &= v_0 \mathbf{V}(\theta_i) \\ \dot{\theta}_i &= h(\mathbf{x}_i) + \eta \xi_i(t) \end{aligned}$$

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

Interaction with "obstacles":

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

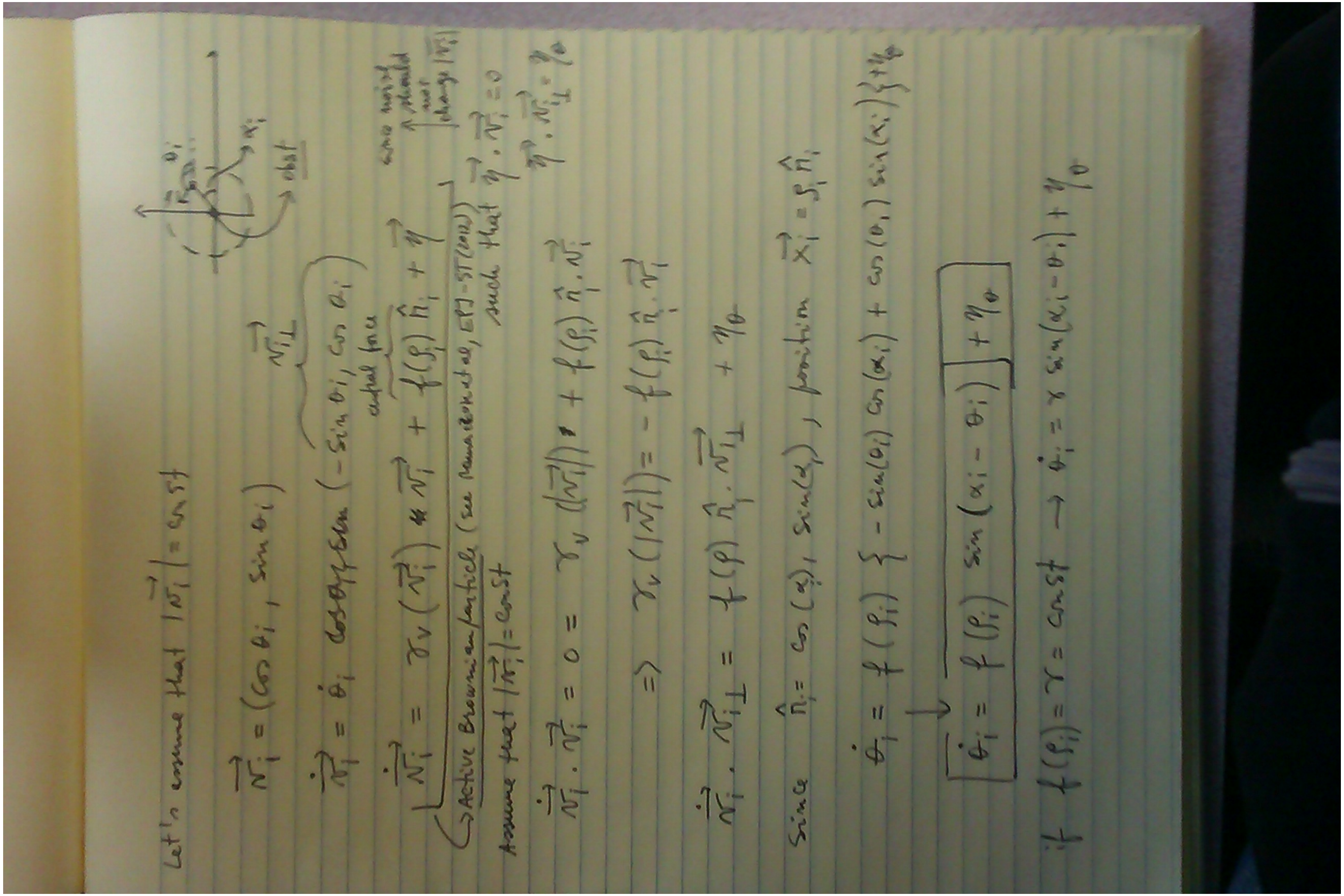


O. Chepizhko, F. Peruani, PRL (2013)

An active "Lorentz" gas

The next slide shows some simple (hand written) calculations that I added after my talk to clarify that a active particles moving at constant speed and being exposed to a (short-range) central force has to have the functional form (symmetry) of the model you showed you in the previous slide. Hope this clarify the issue. There is always a sin(\alpha - \theta) [we can add a minus or plus in order to have an attractive and repulsive central force]. Let me add that details at the level of the microscopic model (that not involve a change of symmetry or a new coupling such as density dependent speed, etc) should not have an impact on the resulting macroscopic behavior.

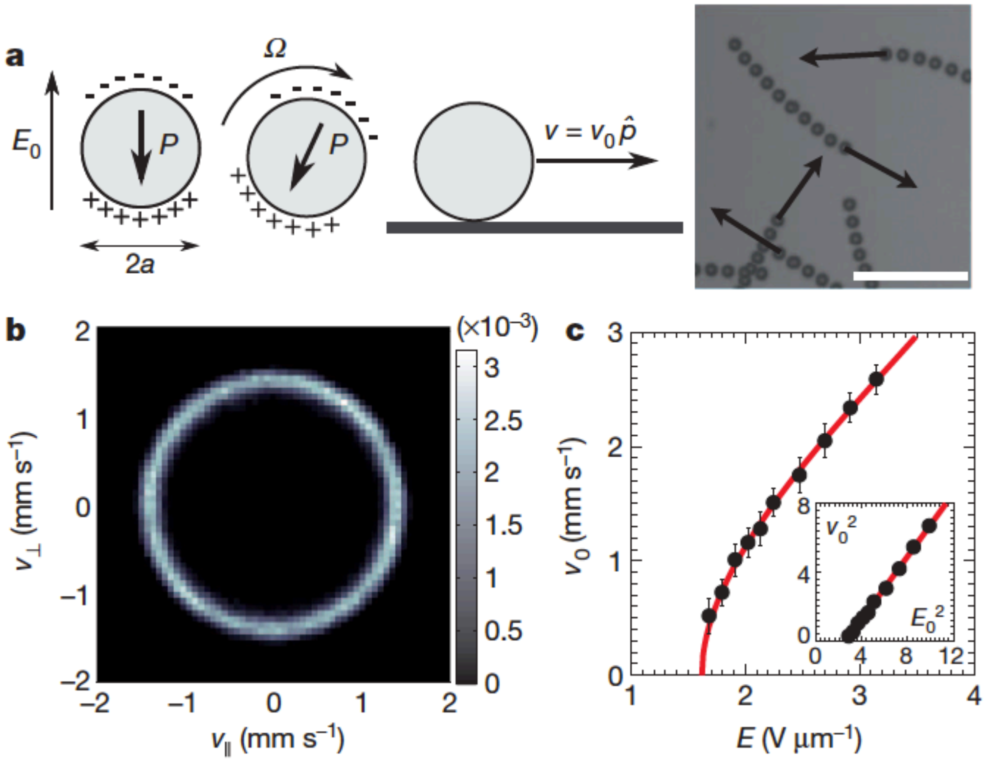
An active "Lorentz" gas



An active "Lorentz" gas

• **Is there a physical/biological realization of such a model?**

Quincke rollers!



$$\dot{r}_i = v_0 \hat{p}_i$$

$$\dot{\theta}_i = \frac{1}{\tau} \sum_{i \neq j} \frac{\partial}{\partial \theta_i} H_{\text{eff}}\left(r_i - r_j, \hat{p}_i, \hat{p}_j\right)$$

$$H_{\text{eff}}\left(r, p_i, p_j\right) = A(r)\hat{p}_i \cdot \hat{p}_j + B(r)\hat{p}_i \cdot \hat{r} + C(r)\hat{p}_i \cdot (2\hat{r}\hat{r} - I) \cdot \hat{p}_j$$

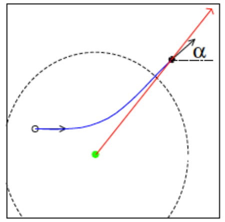
Bricard, Caussin, Desreumaux, Dauchot, Bartolo, Nature (2013)

Experiments with obstacles are being performed!

This will be very important for the second half of the talk.

An active “Lorentz” gas

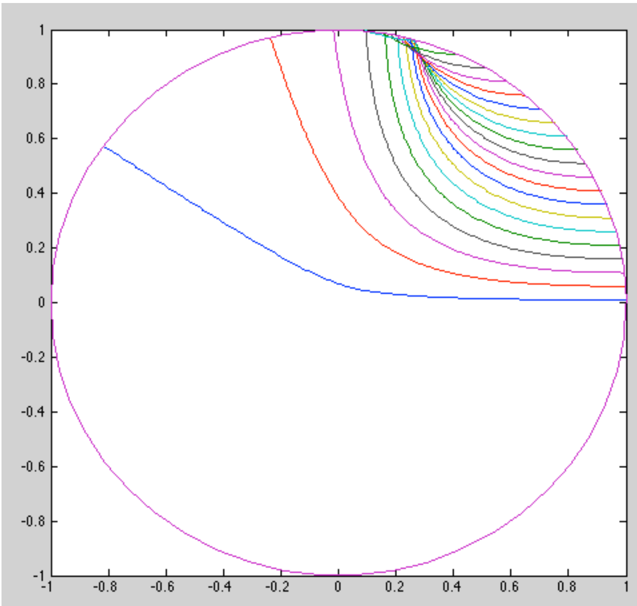
- **The scattering process:**



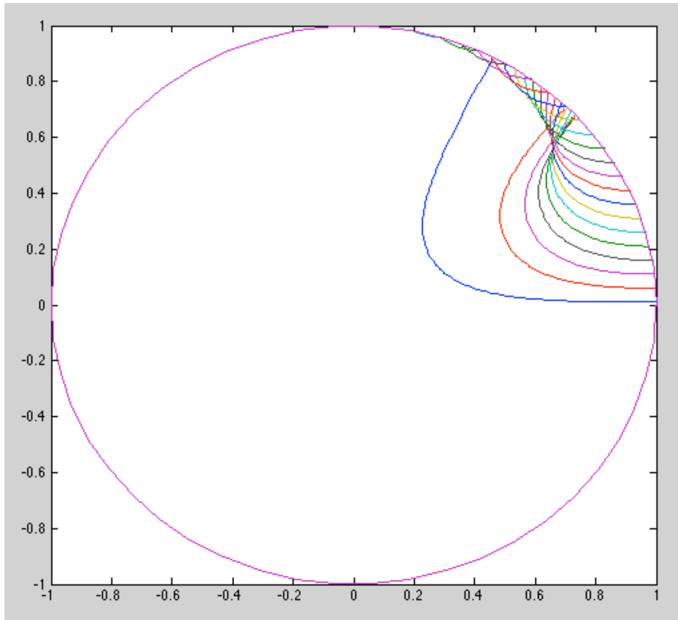
$$\dot{\mathbf{x}}_i = v_0 \mathbf{V}(\theta_i)$$

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

γ=1



γ=5

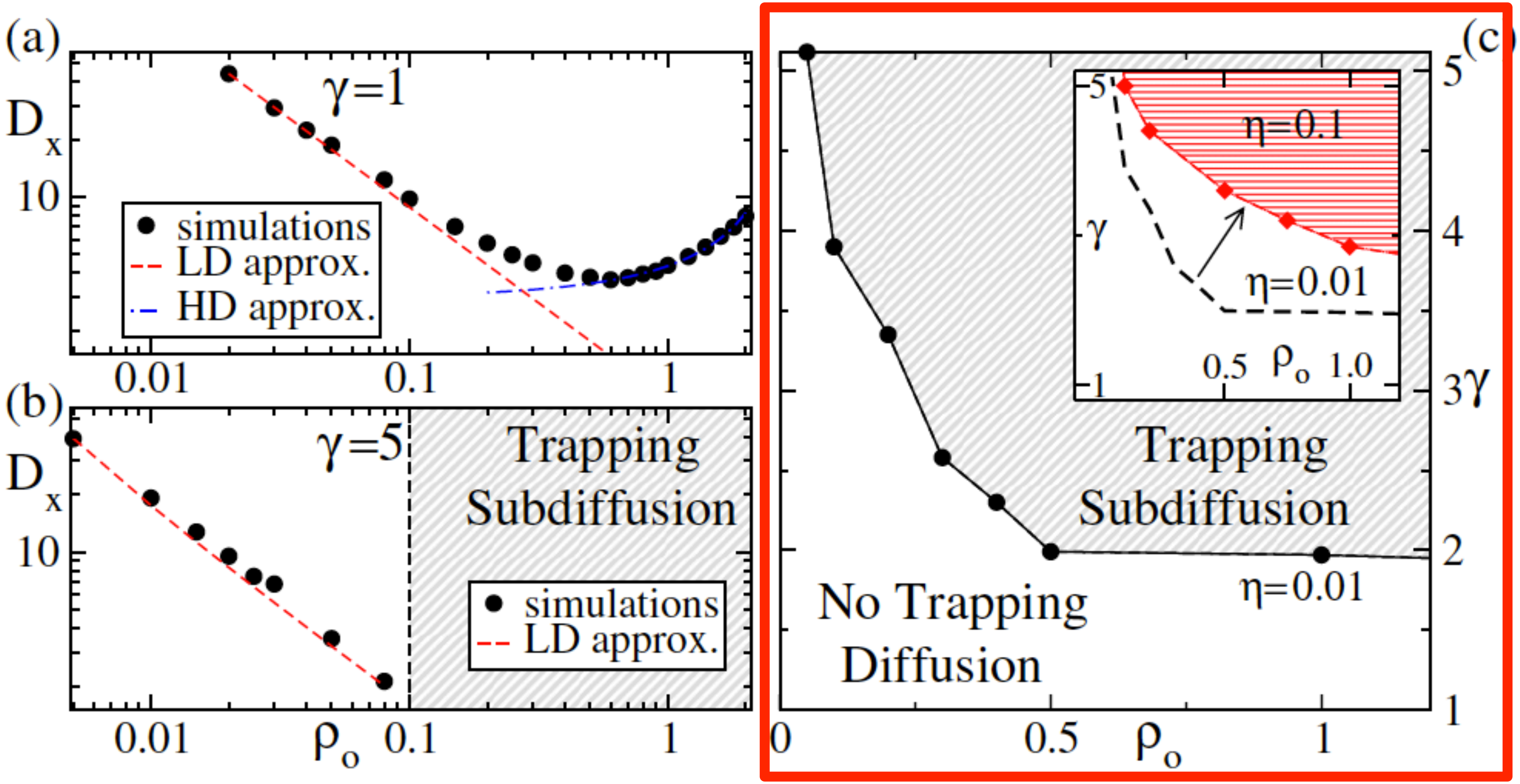


- The lack of angular momentum conservation prevents us from deriving an effective potential from where to compute, among other things, the maximum penetration distance.
- Another remarkable consequence of the lack of conserved quantities is the fact that scattered angle is no longer bijective with respect to the impact parameter.

An active “Lorentz” gas

- **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!

(These findings can be understood theoretically!)

An active "Lorentz" gas

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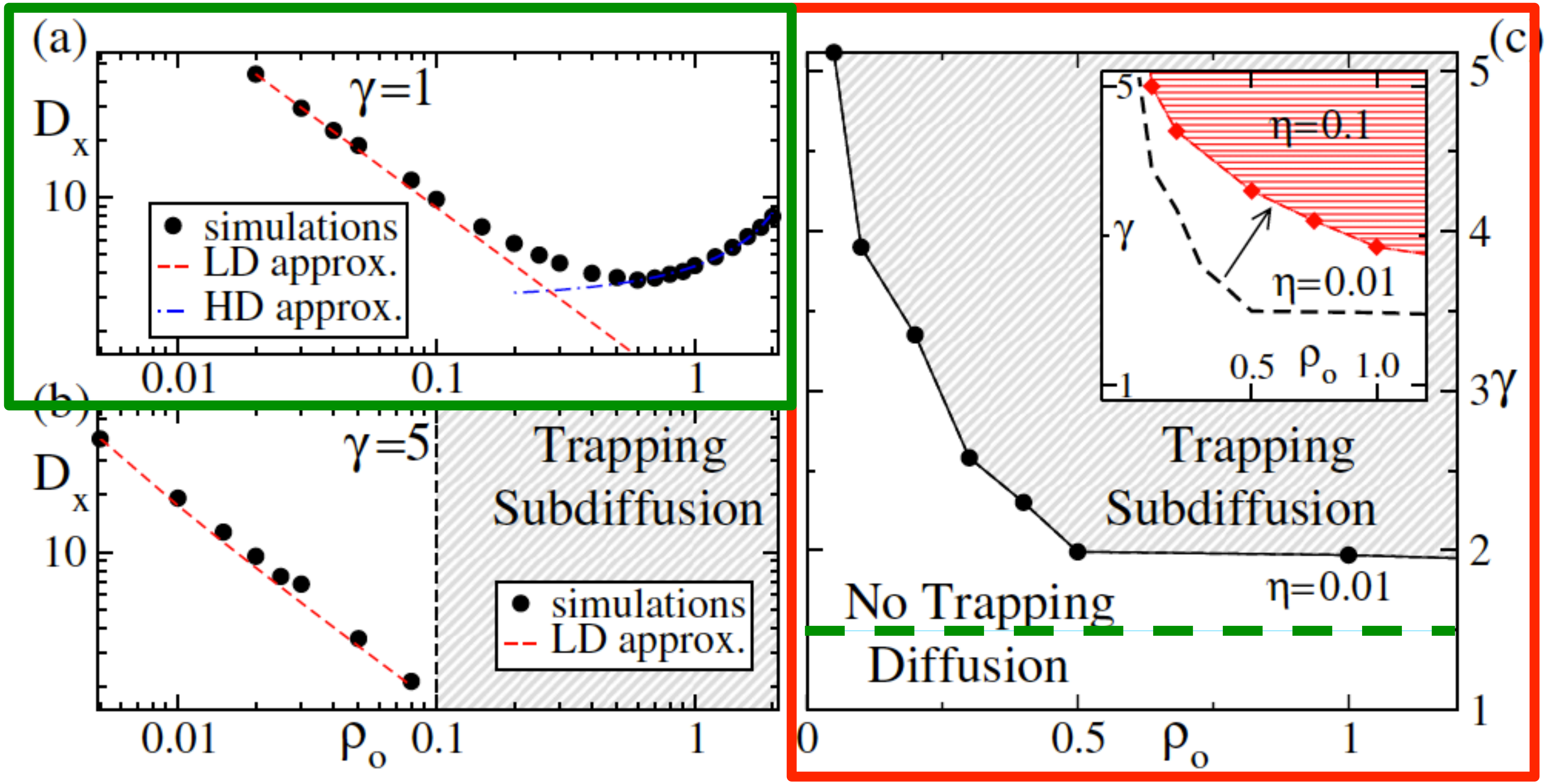

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An active "Lorentz" gas

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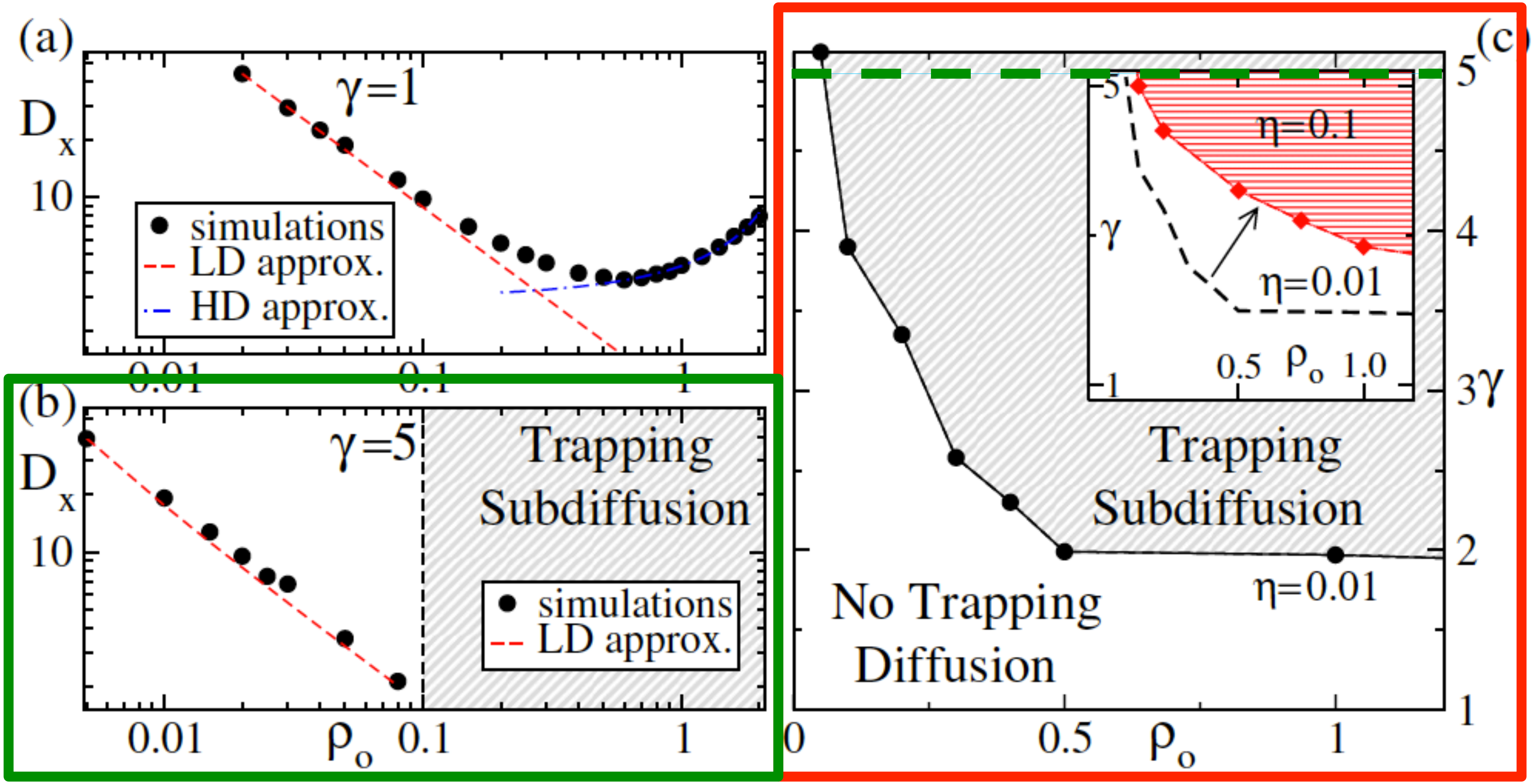

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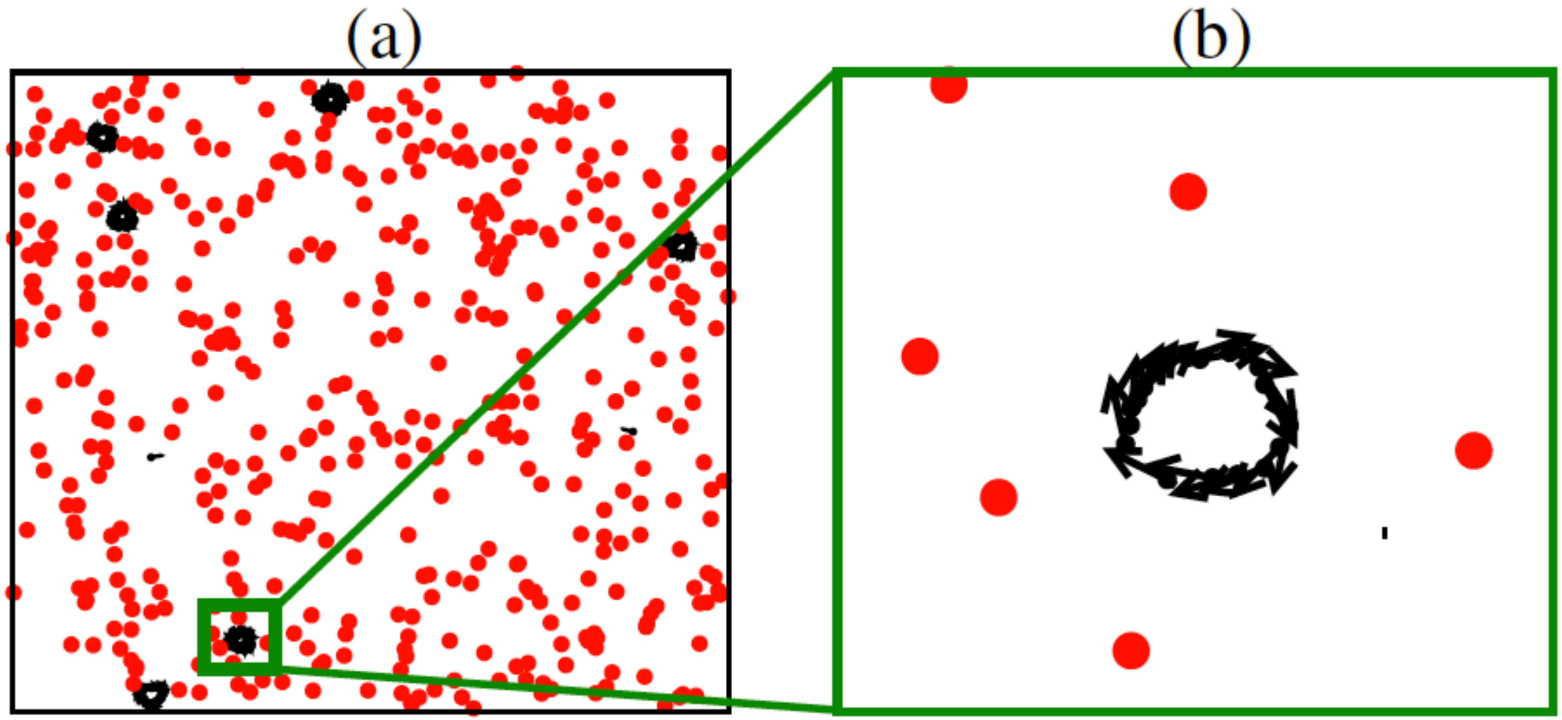
An active “Lorentz” gas

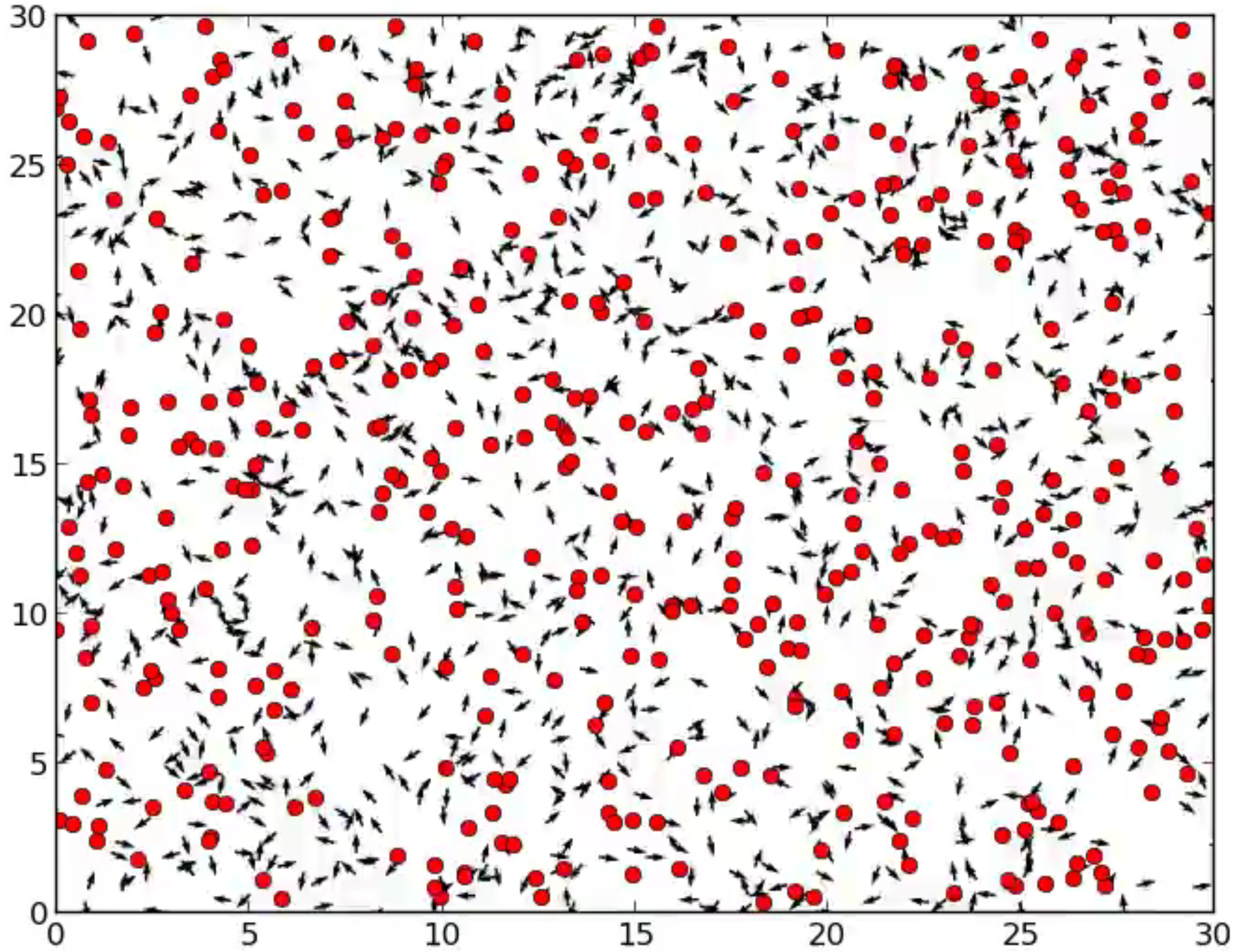
- **How is possible to trapped particles moving at constant speed?**



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

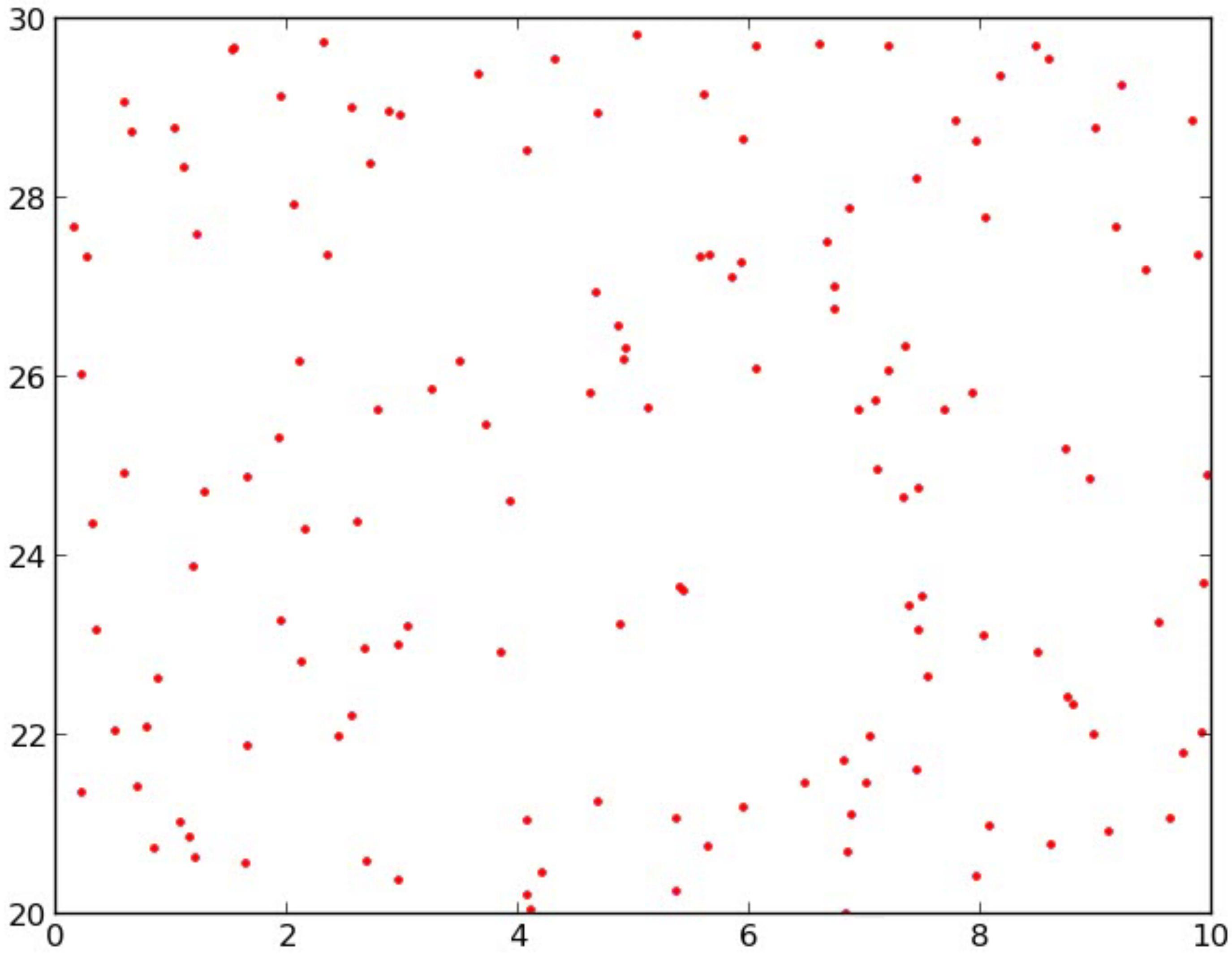
Remember that noise is present. These orbits are not absorbing, and particle can escape.

An active "Lorentz" gas



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

An active “Lorentz” gas



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

An active "Lorentz" gas

- **<u>How can we understand the observed behavior?</u>**

We look for a coarse-grained description of the problem in terms of $p(\mathbf{x}, \theta, t)$

whose temporal evolution can be expressed as:

$$\partial_t p + v_0 \nabla . [\mathbf{V}(\theta) p] = D_\theta \partial_{\theta\theta} p + F[p(\mathbf{x}, \theta, t), \rho_o(\mathbf{x})]$$

Interactions with obstacles

There are two limiting cases where F[.] can be specified:

- **<u>Low density (LD) approximation</u>**

- **<u>High density (HD) approximation</u>**

(with respect obstacle density)

An active "Lorentz" gas

• **<u>Low density (LD) approximation</u>**

We assume that ⟶ $D_\theta^{-1} v_0 >> \rho_o^{-1/2}$

↓

This implies that in between obstacles we can assume that particles move ballistically.

If we look at time-scales larger than R/v0, we can assume that the interactions with obstacles can be described as sudden jumps in the moving direction of the particle:

$$\begin{aligned} F[p] &= -\lambda(\rho_o)\, p(x,\theta,t) + \int_0^{2\pi} d\theta' T(\theta,\theta') p(x,\theta',t) \\ &\approx \frac{\lambda(\rho_o)\epsilon_\theta^2}{6} \partial_{\theta\theta} p\,, \end{aligned} \tag{5}$$

An active "Lorentz" gas

- **Low density (LD) approximation**

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$$\approx \frac{\lambda(\rho_o)\epsilon_\theta^2}{6} \partial_{\theta\theta} p\,, \qquad (5)$$

Top-hat simplification: $T(\theta,\theta';\mathbf{x}) \simeq \lambda(\rho_o) T(\theta,\theta') \approx [\lambda(\rho_o)/(2\epsilon_\theta)]\, \Theta(\epsilon_\theta - |\theta-\theta'|)$

where $\lambda(\rho_o) \approx v_o \rho_o \sigma_o$ and $\sigma_o = 2R$

An active "Lorentz" gas

- **Low density (LD) approximation**

We define $\longrightarrow$ $$\tilde{D}_\theta = D_\theta + \lambda(\rho_o)\epsilon_\theta^2/6$$

and perform a moment expansion by using:

$$\begin{aligned} P_x(\mathbf{x},t) &= \int d\theta \cos(\theta) p \quad & Q_s(\mathbf{x},t) &= \int d\theta \sin(2\theta) p \\ P_y(\mathbf{x},t) &= \int d\theta \sin(\theta) p \quad & Q_c(\mathbf{x},t) &= \int d\theta \cos(2\theta) p \end{aligned}$$

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

This allows us to rewrite the previous 4-variable equations as a system of 3-variable equations:

$$\begin{aligned} \partial_t \rho &= -v_0 \nabla.\mathbf{P} \\ \partial_t P_x &= -\frac{v_0}{2}\nabla.\left[Q_c + \rho, Q_s\right] - \tilde{D}_\theta P_x \\ \partial_t P_y &= -\frac{v_0}{2}\nabla.\left[Q_s, \rho - Q_c\right] - \tilde{D}_\theta P_y \end{aligned}$$

Since there is no induced order (neither ferromagnetic nor nematic), we close the system by assuming: $\partial_t Q_c = \partial_t Q_s = 0$ and $Q_c = Q_s = 0$

An active "Lorentz" gas

• **Low density (LD) approximation**

Under all these assumptions, we arrive to the following asymptotic equation for ρ(x,t):

$$\partial_t \rho = \nabla . \left[\frac{v_0^2}{2\tilde{D}_\theta} \nabla \rho \right]$$

$$D_x = v_0^2 / \left[2 \left(D_\theta + \Lambda_0 \rho_o \right) \right]$$

$$\Lambda_0 = v_0 \sigma_0 \epsilon_\theta^2 / 6$$

An active “Lorentz” gas

• **High density (HD) approximation**

At high obstacle densities, active particles sense always several obstacle around them, which forces us to leave the Boltzmann-like for the Fokker-Planck approach.

At high obstacle densities, the interaction with obstacles can then be modeled as:

$$F = \partial_\theta \left[I p(\mathbf{x}, \theta, t) \right]$$

where I is the average “torque” felt by a particle at (x,θ), which takes the form:

$$I = \frac{\gamma}{n(\mathbf{x})} \sum_j \sin(\theta - \alpha_j) = \frac{\gamma \Gamma(\mathbf{x})}{n(\mathbf{x})} \sin(\theta - \psi(\mathbf{x}))$$

Applying the usual tricks as for Kuramoto model.

An active “Lorentz” gas

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Since obstacles are located at random, this is equivalent to summing n(x) random vectors!

An active "Lorentz" gas

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Replacing the above sum by its average, we can express:

$$I \sim \sin(\theta - \psi(\mathbf{x}))/\sqrt{n}$$ where $n \approx \pi R^2 \rho_o$

An active "Lorentz" gas

• **High density (HD) approximation**

After performing the moment expansion procedure used for the LD approximation, we arrive to:

$$\begin{aligned}\partial_t \rho &= \frac{v_0^2}{2D_\theta}\nabla^2\rho - \frac{\gamma v_0}{2D_\theta R\sqrt{\pi\rho_0}}\nabla.\left[(\cos(\psi),\sin(\psi))\rho\right] \\ &= \frac{v_0^2}{2D_\theta}\nabla^2\rho - \frac{\gamma v_0}{2D_\theta R\sqrt{\pi\rho_0}}\nabla.\left[\frac{\rho\nabla\rho_o(\mathbf{x})}{||\nabla\rho_o(\mathbf{x})||}\right], \quad (11)\end{aligned}$$

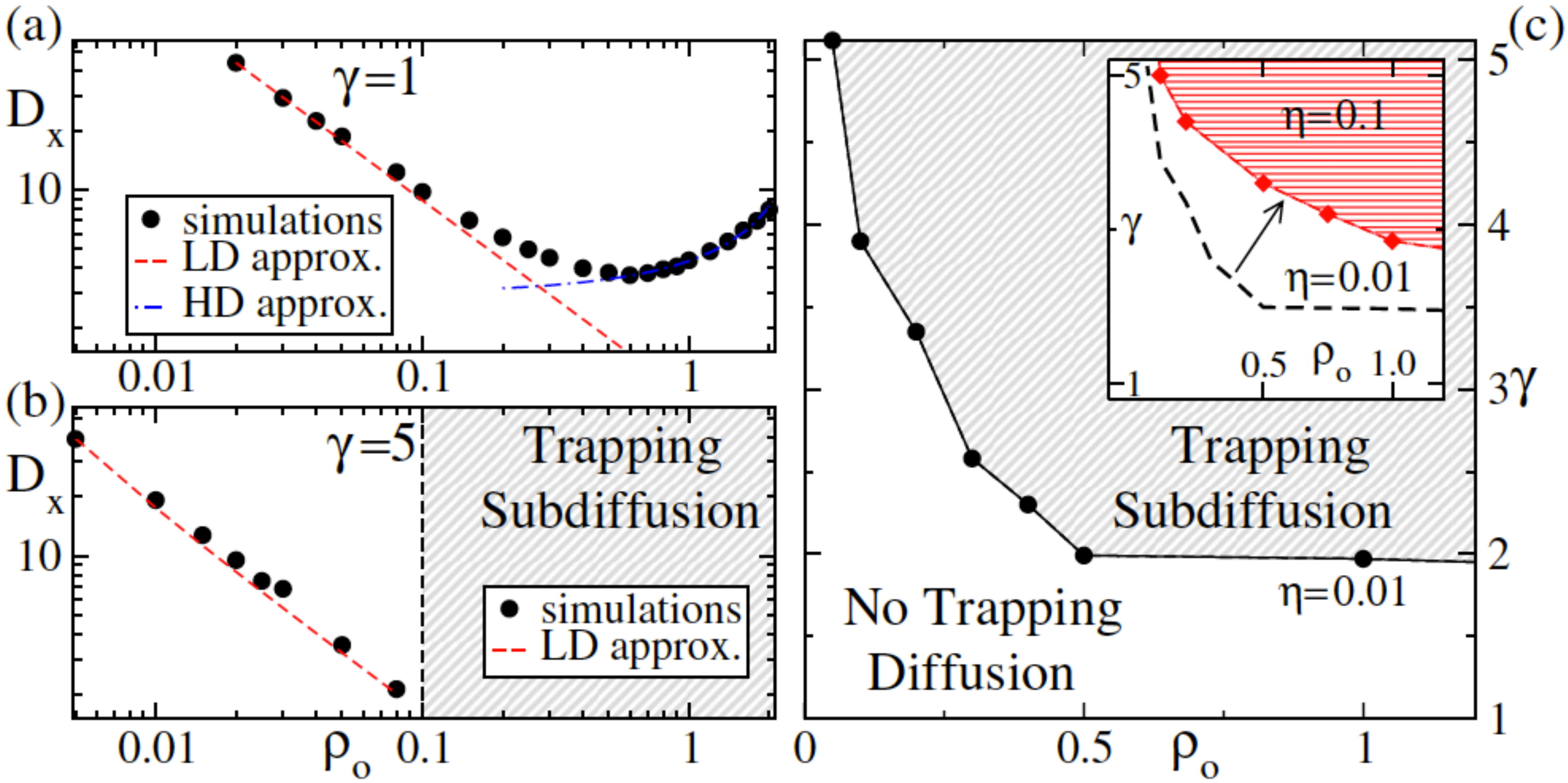
From this we learn two important things:

- **The convective term dominates the asymptotic dynamics of ρ.**
- **As the density of obstacles increases, the diff. coeff. increase.**

$$D_x \sim 1/\left[\rho_c - \Lambda_1 \rho_o\right]$$

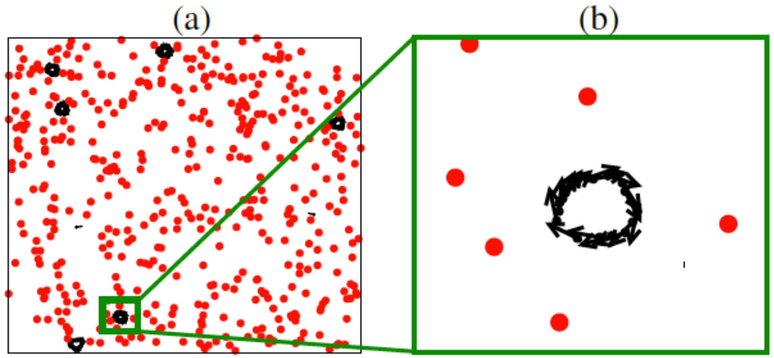
An active "Lorentz" gas

- **Comparison between the LD and HD and simulations**



An active "Lorentz" gas

- **Why do we observe subdiffusion?**



$$\sigma^2(t) = \langle \mathbf{x}^2(t) \rangle$$

If we imagine an array of traps, the MSD has to be proportional to the number of jumps made according to the CLT.

$$\sigma^2(t) \propto n_J(t)$$

→ The problem reduces to know how many jumps our particle performs during t !

If every trap is characterized by an average $<\tau_t>$, this is simply $t/<\tau_t>$

An active “Lorentz” gas

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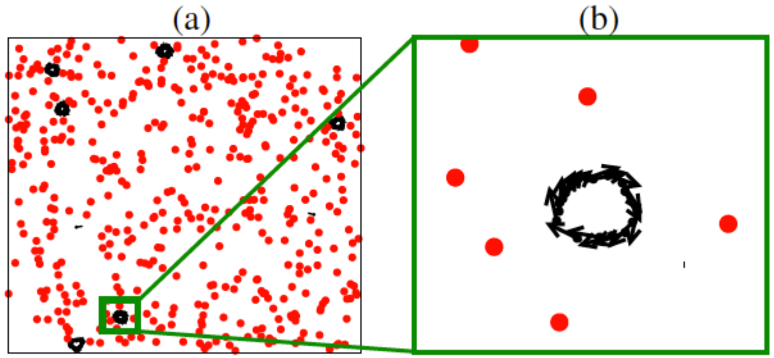
If we imagine an array of traps, the MSD has to be proportional to the number of jumps made according to the CLT.



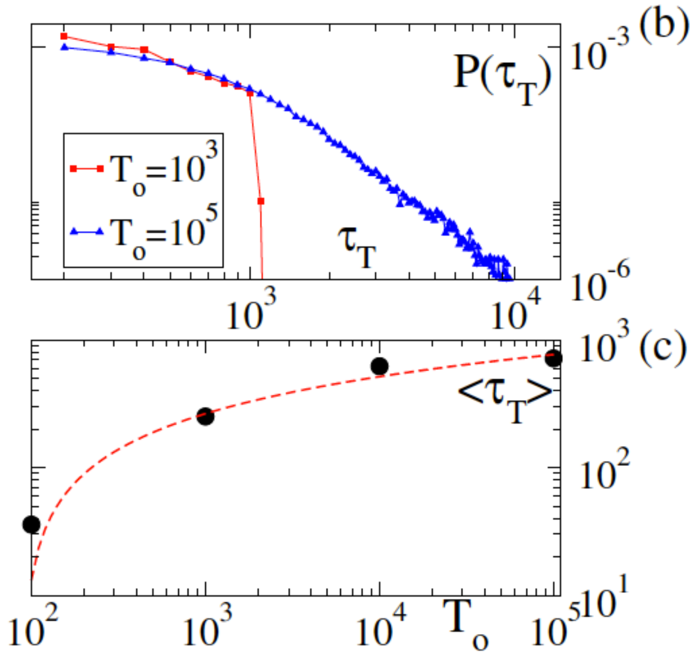
$$\sigma^2(t) \propto n_J(t)$$

The problem reduces to know how many jumps our particle performs during t !

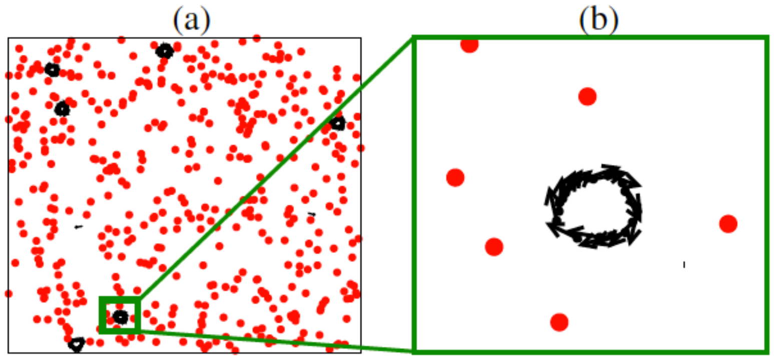
If every trap is characterized by an average $<\tau_t>$, this is simply $t/<\tau_t>$

• **Measurement on** $<\tau_t>$

$<\tau_t>$ depends on the observation time !!!



An active "Lorentz" gas



- **<u>Why do we observe subdiffusion?</u>**

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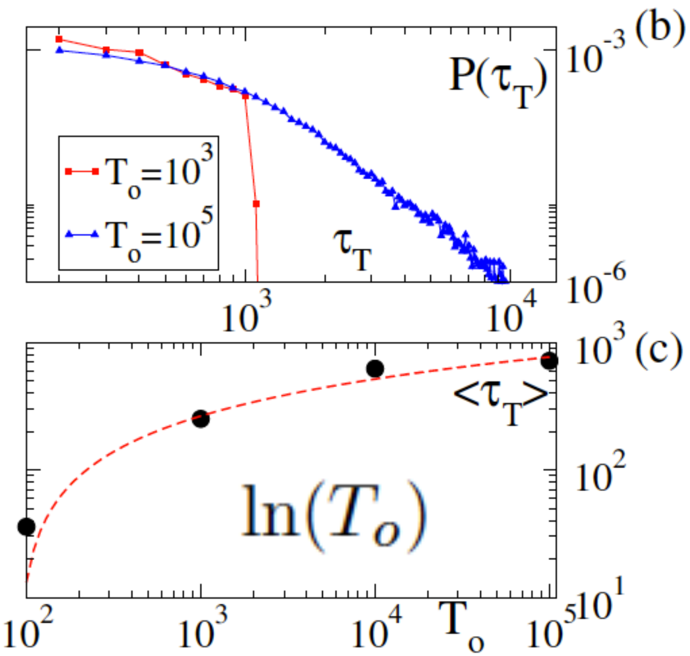

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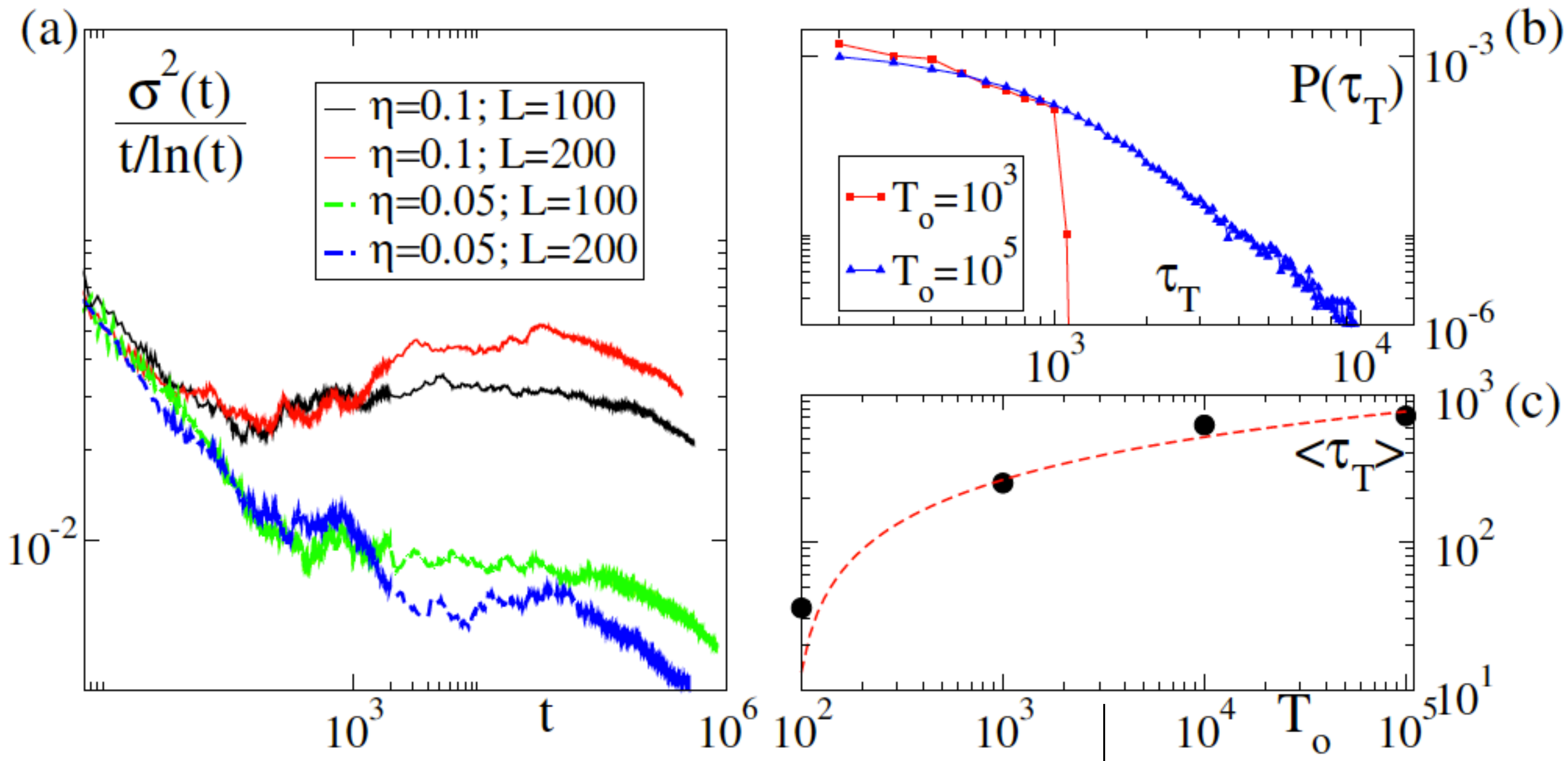

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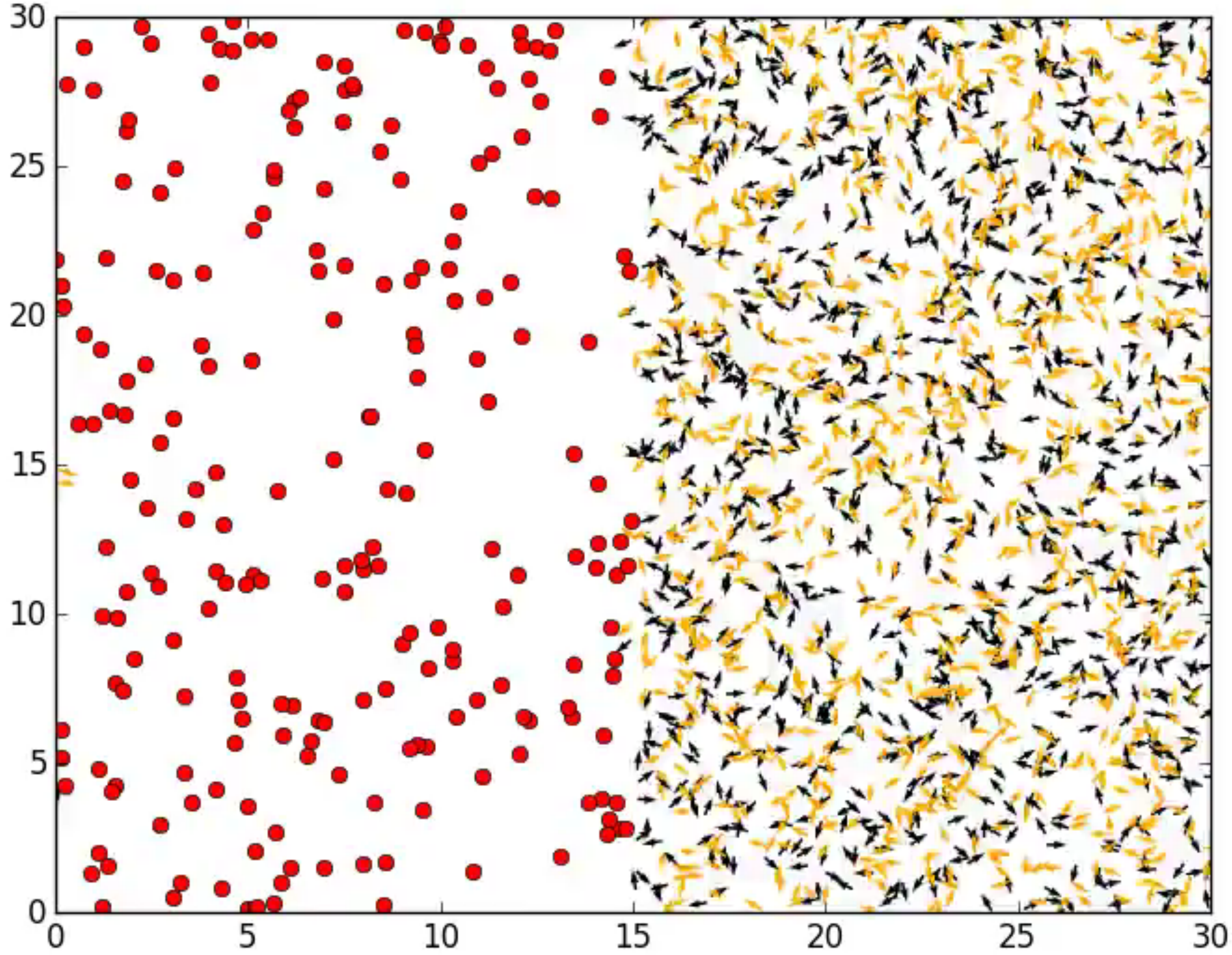
An active "Lorentz" gas

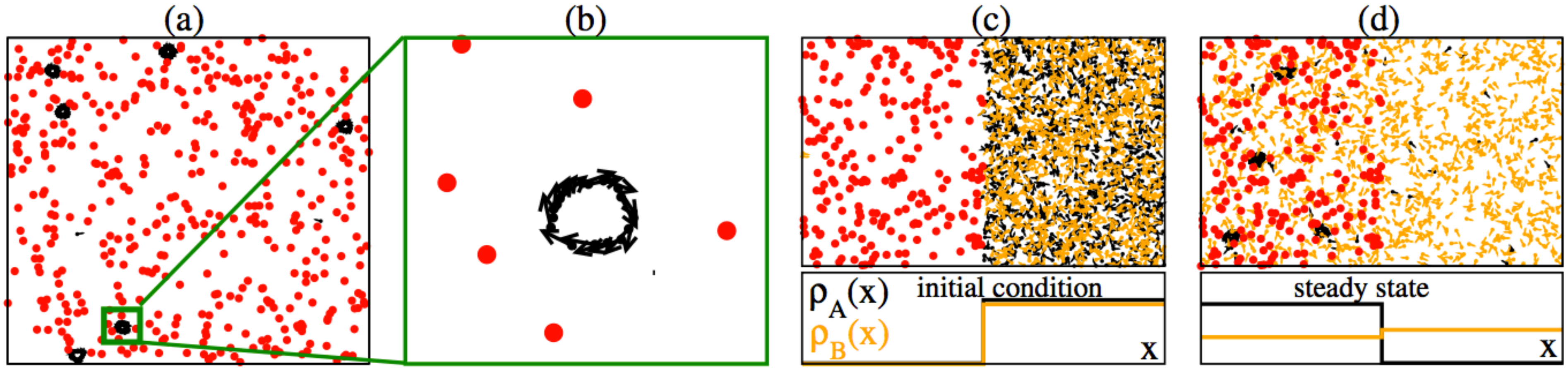
- **Filtering**

$\gamma_A > \gamma_B$



An active “Lorentz” gas

• **We can use the traps to fabricate a filter of SPPs!** $\gamma_A > \gamma_B$



Results:

- The diffusion coefficient exhibits a minimum with obstacle density (small γ)
- Spontaneous trapping of particles (moving at constant speed) occurs
- Trapping leads to subdiffusive behavior
- These fact can be used to fabricate a filter of active particles!

O. Chepizhko, F. Peruani, PRL (2013)

Collective motion in heterogeneous media

-- Adding particle-particle (p-p) interactions --

Motivation:

Does the environment have an impact on the collective behavior?

O. Chepizhko, E. Altmann, F. Peruani, PRL (2013)

Collective motion in heterogeneous media

- **A minimal continuum time SPP model with obstacles:**

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

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

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

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

O. Chepizhko, E. Altmann, FP, Phys Rev Lett (2013)

Collective motion in heterogeneous media

- **A minimal continuum time SPP model with obstacles:**

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

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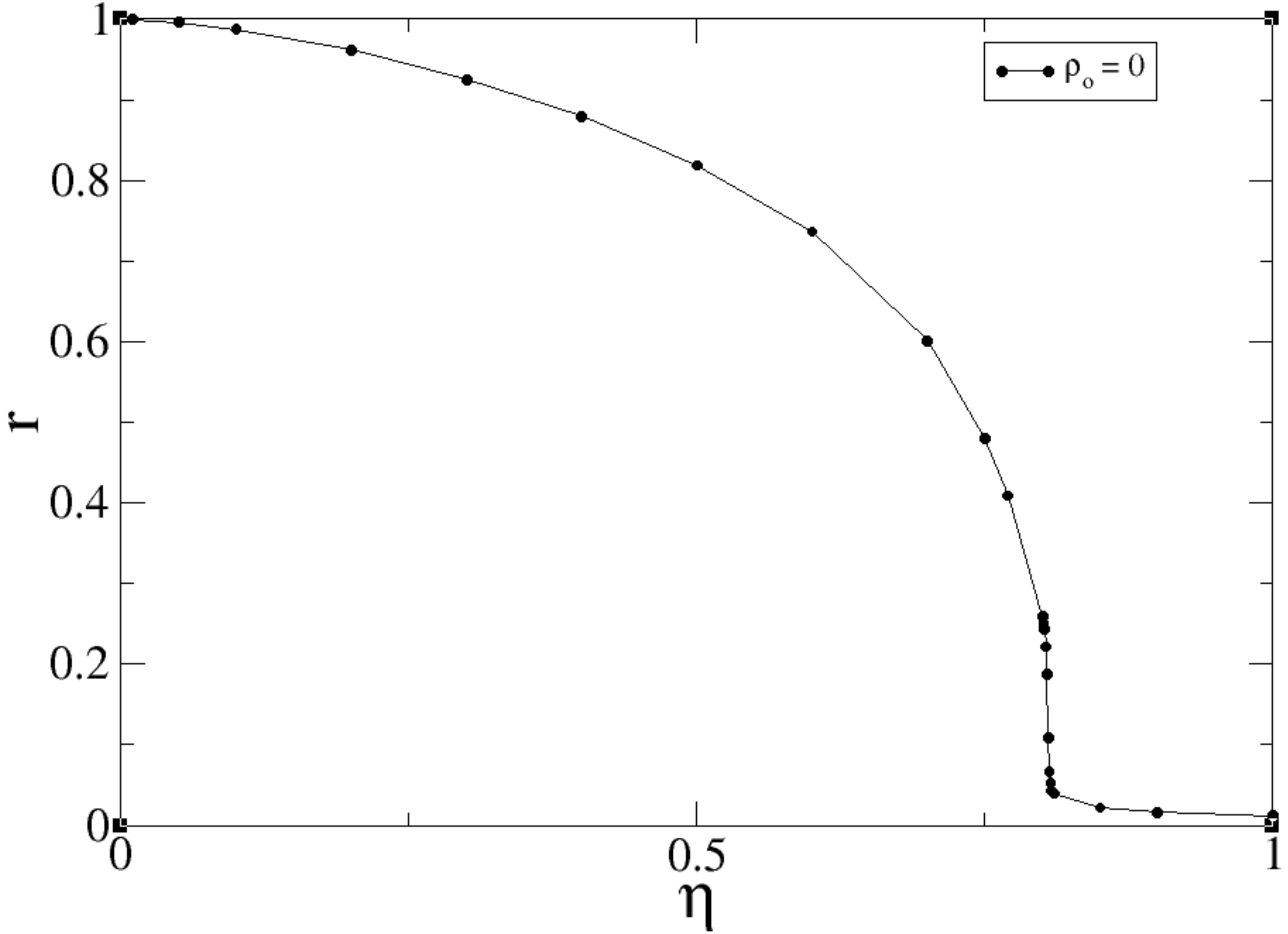
Order parameter → $r = \langle r \rangle_t = \langle \left| \frac{1}{N_b} \sum_{i=1}^{N_b} e^{i\theta_i(t)} \right| \rangle_t$ [equiv. to the magnetization]

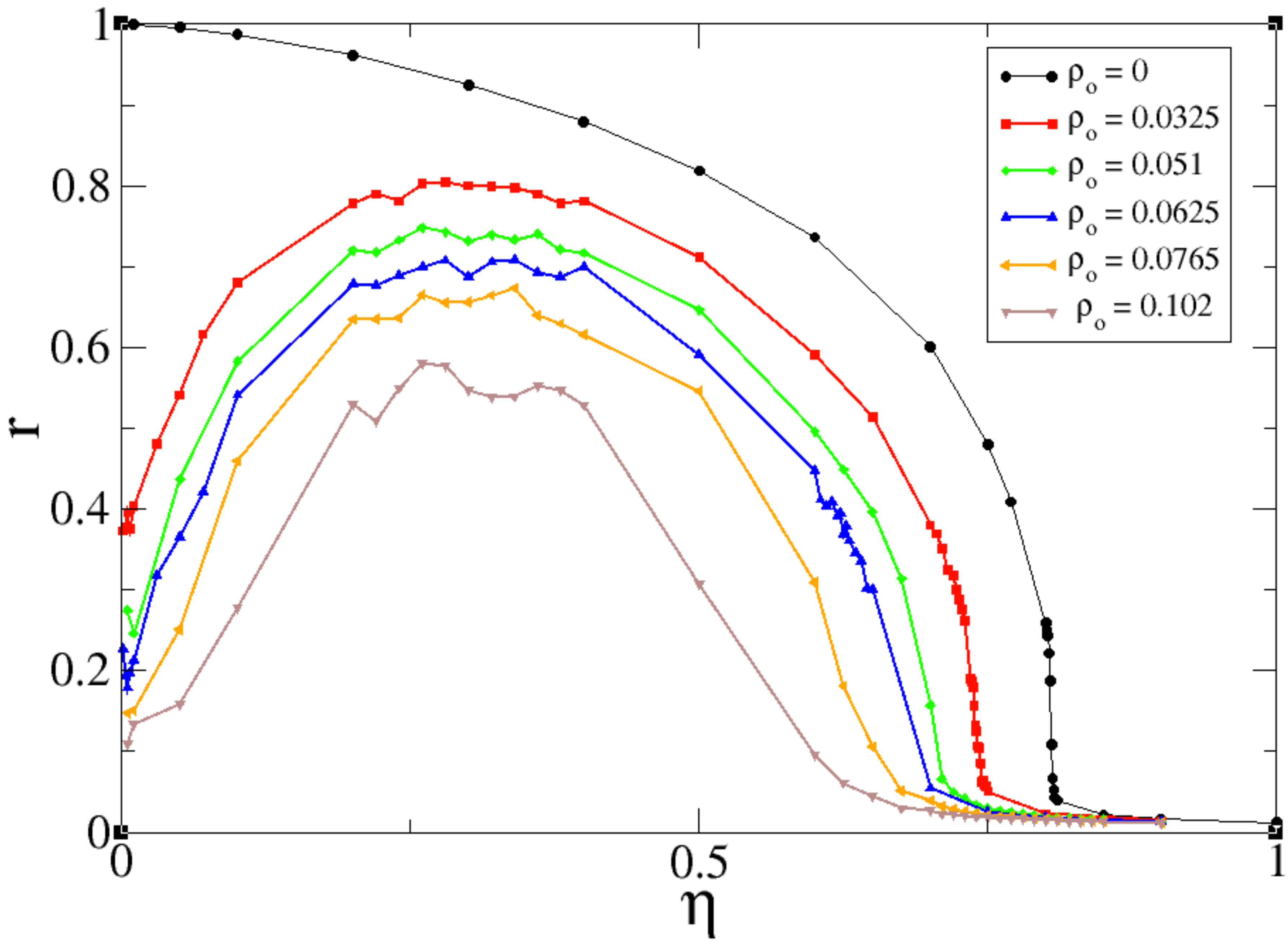
Susceptibility → $\chi = \langle (r(t) - r)^2 \rangle_t$

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

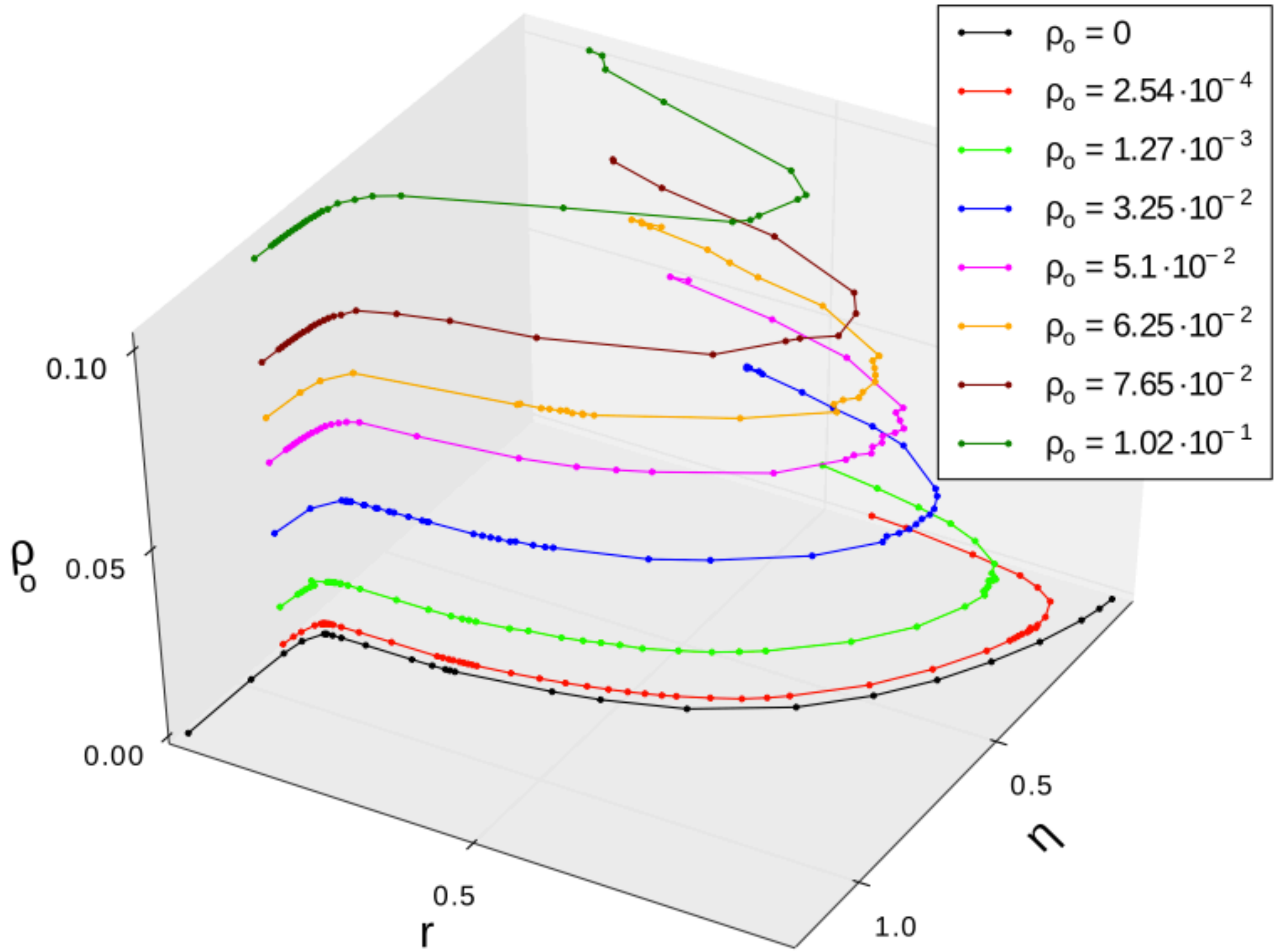
Collective motion in heterogeneous media



Collective motion in heterogeneous media



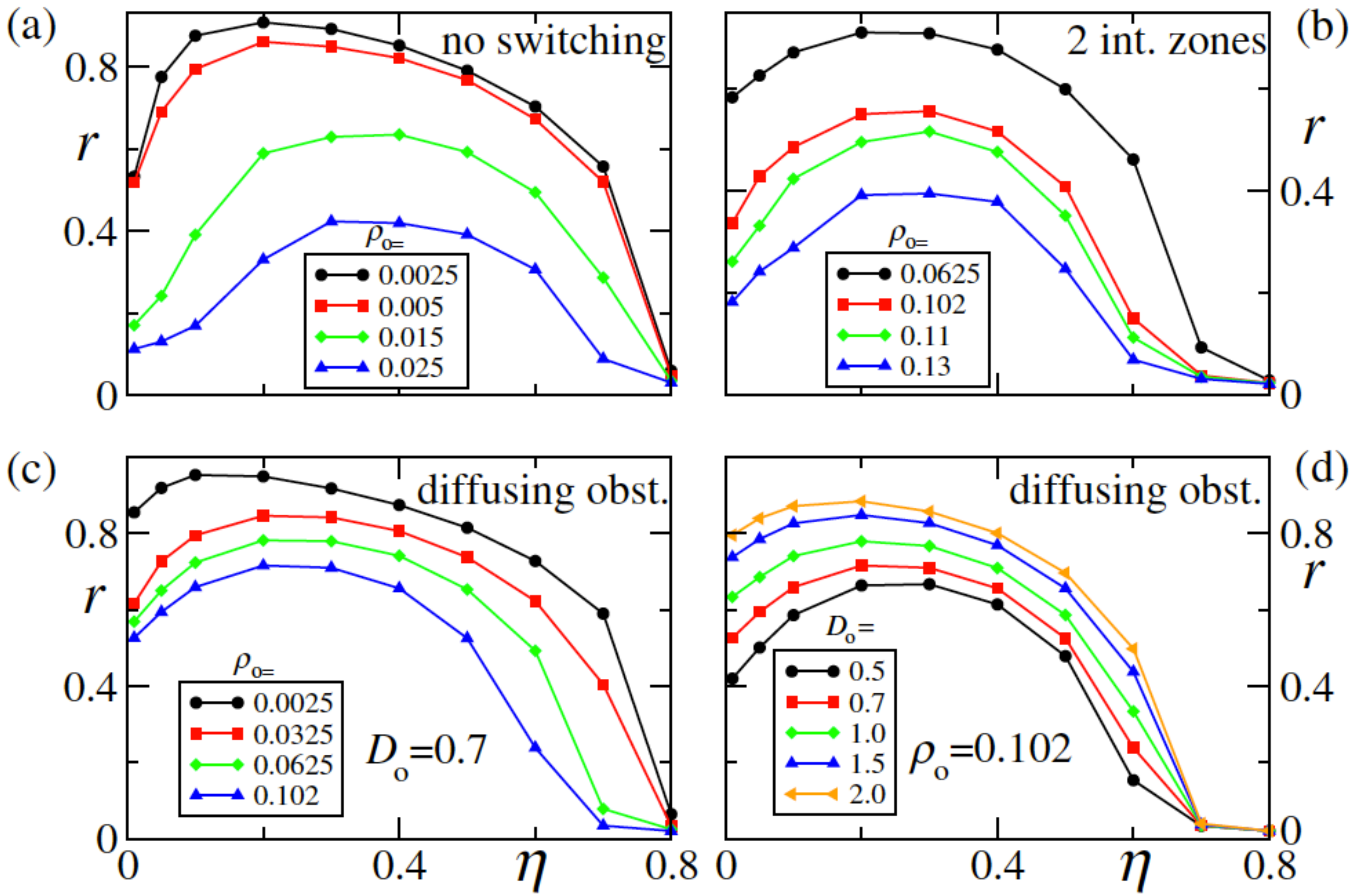
Collective motion in heterogeneous media



There is an optimal noise value that maximizes collective motion !

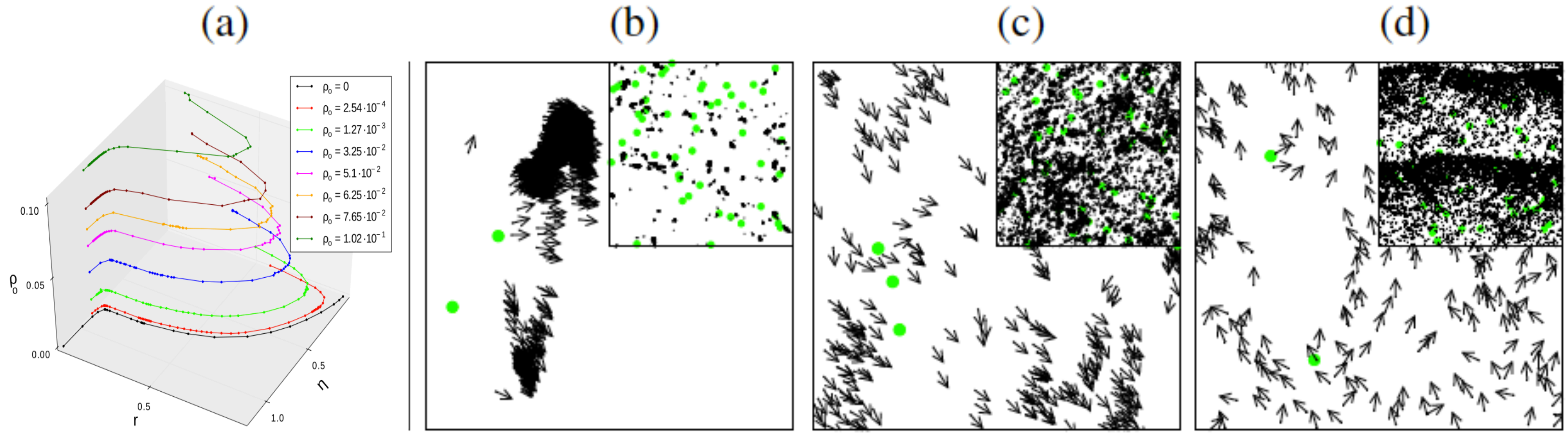
Collective motion in heterogeneous media

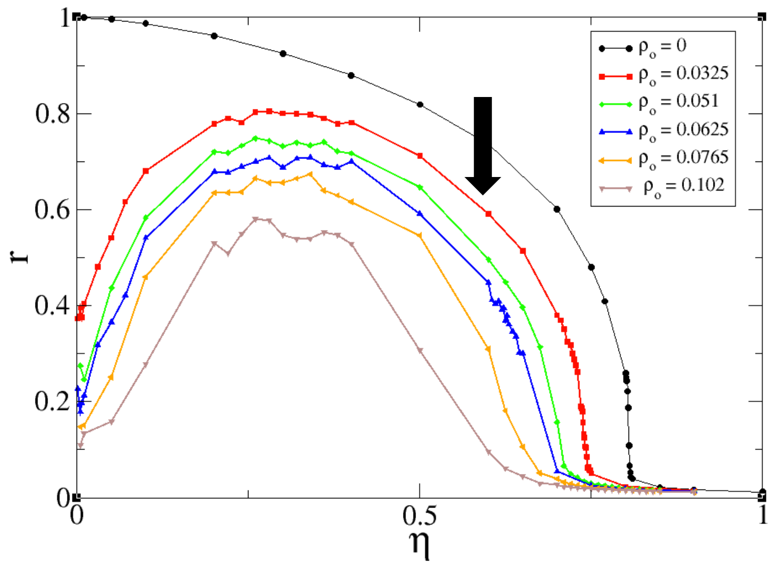
- **Are these results model-dependent?**



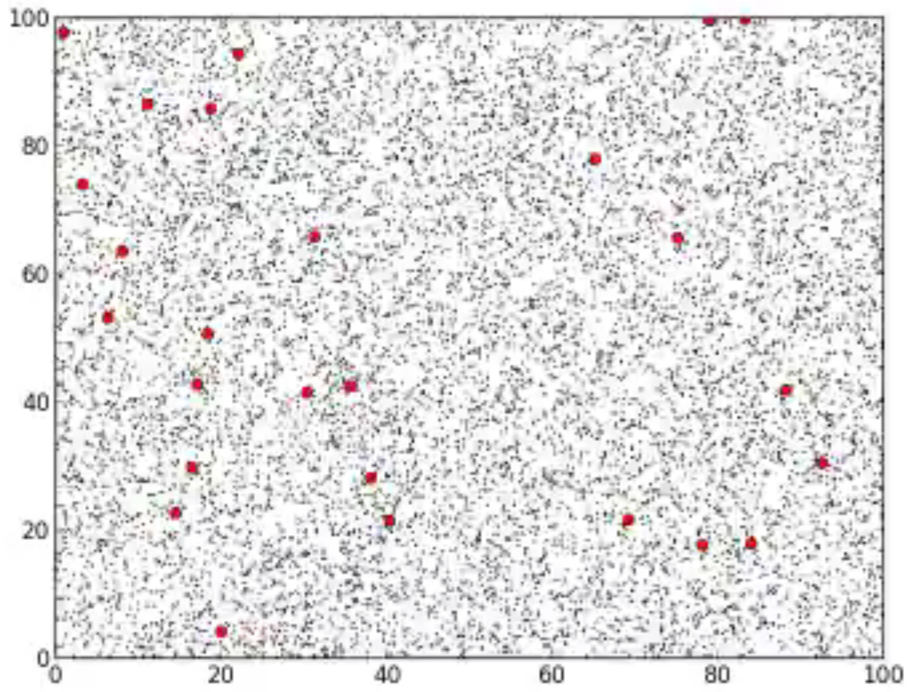
The same behavior is observed in all tested variants of the model, including diffusive obstacles !!!

Collective motion in heterogeneous media

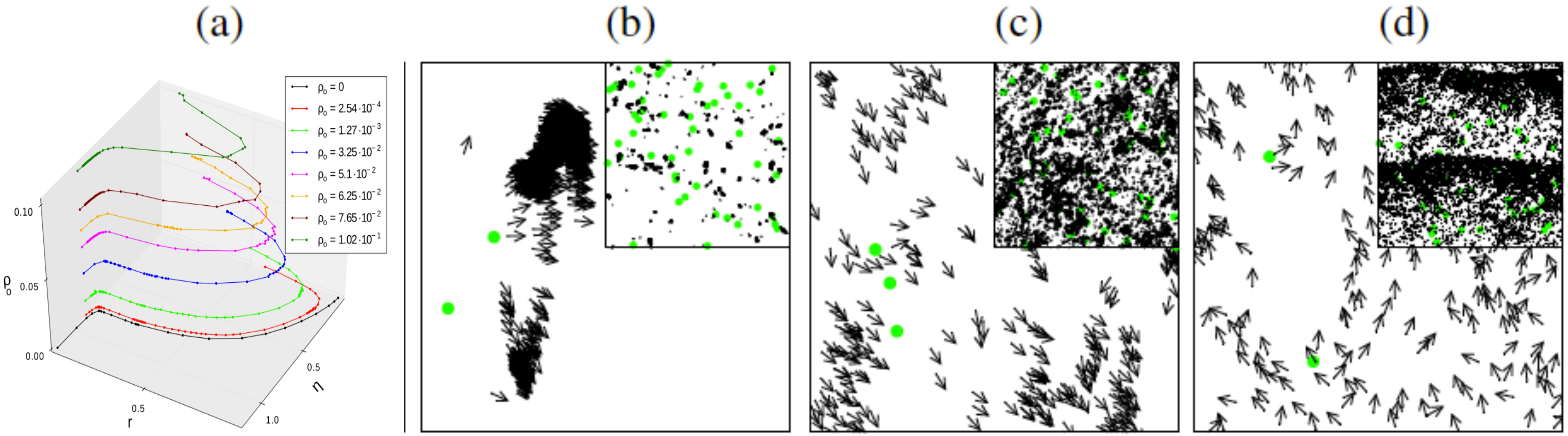


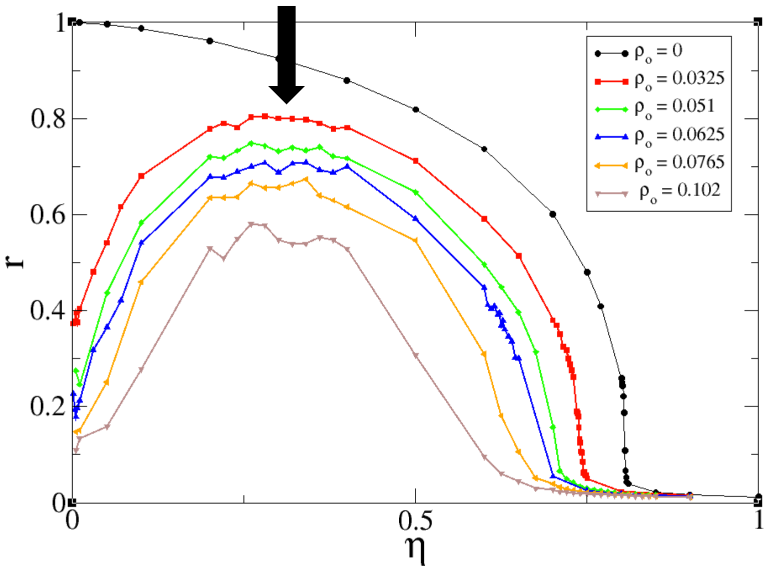


N=10000



Collective motion in heterogeneous media





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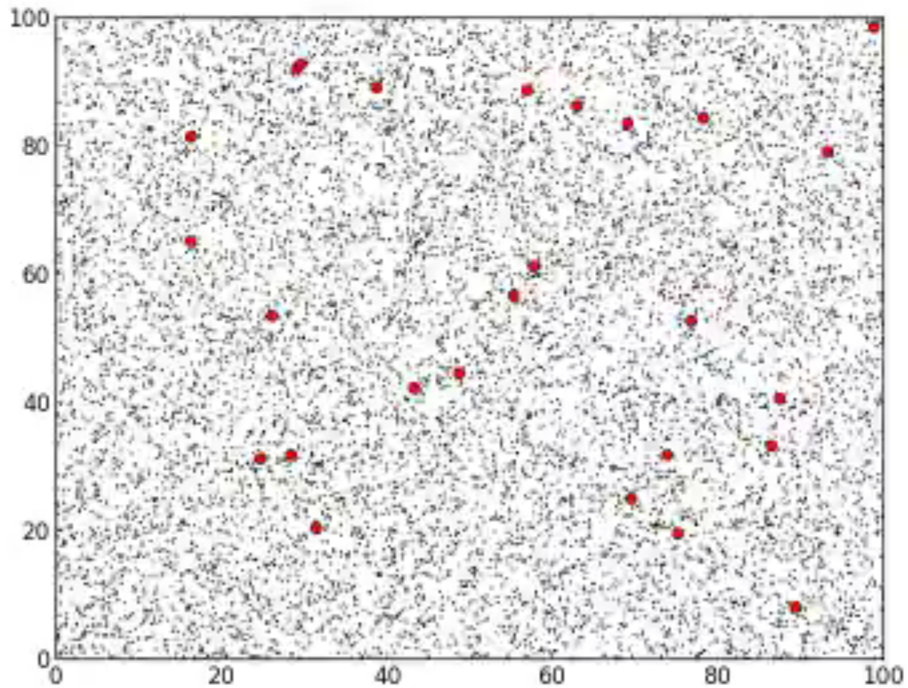
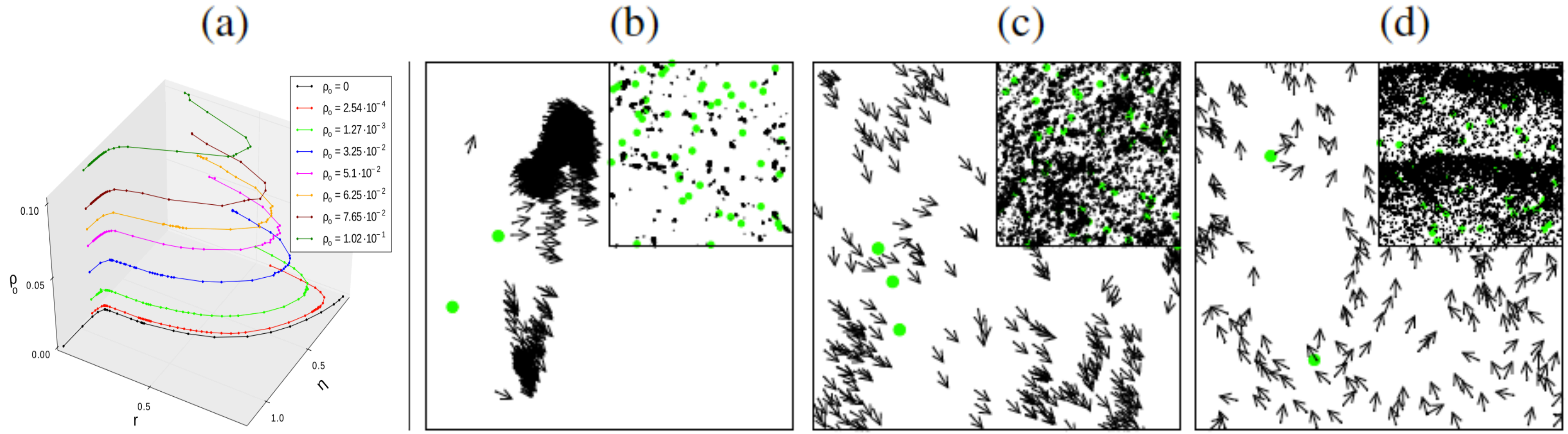
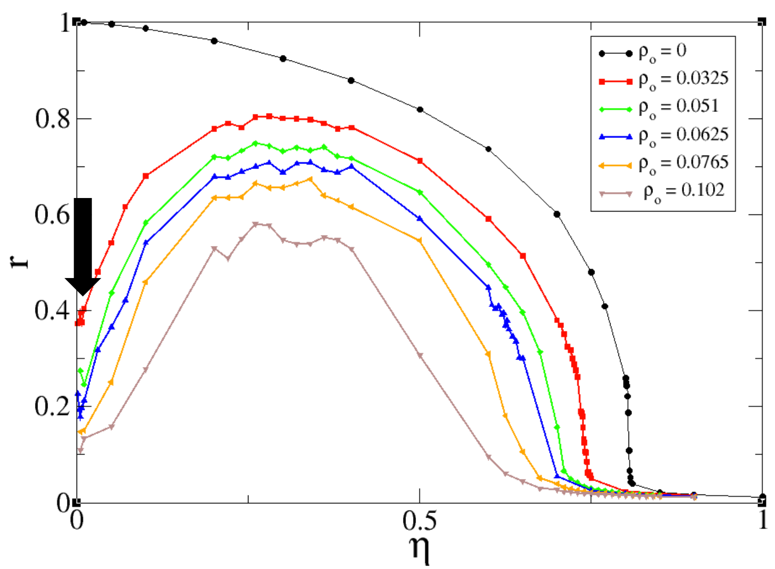
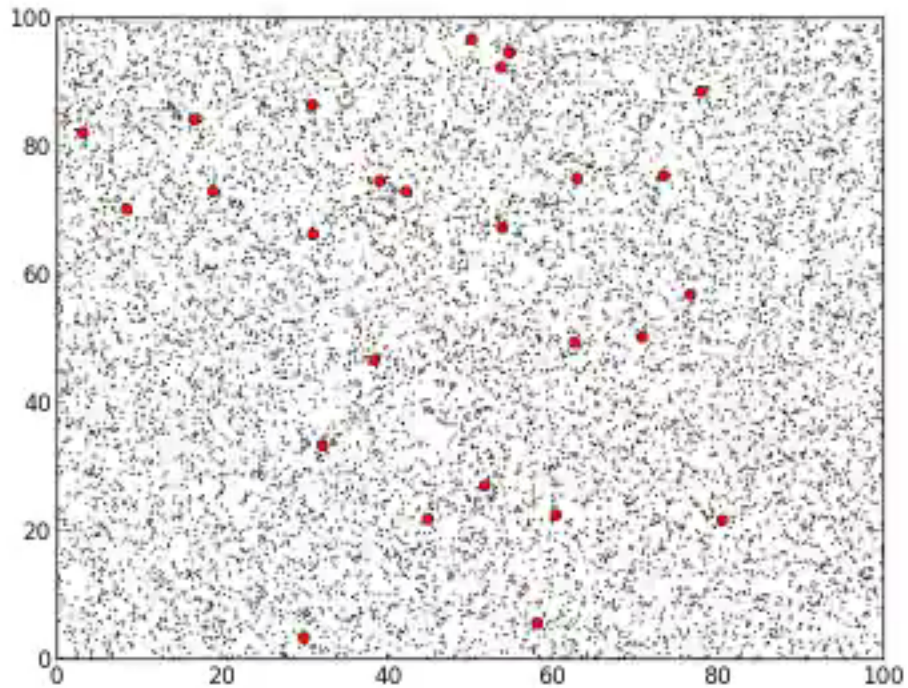


Collective motion in heterogeneous media



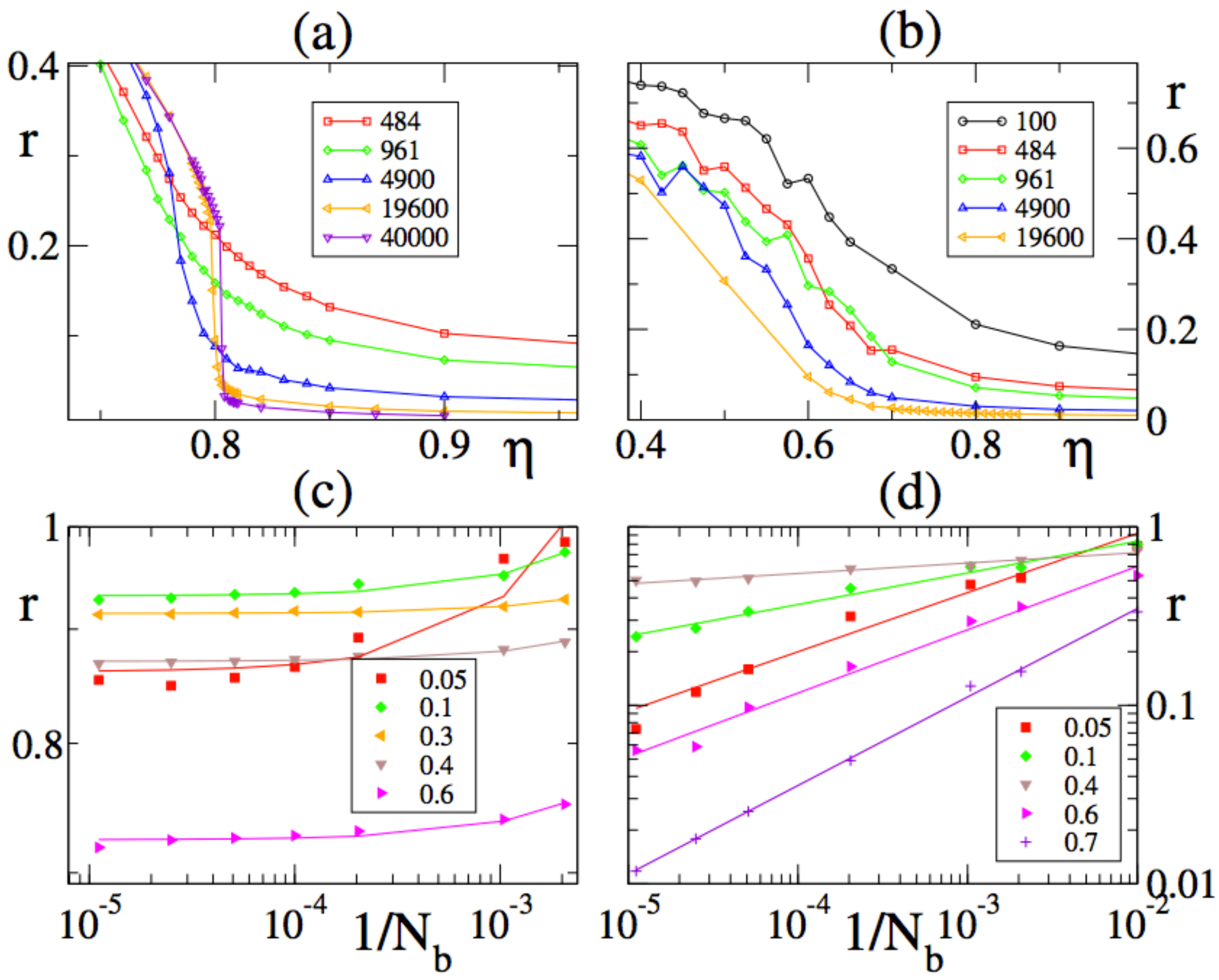


N=10000



Collective motion in heterogeneous media

• **<u>Long-range order vs. quasi long-range order:</u>**



$\rho_o = 2.55\,10^{-3}$ $\rho_o = 0.102$

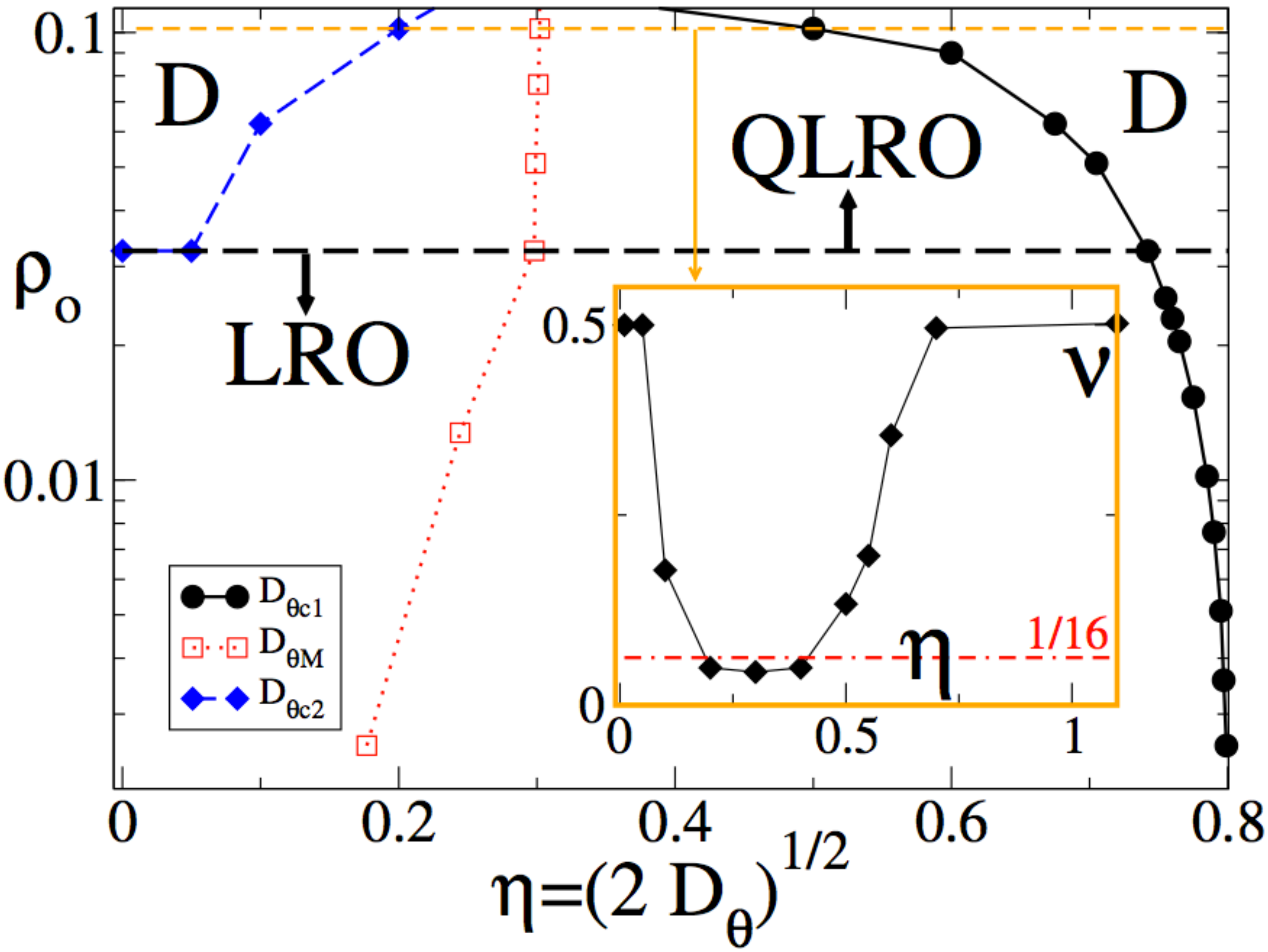
Long-range order

$$r \sim r_\infty(\eta)\exp(A(\eta)N_b)$$

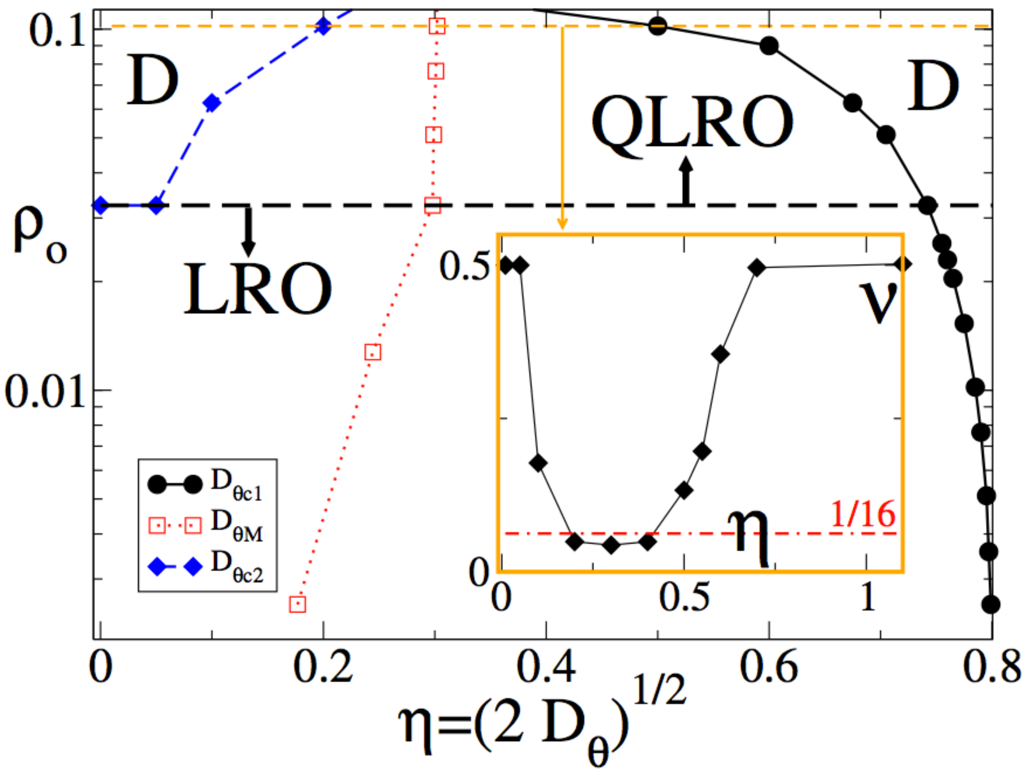
Quasi long-range order

$$r \propto N_b^{-\nu(D_\theta,\rho_o)}$$

• **Phase diagram:**



Collective motion in heterogeneous media



Results:

- There is an optimal noise (resp. obst. density) that maximizes collective motion
- Due to the presence of obstacles/defects, the system exhibit QLRO!!!
- (At very low obst. densities, the numerical results are consistent w/ LRO, but …)

O. Chepizhko, E. Altmann, F. Peruani, PRL (2013)

Acknowledement

Oleksandr (Sasha) Chepizhko

Thanks for you attention!

Some references:

Chepizkho, Peruani, PRL (2013)
Chepizkho, Altmann, Peruani, PRL (2013)