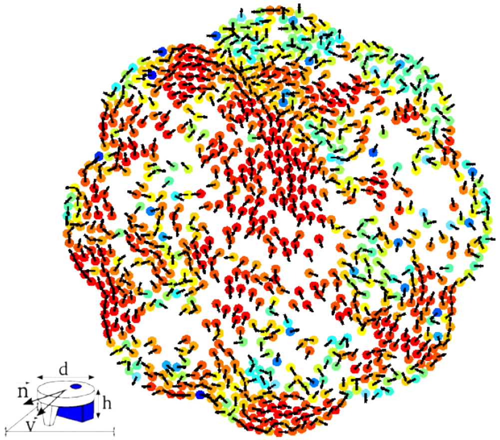
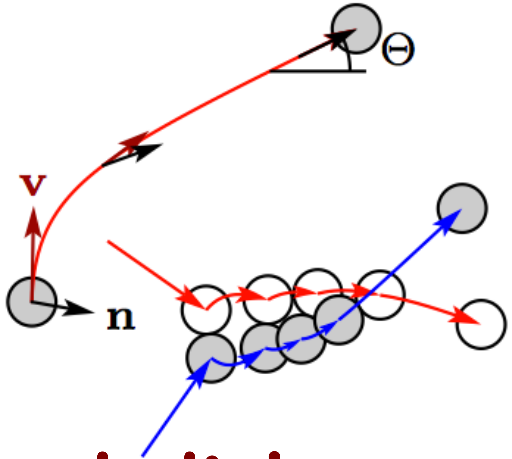
ESPCI ParisTech — CNRS — UMR Gulliver

EC2M Effets Collectifs & Matière Molle





Self-propelled hard disks

a “simple” active liquid

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Michael Schindler
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Kyoto 08/2015

Overview

- **Introduction**
  - Active liquids
  - Self-propelled disks

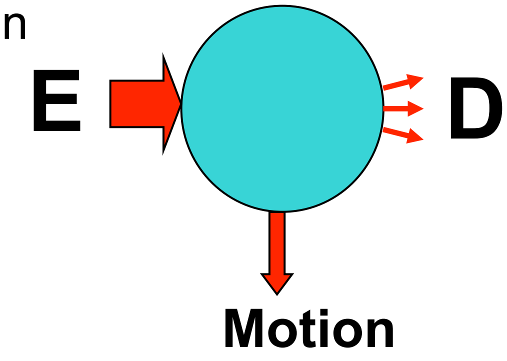
- **“Experimental” realization**
  - Walking grains and In-silico extrapolation

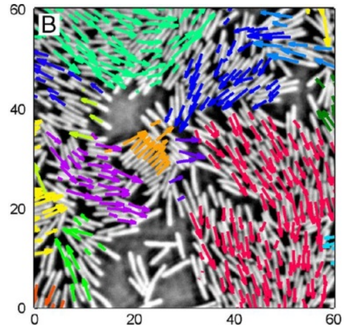
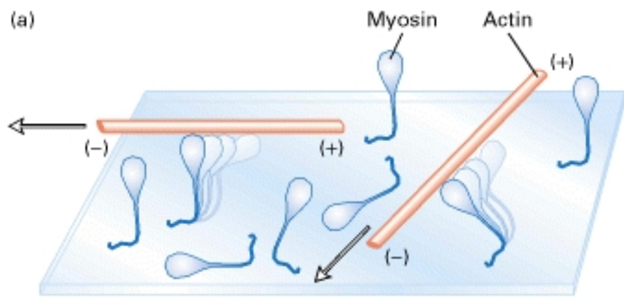
=>Self propelled disks exhibit a transition to polar collective motion

- **Models and Theoretical description**
  - Where does the alignment come from ? What *is* the alignment ?
  - How does it compare to the Vicsek alignment rule ?
  - Are the differences significant ?

Active liquids

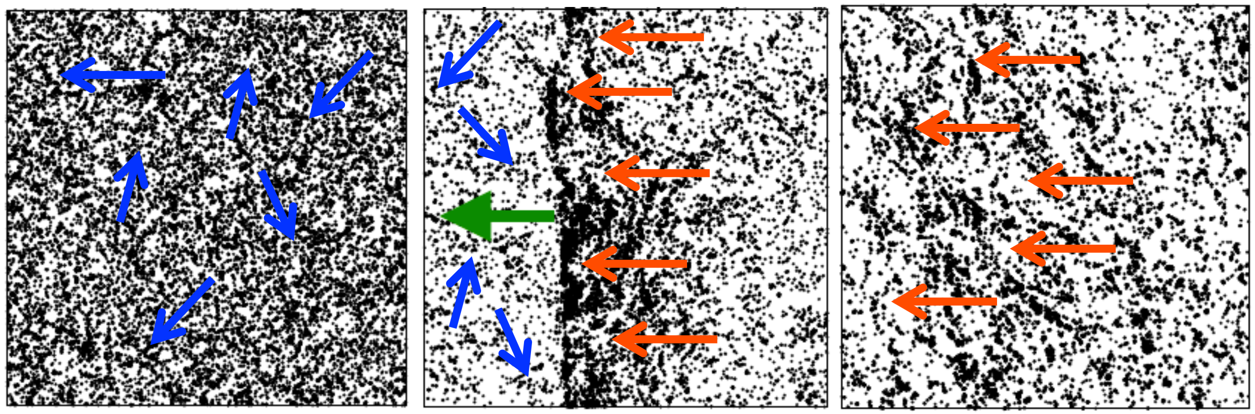
- A commonly accepted definition of an active fluid :
  - Out of equilibrium fluid composed of particles the motion of which results from the dissipation of the energy received homogeneously at the scale of each particle.

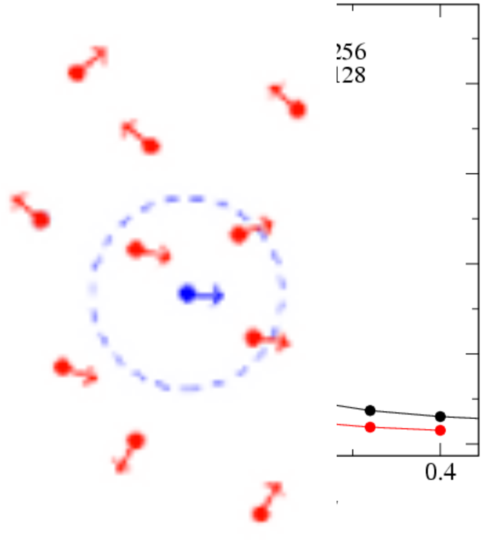


Birds	Crikets	Bacteria	Actin filaments on myosine
			
20cm	1cm	10μm	100nm-10μm

Transition to collective motion : the Vicsek Model

- Over damped, Self Propelled Point Particles, $V = V_0\ \mathbf{n}$
- Noisy Alignment with neighbors (within some range)
- Diffusive Noise

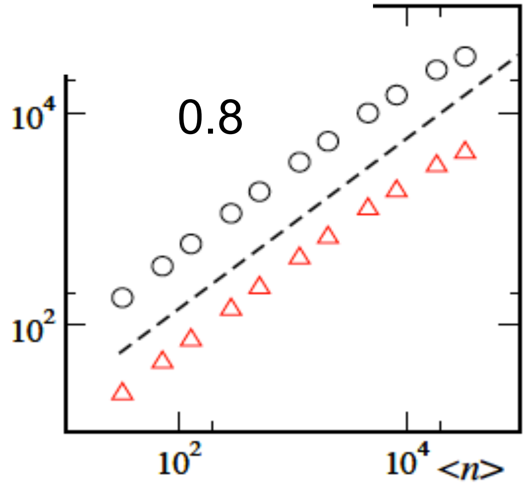




⇒ Discontinuous transition to collective motion

⇒ fast domain growth leading to high-density/high order solitary bands/sheets (2D/3D)

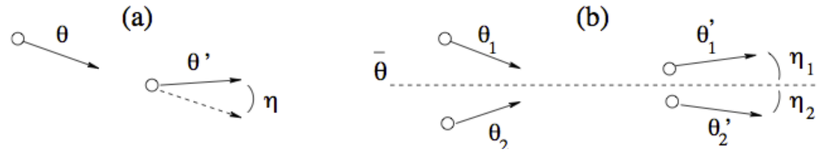
⇒ Giant density fluctuations in the homogeneous polar state



PRE, *77*(4), 6113 2008.

Continuous description Bertin, Droz, Grégoire, J. Phys. A: Math. Theor. **42** (2009)

- Binary interaction version



- Boltzmann equation (molecular chaos)

$$\frac{\partial f}{\partial t}(\mathbf{r},\theta,t) + \mathbf{e}(\theta)\cdot\nabla f(\mathbf{r},\theta,t) = I_{\mathrm{dif}}[f] + I_{\mathrm{col}}[f]$$

- Hydrodynamics equations

$$\begin{aligned}\frac{\partial \mathbf{w}}{\partial t} + \gamma(\mathbf{w}\cdot\nabla)\mathbf{w} &= -\frac{1}{2}\nabla(\rho - \kappa \mathbf{w}^2) \\ &+ (\mu - \xi \mathbf{w}^2)\mathbf{w} + \nu\nabla^2\mathbf{w} - \kappa(\nabla\cdot\mathbf{w})\mathbf{w}\end{aligned} \quad (8)$$

where the different coefficients are given by

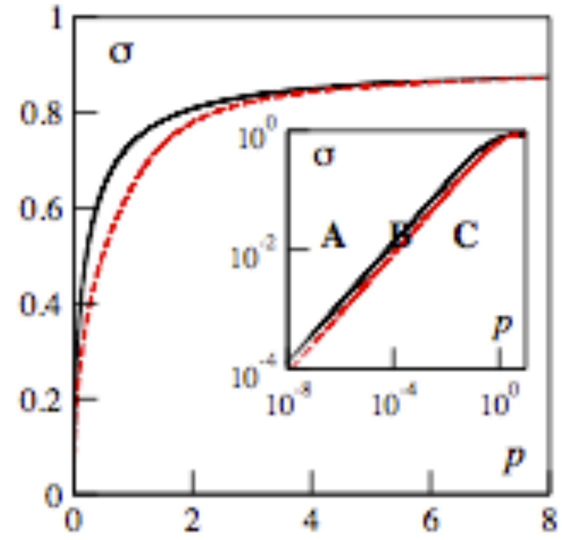
$$\nu = \frac{1}{4}\left[\lambda\left(1 - e^{-2\sigma_0^2}\right) + \frac{4}{\pi}\rho\left(\frac{14}{15} + \frac{2}{3}e^{-2\sigma^2}\right)\right]^{-1} \quad (9)$$

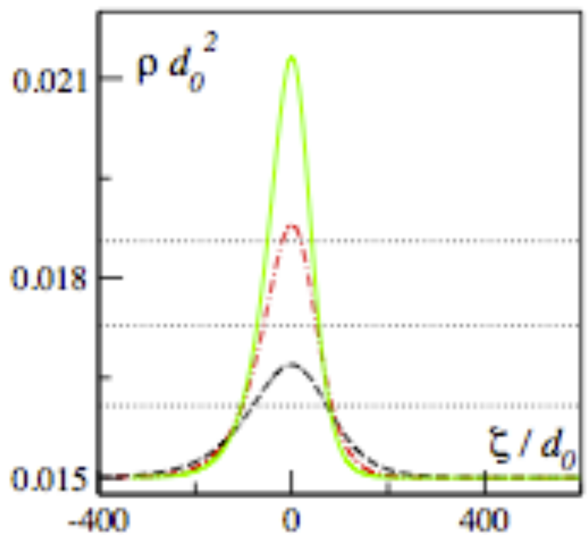
$$\gamma = \frac{8\nu}{\pi}\left(\frac{16}{15} + 2e^{-2\sigma^2} - e^{-\sigma^2/2}\right) \quad (10)$$

$$\kappa = \frac{8\nu}{\pi}\left(\frac{4}{15} + 2e^{-2\sigma^2} + e^{-\sigma^2/2}\right) \quad (11)$$

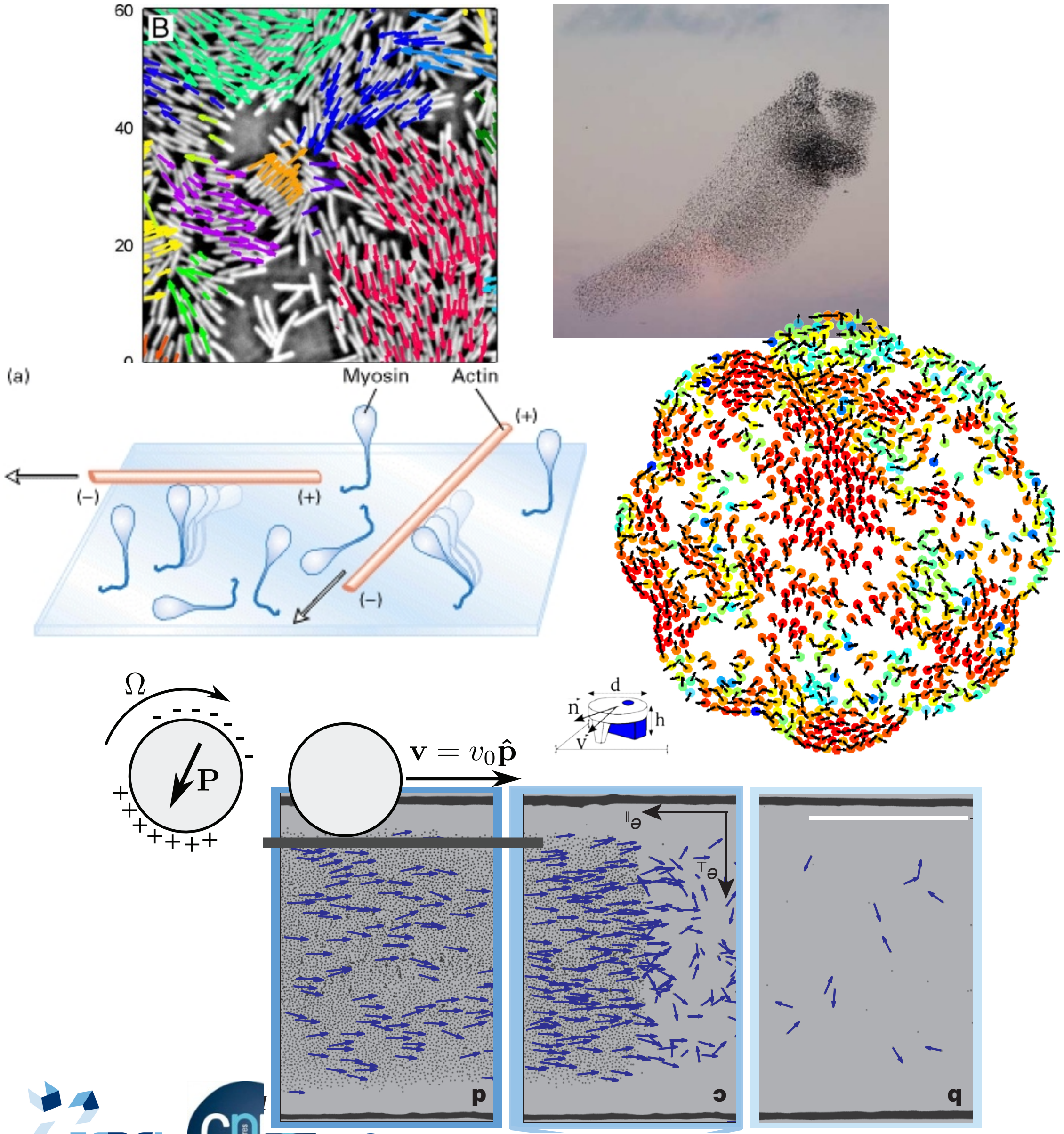
$$\mu = \frac{4}{\pi}\rho\left(e^{-\sigma^2/2} - \frac{2}{3}\right) - \lambda\left(1 - e^{-\sigma_0^2/2}\right) \quad (12)$$

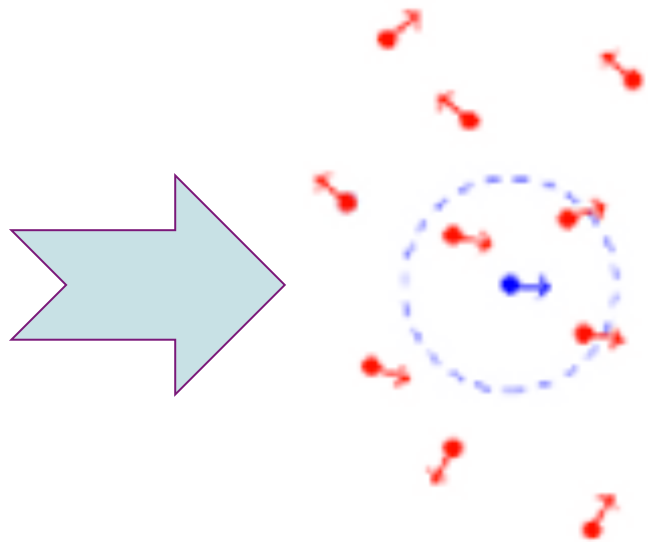
$$\xi = \frac{64\nu}{\pi^2}\left(e^{-\sigma^2/2} - \frac{2}{5}\right)\left(\frac{1}{3} + e^{-2\sigma^2}\right) \quad (13)$$





The underlying expectation ...





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Is it reasonable ?

	Alignment	Phases	Giant density fluct.
Rolling colloids	with (hydro origin)	Iso -> polar bands -> hom. polar phase	No
Actin filaments	with (steric origin)	Iso -> polar clusters -> polar bands ?	irrelevant
Bacteria	with (steric origin)	Iso -> polar clusters	irrelevant
Walking disks	A priori without	Iso -> polar clusters	irrelevant
Janus colloids	? (hydro origin)	Iso -> apolar active clusters	No
Surfing colloids	? (hydro origin)	Iso -> apolar active clusters	No

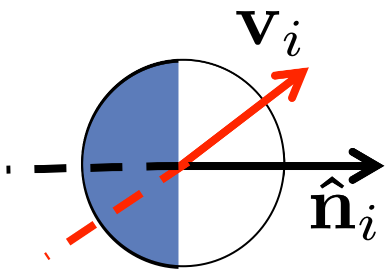
To date, not a single experimental system follows the Vicsek scenario

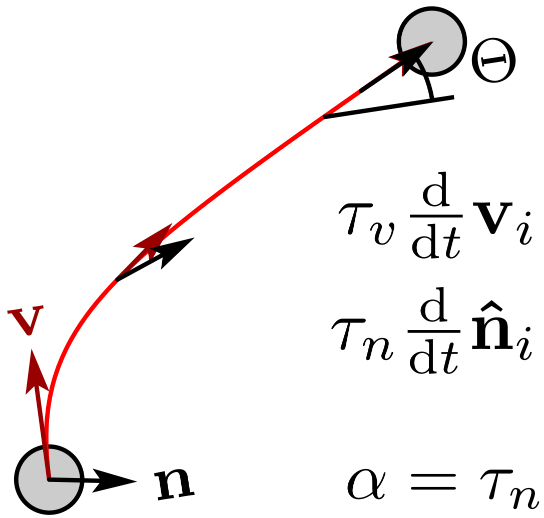
- Is it because of “complicated” but irrelevant factors ?
- Or more deeply the microscopic dynamics does not yield effectively to Vicsek-like alignment and the associated transition scenario?

Self-propelled disks

- **The simplest active particle with hard core repulsion**
  - Standard hard or soft repulsion
  - No shape anisotropy
  - No explicit alignment rule

- **2 positional +1 orientational degrees of freedom**
  (+ their time derivative)





$$\tau_v \frac{\mathrm{d}}{\mathrm{d}t}\mathbf{v}_i = \hat{\mathbf{n}}_i - \mathbf{v}_i,$$

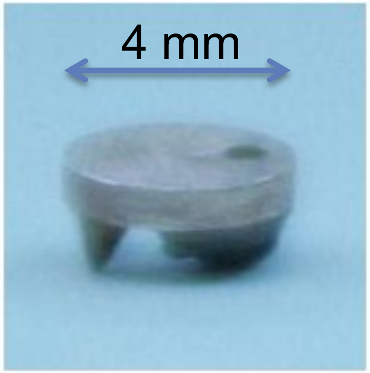
$$\tau_n \frac{\mathrm{d}}{\mathrm{d}t}\hat{\mathbf{n}}_i = (\hat{\mathbf{n}}_i \times \hat{\mathbf{v}}_i) \times \hat{\mathbf{n}}_i.$$

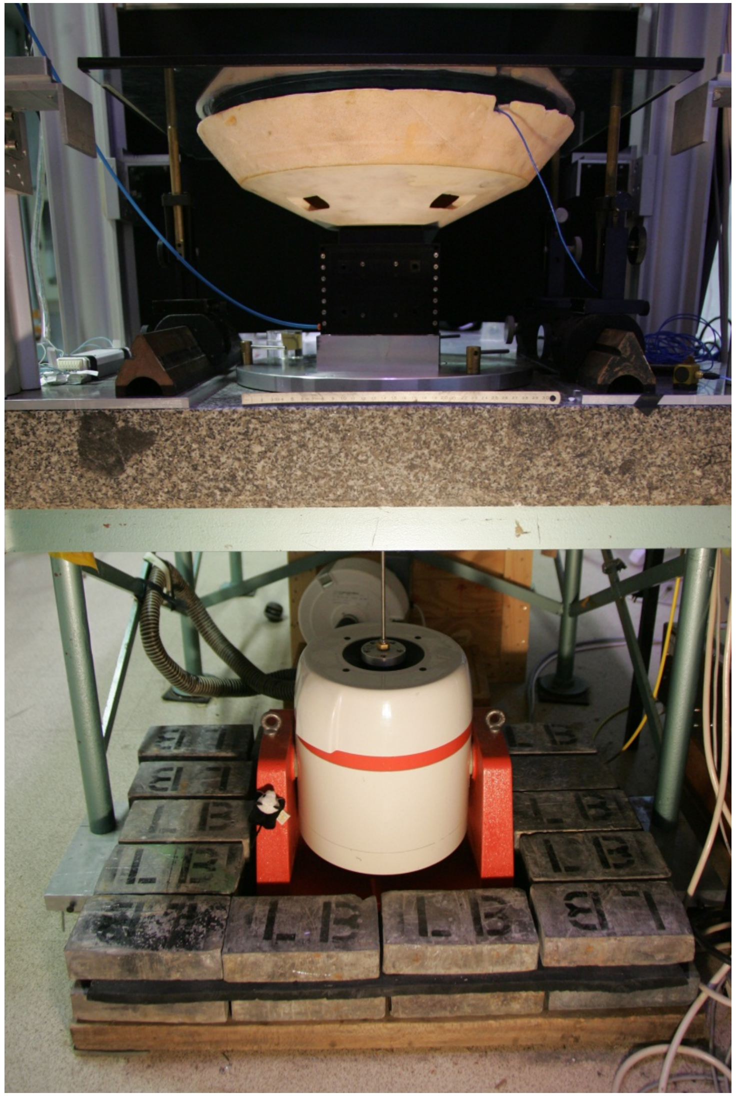
$\alpha = \tau_n / \tau_v$, persistence of $\hat{\mathbf{n}}_i$: key control parameter

Experiments : Vibrated polar disks

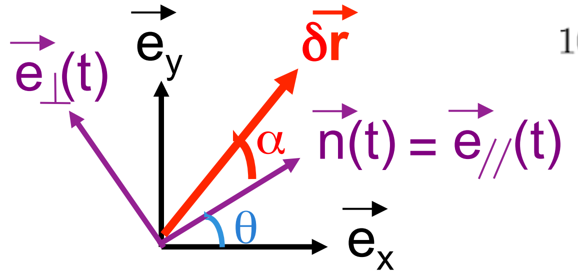
- Goals :
  - A well controlled 2D experiment
  - Particles,
    - Hard disk interactions
    - NO a priori alignment
  - Polar self propulsion

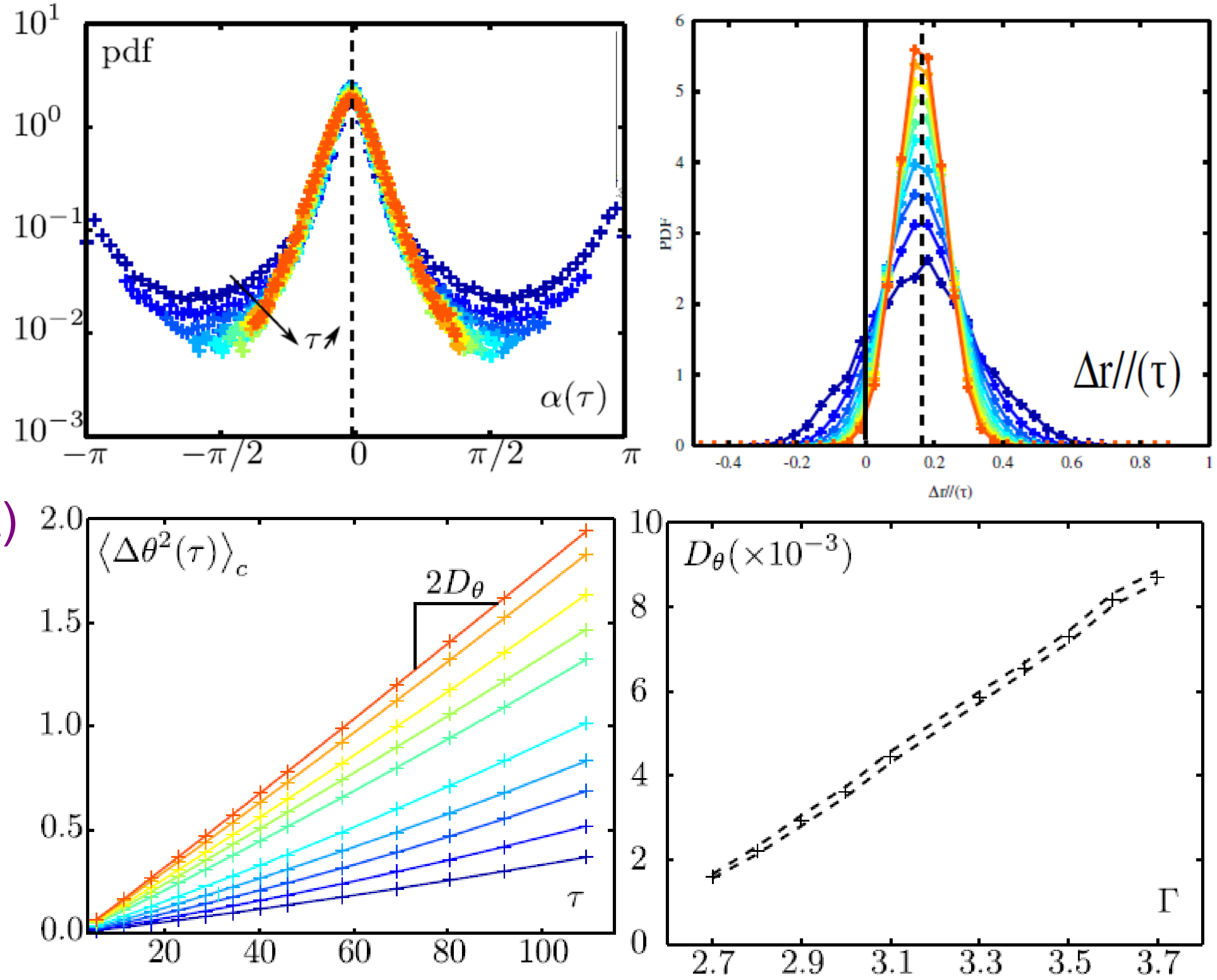
- Achieved with :
  - A well controlled vibration set-up (square air bearing slide) (f=115Hz)
  - Specifically designed walkers





Self propulsion





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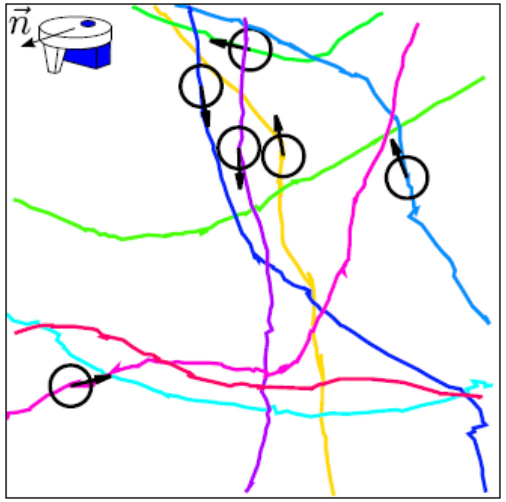
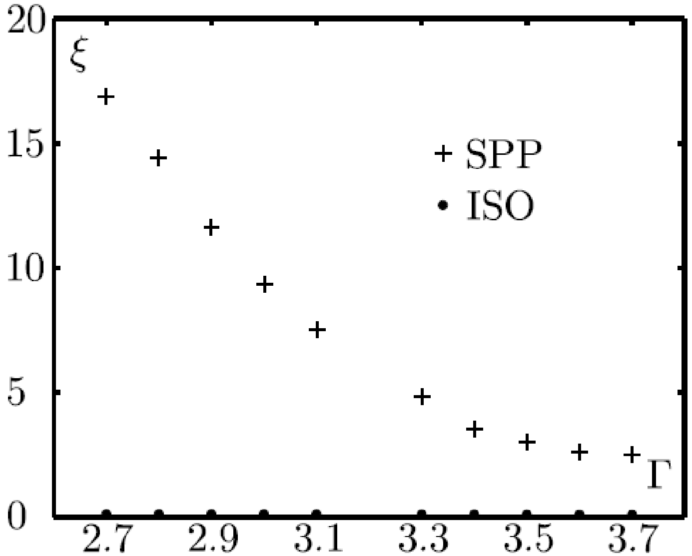
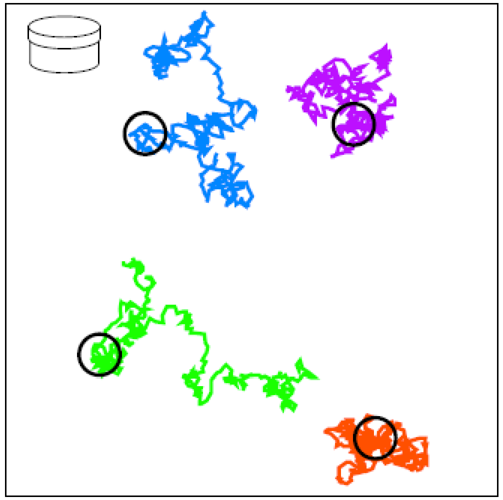
Individual motions of SPP vs. ISO:

Varying the natural control parameter Γ in the range $2.8<\Gamma<3.8$:





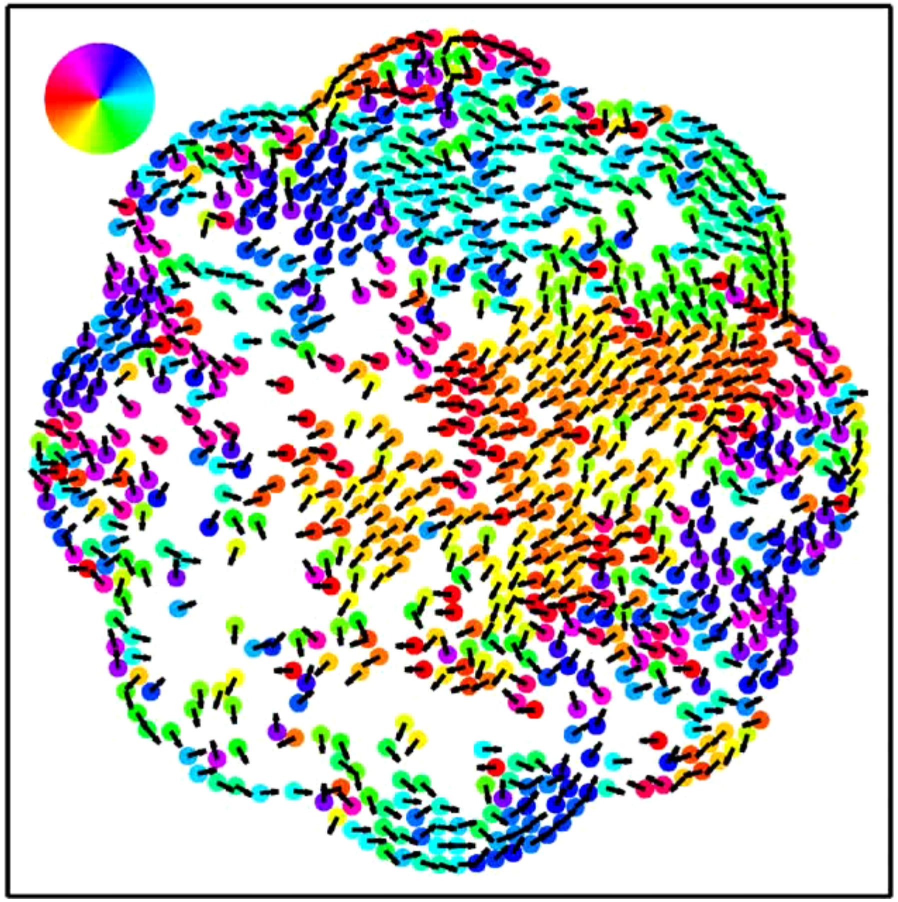


- SPP move along their polarity with an almost constant velocity V_0
  The angular exponential diffusion (noise) increases linearly with Γ

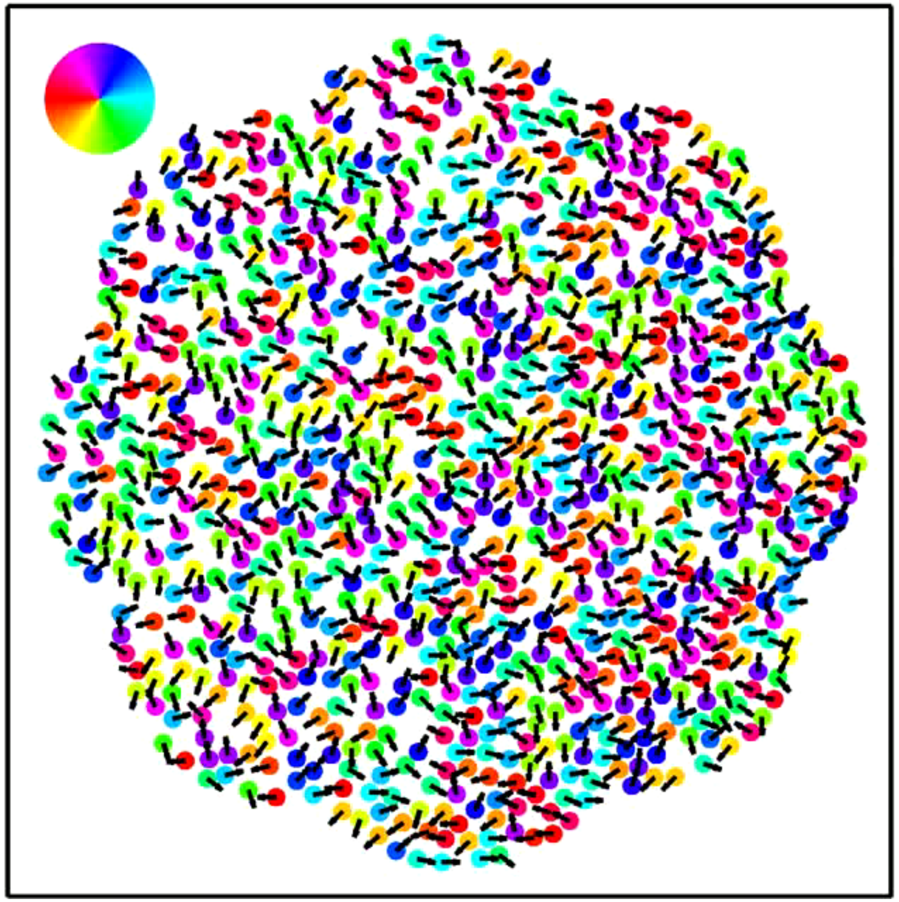
  => Persistence length: $\xi = V_0/D_\theta$

- By comparison ISO particles behave as standard diffusive particles
- Interactions : Hard core repulsion / No built-in alignment

Collective behaviors (Φ=0.47, Γ=2.7)



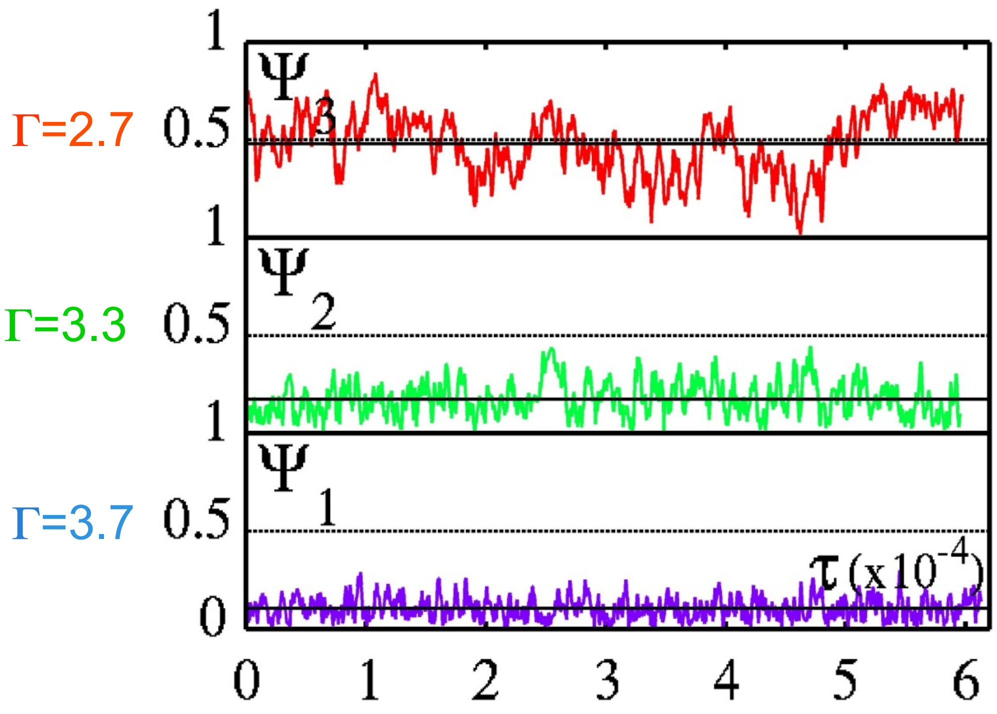
SPP

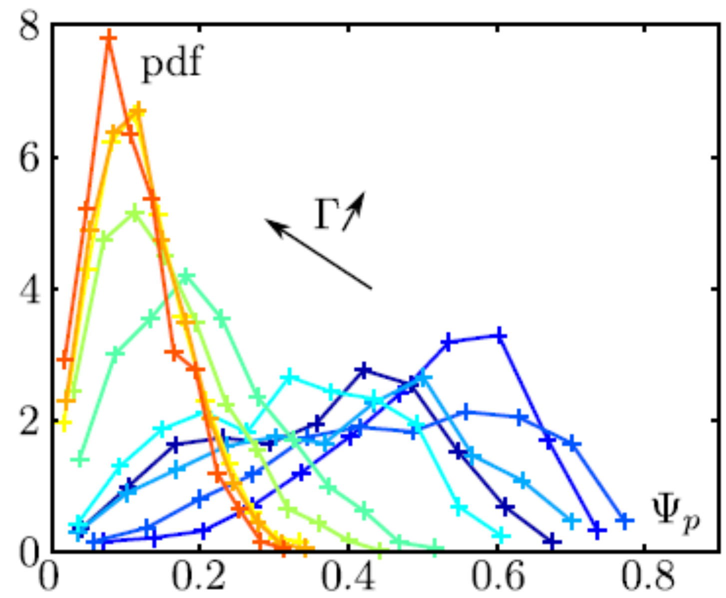


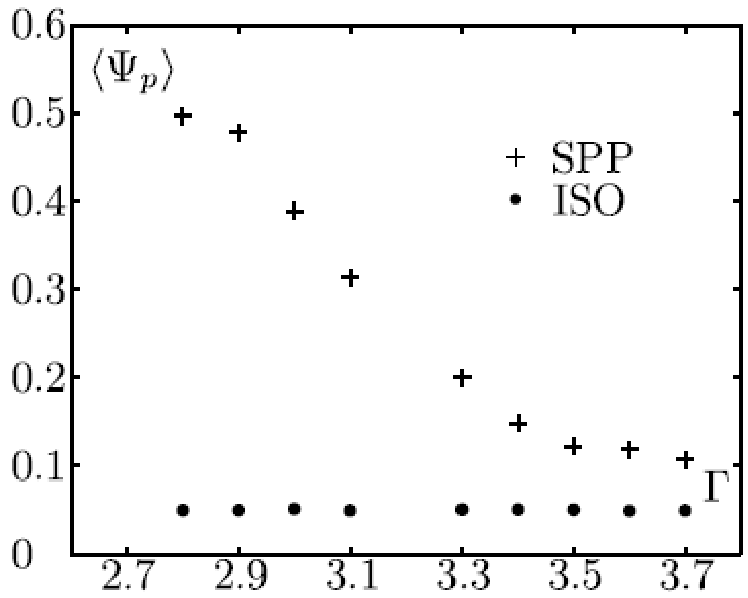
ISO

… collective motion and polar ordering

$$\Psi(t) = |\langle \vec{u}_i(t) \rangle|$$







In silico extrapolation :

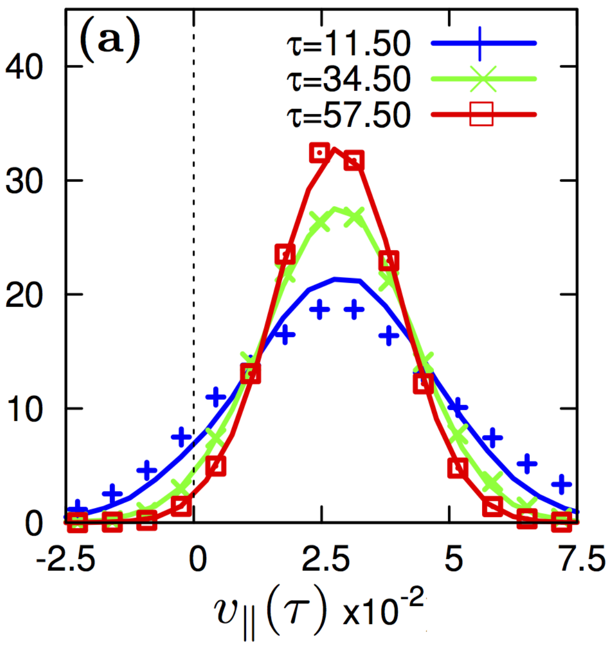
PRL 110 208001 (2013)

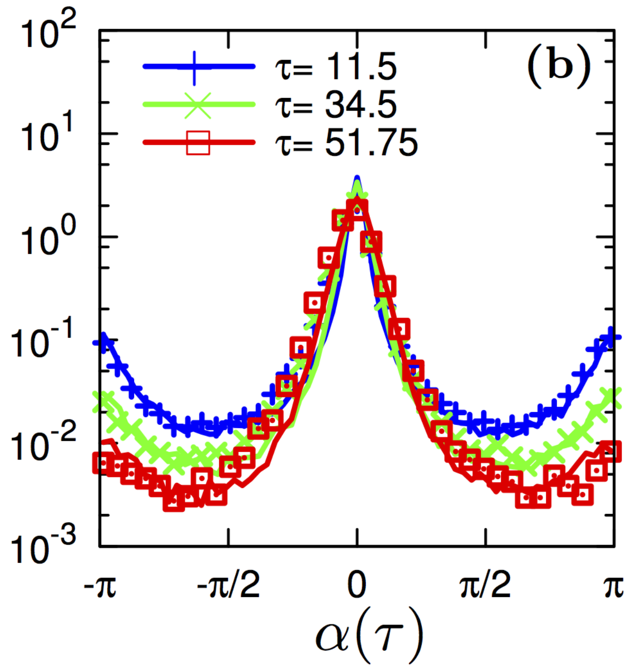
$$m\frac{d\mathbf{v}}{dt} = \underbrace{-\alpha F_0 \mathbf{v}}_{\text{friction}} + \underbrace{F_0 \mathbf{n}}_{\text{moteur}} + \underbrace{F_0 \left(\varepsilon_{\parallel} \eta\, \mathbf{n} + \varepsilon_{\perp} \eta' \mathbf{e}_{\perp}\right)}_{\text{bruit actif}}$$

+ slightly inelastic collisions

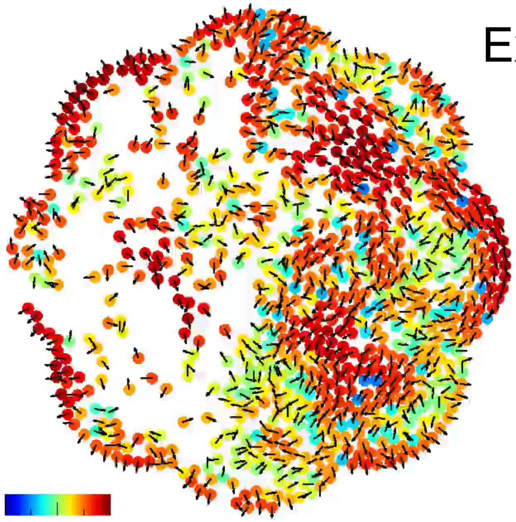
$$\frac{d\mathbf{n}}{dt} = \mathbf{\Omega} \times \mathbf{n} \qquad \mathbf{\Omega} = \frac{\mathbf{n} \cdot \hat{\mathbf{v}}}{\tau_{\varphi}} (\mathbf{n} \times \hat{\mathbf{v}})$$

+ Mapping the model on the experimental system via the one particle dynamics

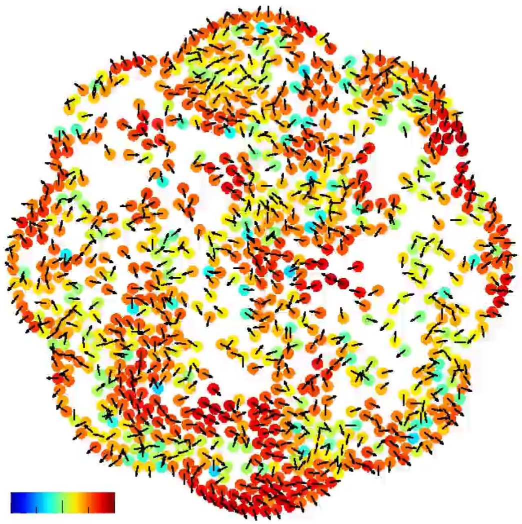




In silico extrapolation

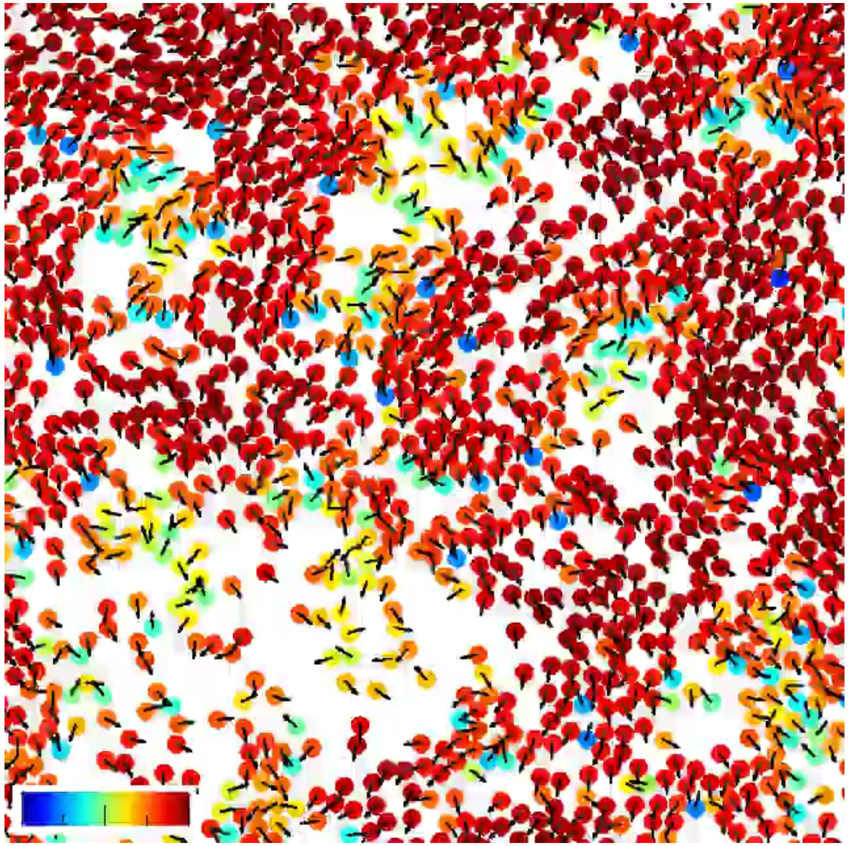


Experiment



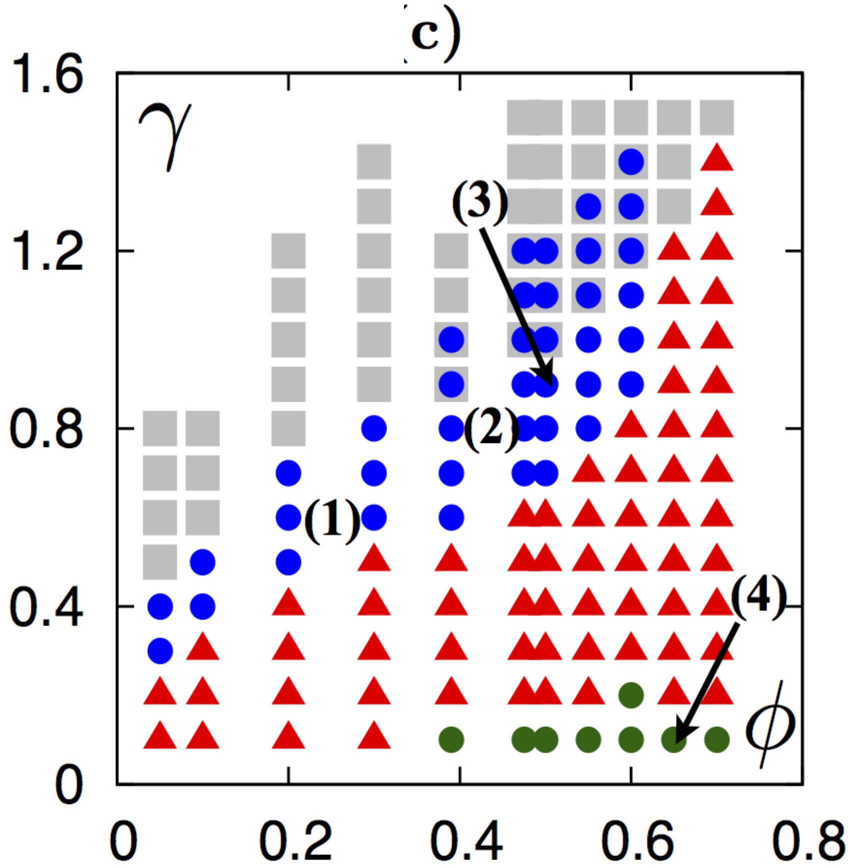
Model

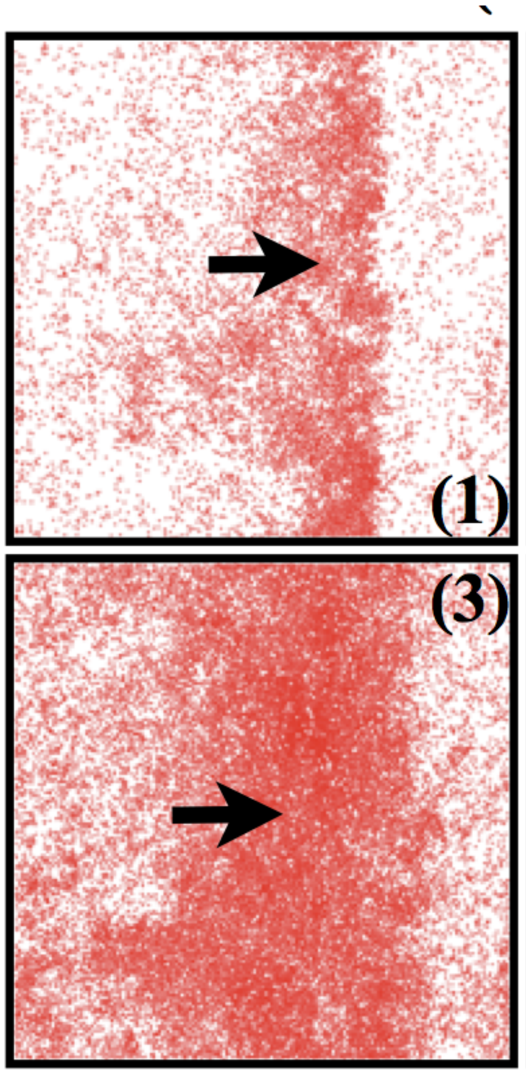
Periodic boundary conditions



More quantitatively

$$\gamma^2 = \frac{D_{//}}{D_{//}^{\Gamma=2.7}} = \frac{D_{perp}}{D_{perp}^{\Gamma=2.7}}$$





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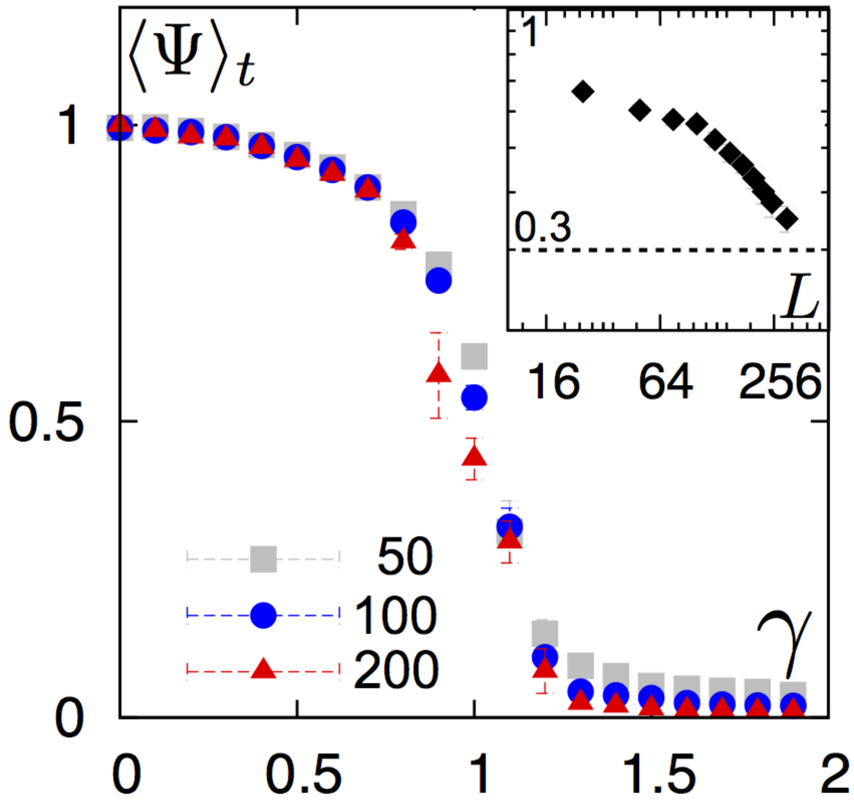


γ=1: parameters values match experimental individual dynamics

The order parameter <Ψ>≈0.5 and decreases with system size

⇒ The experiment sits right below the thermodynamic limit transition

⇒ The order correlation length is larger than the system size

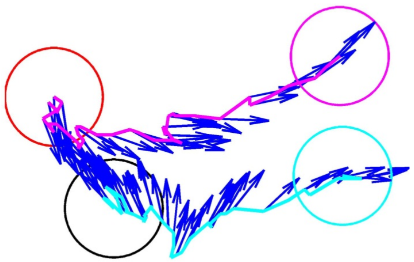
γ≠1 : more or less noise

Transition from disordered to polar phase

Altogether

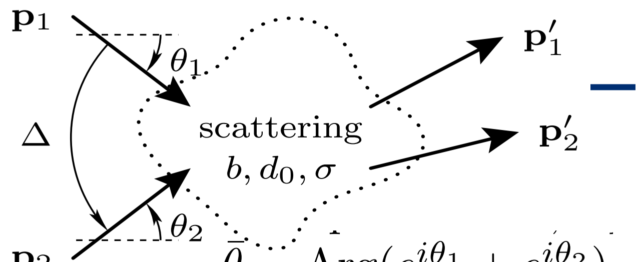
=>Self propelled disks
exhibit a transition to polar collective motion

- **Questions**
  - Where does the alignment come from ?
  - How does it compare to the Vicsek alignment rule ?
  - Are the differences significant ?



???

To answer these questions



$$\bar{\theta} = \mathrm{Arg}(e^{i\theta_1} + e^{i\theta_2})$$

$$\Delta = \theta_1 - \theta_2$$

- Binary interaction scattering event

  don't conserve momentum $\mathbf{P}(t) = \int \mathrm{d}\theta f(\theta,t)\hat{\mathbf{e}}(\theta)$

- Boltzmann equation (molecular chaos)

$$\frac{\partial f}{\partial t}(\mathbf{r},\theta,t) + \mathbf{e}(\theta)\cdot\nabla f(\mathbf{r},\theta,t) = I_{\mathrm{dif}}[f] + I_{\mathrm{col}}[f]$$

- Restricting to the study of homogeneous phases

- Compute the dynamics of the order parameter $\psi(t) = |\mathbf{P}(t)|$.

$$\frac{\mathrm{d}\psi}{\mathrm{d}t} = \lambda\Phi_f\left[(\hat{\mathbf{p}}\cdot\delta\mathbf{p})\cos\bar{\theta}\right] - D\psi,$$

- Ansatz (instead of a Fourier expansion) for the angular distribution

$$f(\theta,t) = f_{\psi(t)}(\theta) \qquad f_\psi(\theta) = \frac{e^{\kappa\cos\theta}}{2\pi I_0(\kappa)}, \qquad \text{with} \quad \frac{I_1(\kappa)}{I_0(\kappa)} = \psi,$$

= > A closed form equation for the order parameter

Generic form for homogeneous polar liquids

- A closed form equation for the order parameter

$$\frac{\mathrm{d}\psi}{\mathrm{d}t} = \lambda \Phi_\psi[\mathbf{p}\cdot\delta\mathbf{p}] - D\psi$$

$$\Phi_\psi[\dots] = \int_0^\pi \frac{\mathrm{d}\Delta}{\pi} \int \mathrm{d}\zeta\, K(\Delta,\zeta) g(\psi,\Delta)(\dots)$$

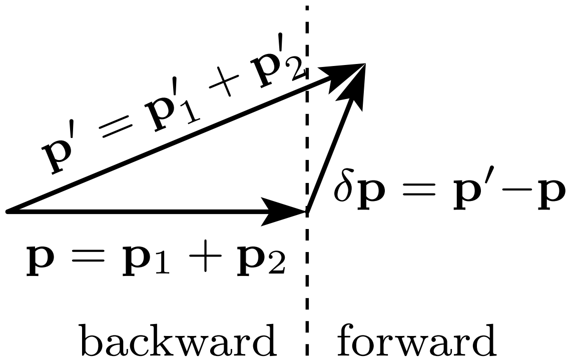
- Linearized around the isotropic state

$$\frac{1}{\lambda}\frac{\mathrm{d}\psi}{\mathrm{d}t} \simeq (\mu - D/\lambda)\psi - \xi\psi^3$$

$$\mu := \langle \mathbf{p}\cdot\delta\mathbf{p}\rangle_0,$$

$$\xi := \langle (\tfrac{1}{2} - \cos\Delta)\, \mathbf{p}\cdot\delta\mathbf{p}\rangle_0$$

$$\langle\dots\rangle_0 = \frac{1}{2\pi}\int_{-\pi}^{\pi} \mathrm{d}\Delta \int \mathrm{d}\zeta\, K(\Delta,\zeta)(\dots)$$

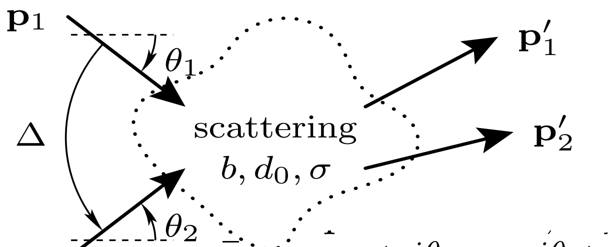


Let's use it … $\frac{1}{\lambda}\frac{\mathrm{d}\psi}{\mathrm{d}t} \simeq (\mu - D/\lambda)\psi - \xi\psi^3$

$$\mu := \langle \mathbf{p}\cdot\delta\mathbf{p}\rangle_0,$$
$$\xi := \langle (\tfrac{1}{2} - \cos\Delta)\, \mathbf{p}\cdot\delta\mathbf{p}\rangle_0$$

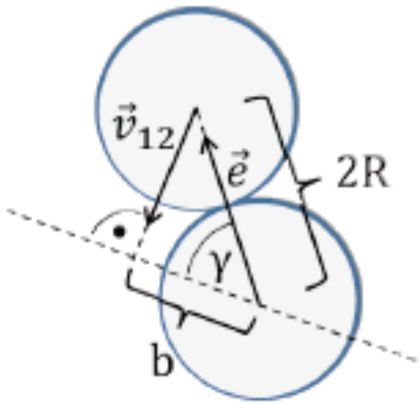
$$\langle \dots \rangle_0 = \frac{1}{2\pi}\int_{-\pi}^{\pi}\mathrm{d}\Delta \int \mathrm{d}\zeta\, K(\Delta,\zeta)(\dots)$$

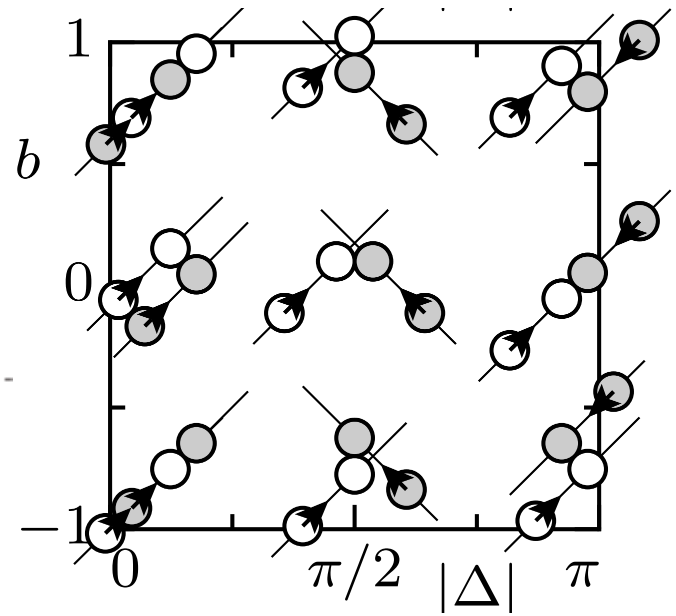
- For colliding particles, the collision rate : $K(\Delta) \propto |\sin(\Delta/2)|$
- $\int_\zeta \mathbf{p}\cdot\delta\mathbf{p}$ is the relevant quantity to compute



$\bar{\theta} = \mathrm{Arg}(e^{i\theta_1} + e^{i\theta_2})$

$\Delta = \theta_1 - \theta_2$



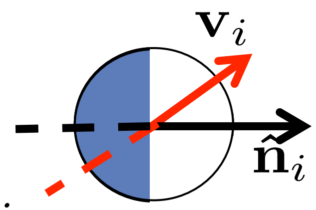


Simulations of binary scattering events

$$\tau_v \frac{\mathrm{d}}{\mathrm{d}t}\mathbf{v}_i = \hat{\mathbf{n}}_i - \mathbf{v}_i,$$

$$\tau_n \frac{\mathrm{d}}{\mathrm{d}t}\hat{\mathbf{n}}_i = (\hat{\mathbf{n}}_i \times \hat{\mathbf{v}}_i) \times \hat{\mathbf{n}}_i.$$

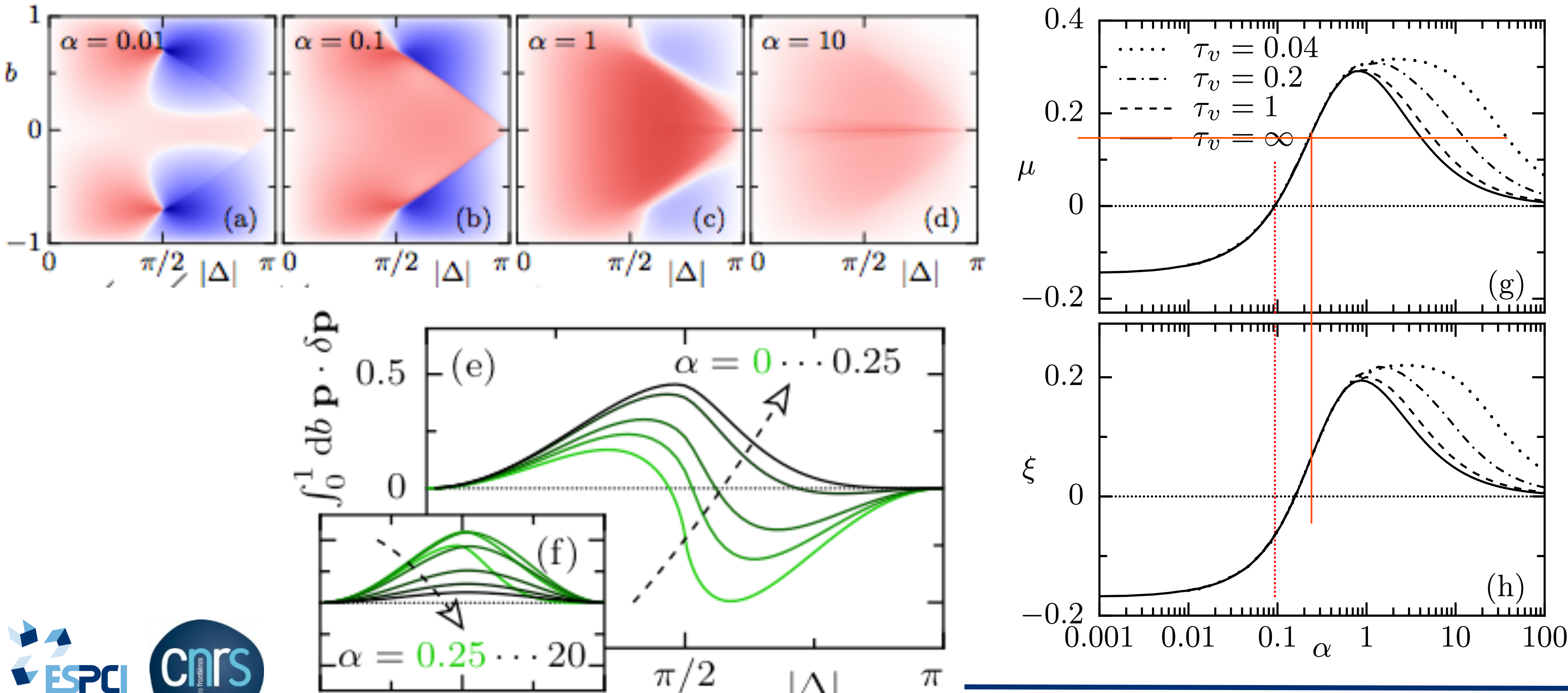
$\alpha = \tau_n / \tau_v$, persistence of $\hat{\mathbf{n}}_i$



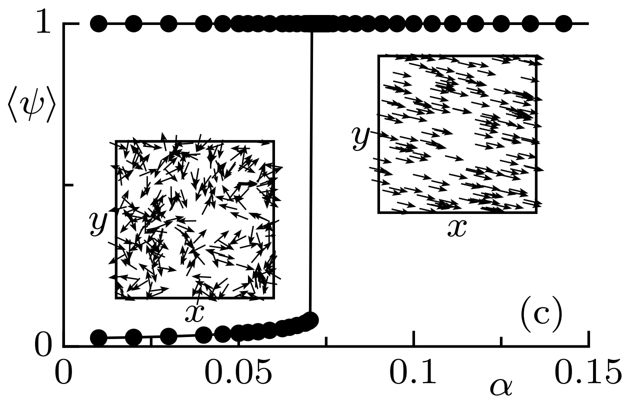
$$\frac{1}{\lambda}\frac{\mathrm{d}\psi}{\mathrm{d}t} \simeq (\mu - D/\lambda)\psi - \xi\psi^3$$

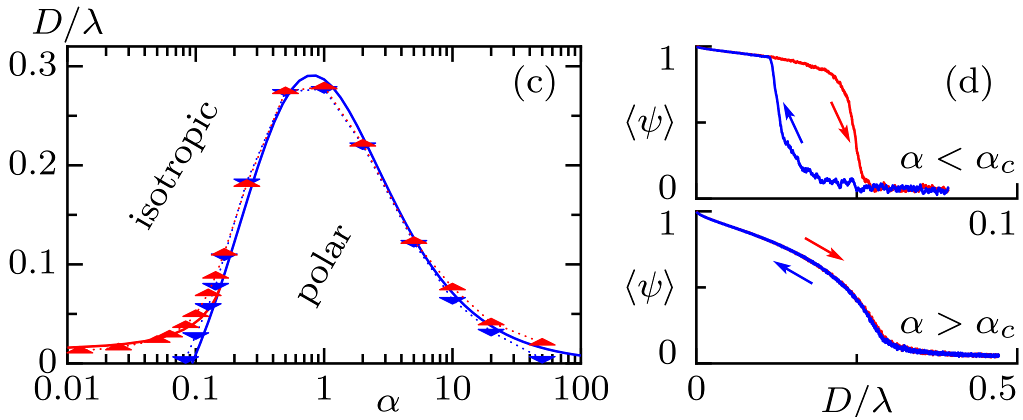
$$\mu := \langle \mathbf{p}\cdot\delta\mathbf{p} \rangle_0,$$

$$\xi := \langle (\tfrac{1}{2} - \cos\Delta)\, \mathbf{p}\cdot\delta\mathbf{p} \rangle_0$$



Consequences for the transition between hom. phases





- A strongly first order transition in the absence of self-diffusion (D=0)
- A triciritical point at finite D>0, towards a second order transition
- A re-entrant transition for α >1 (when the polarity is too much persistent)
- Nota Bene :
  - Multiple re-collisions are not essential
  - One can capture the form of pδp (b,Δ) for α=0 from simple geom. arguments
  - Inelastic HS behave in a similar way

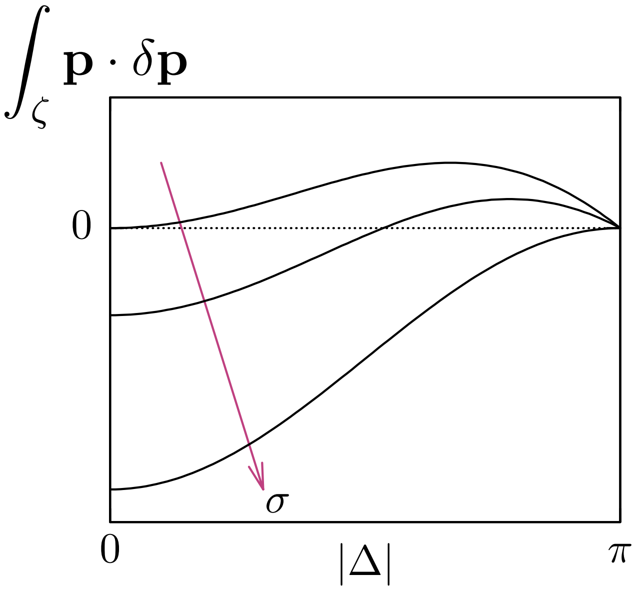
What about the Vicsek aligning rules?

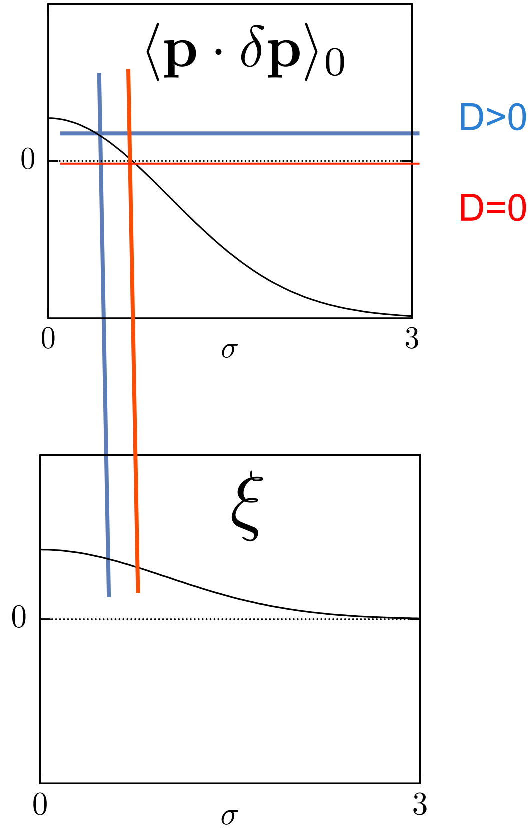
- Viscek like alignment

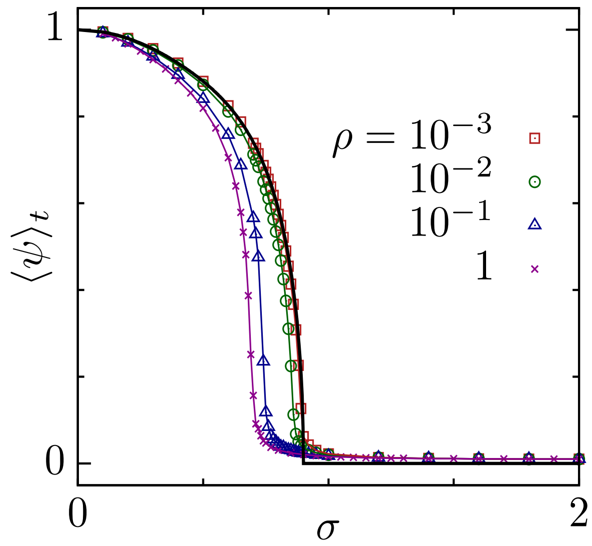
$$\theta'_1 = \bar{\theta} + \eta_1 \qquad \theta'_2 = \bar{\theta} + \eta_2$$

$$\mathbf{p}\cdot\delta\mathbf{p} = |\mathbf{p}|(\cos\eta_1 + \cos\eta_2 - |\mathbf{p}|)$$

$$\int_\zeta \mathbf{p}\cdot\delta\mathbf{p} = 2\cos\frac{\Delta}{2}\left(2e^{-\sigma^2/2} - 2\cos\frac{\Delta}{2}\right)$$







Summary

- Hard core repulsion + Self propulsion => effective alignment.
  - => steric orientation is not necessary
  - => hard or soft disks systems can not be claimed without “alignment”

- Alignment
  - $\langle \mathbf{p} \cdot \delta \mathbf{p} \rangle_0$ is the physically meaningful quantity

- Transition to collective motion
  - A rich phase diagram with a transition from 1rst to 2^{nd} order, controlled by the level of noise
  - The Viscek aligning rule is not a good effective description of the alignment in systems of hard disks

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- Julien Deseigne and Hugue Chaté (CEA-Saclay) — Walking grains
- Christoph Weber, Timo Hanke and Erwin Frey (Munich) — Grains in Silico
- Michael Schindler and Khanh Dang Thu Lam (Gulliver) — Theory

Further reading :

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*SoftMatter **8** p. 5629 (2012)*
*PRL **110** 208001 (2013)*
Cond-mat 1410.4520
Cond-mat 1502.07612

Thank you !

(http://www.ec2m.espci.fr)