Active Matter

Lectures for the 2011 ICTP School on Mathematics and Physics of Soft and Biological Matter

Lecture 3: Hydrodynamics of SP Hard Rods

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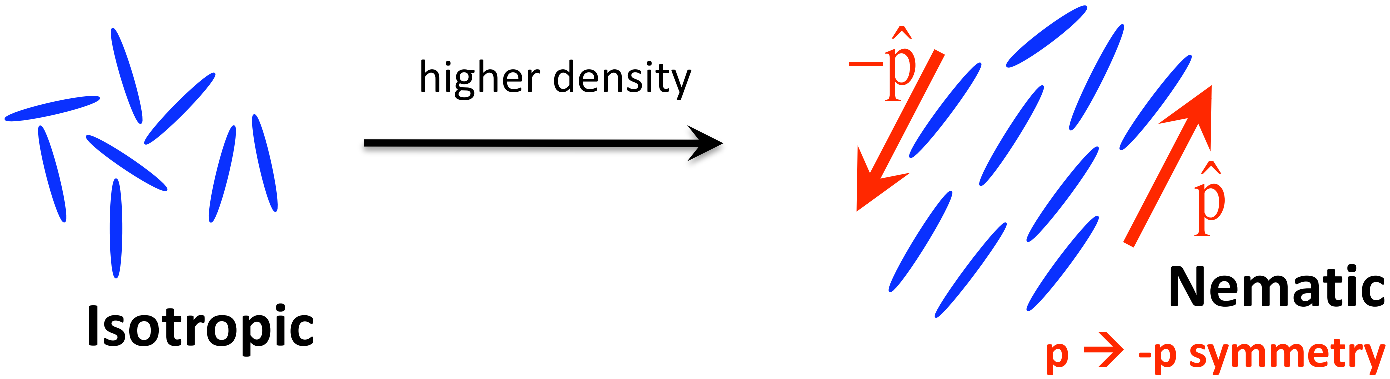
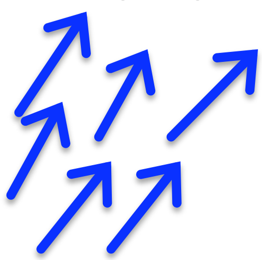
Baskaran & MCM, PRE 77 (2008); PRL 101 (2008); J. Stat. Mech. P04019 (2010)

Excluded volume & Self-Propulsion

- Hard rods order in a nematic phase upon increasing density due solely to entropic **excluded volume effects** (Onsager, 1949)



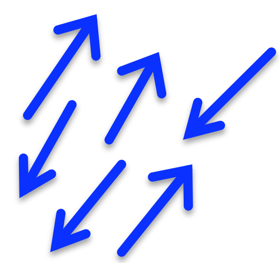
- Do **self-propelled (SP) hard rods** order in polar or nematic phase?



Polar order

Moving phase

Nematic order



Zero mean velocity

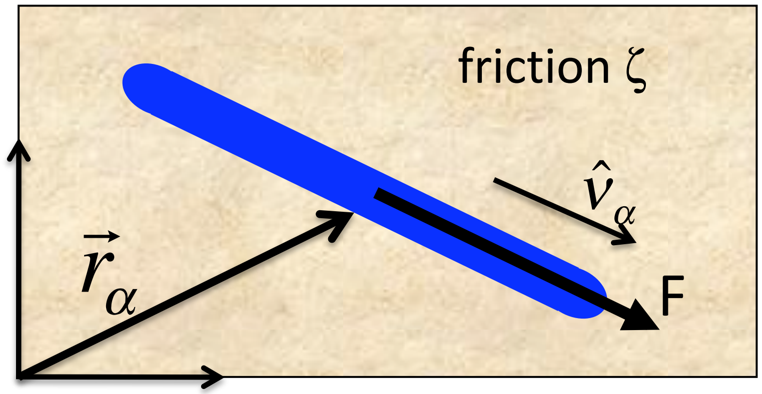
It turns out SP order rods do not exhibit polar order in bulk, but only nematic order. This is because a hard rod collision aligns SP rods regardless of their polarity:

But: many novel properties not present in equilibrium hard rods nematic:

- Self-propulsion enhances nematic order
- Traveling density sound-like wave in both isotropic (at finite wavevector) and ordered states
- Polar packets or clusters at intermediate density (Peruani et al, 2006; Yang et al, 2010; Ginelli et al, 2010)
- Spontaneous phase separation and density segregation: stationary bands

Self-propelled hard rods on a substrate:

Interplay of self-propulsion & excluded volume



- SP speed $v_0=F/\zeta$
- overdamped dynamics
- Noise k_BT_a
- Hard repulsive interactions: energy and momentum conserving collisions

Alignment arises from collision of SP hard rods, it is **not** imposed as a rule (unlike Vicsek-type models)

Langevin dynamics:

$$\begin{cases} \partial_t \vec{v}_i + \underbrace{\overleftrightarrow{\zeta} \cdot \vec{v}_i}_{\text{friction}} = \underbrace{F\hat{v}_i}_{\text{self propulsion}} + \underbrace{\sum_j T(ij)\vec{v}_j}_{\text{interactions}} + noise \\ \partial_t \omega_i + \zeta_r \omega_i = \sum_j T(ij)\ \omega_j + noise \end{cases}$$

Simulations: Peruani et al, PRE 74 (R) 2006; Ginelli et al, PRL 104 (2010); Yang et al, PRE 82 (2010).
Experiments: Deseigne et al PRL 105 (2010).

Langevin dynamics

↓

Smoluchowski equation

(diffusion of in configuration space) $c(\vec{r}, \nu, t)$

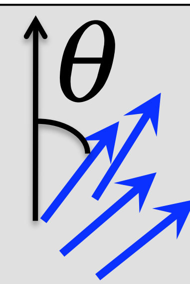
SP enhances longitudinal momentum transfer & modifies Onsager's excluded volume interaction

↓

Hydrodynamic equations:

density of rods ρ

polarization P~<cosθ> → polar order



alignment tensor Q~<cos²θ> → nematic order

Tutorial

From Langevin to Fokker-Planck to hydrodynamics for one particle in one dimension.

R. Zwanzig, Nonequilibrium Statistical mechanics (Oxford University press, 2001), Chapter 1 and 2.

Langevin dynamics

Spherical particle of radius a and mass m, in one dimension

$$m\frac{dv}{dt} = -\zeta v + \eta(t) \qquad \zeta = \qquad \text{friction}$$

noise is uncorrelated in time and Gaussian:

$$\langle \eta(t) \rangle = 0$$
$$\langle \eta(t)\eta(t') \rangle = 2\Delta\delta(t - t')$$

Noise strength Δ

In equilibrium Δ is determined by requiring

$$\lim_{t\to\infty} < [v(t)]^2 >=< v^2 >_{eq}= \frac{k_B T}{m} \qquad \Rightarrow \Delta = \frac{\zeta k_B T}{m^2}$$

Mean square displacement is diffusive

$$< [\Delta x(t)]^2 >= \frac{2k_B T}{\zeta}\left[t - \frac{m}{\zeta}\left(1 - e^{-\zeta t/m}\right)\right] \to \frac{2k_B T}{\zeta} t = 2Dt$$

Fokker-Plank equation

Many-particle systems

When the Langevin equation contains nonlinearities or when dealing with coupled Langevin equations for interacting particles, it is more convenient to work with distribution functions by transforming the Langevin equation(s) into a hierarchy of Fokker Planck equations for noise-averaged distribution functions.
Here I will first show how to do this for a single particle.

First step:

Transform the Langevin equation into a Fokker-Plank equation for the noise-average distribution function

$$f_1(x,p,t) =< \hat{f}_1(x,p,t) >$$

Fokker-Plank equation - 2

Compact notation

$$\begin{aligned} \frac{dx}{dt} &= p/m \\ \frac{dv}{dt} &= -\zeta v - \frac{dU}{dx} + \eta(t) \end{aligned} \quad \Rightarrow \frac{d\mathbf{X}}{dt} = \mathbf{V} + \boldsymbol{\eta}(t)$$

$$\mathbf{X} = \begin{pmatrix} x \\ p \end{pmatrix} \quad \mathbf{V} = \begin{pmatrix} p/m \\ -\zeta v - U' \end{pmatrix} \quad \boldsymbol{\eta} = \begin{pmatrix} 0 \\ \eta \end{pmatrix}$$

Conservation law for probability distribution

$$\int d\mathbf{X}\, \hat{f}(\mathbf{X}, t) = 1 \Rightarrow \quad \partial_t \hat{f} + \frac{\partial}{\partial \mathbf{X}} \cdot \left(\frac{\partial \mathbf{X}}{\partial t} \hat{f} \right) = 0$$

$$\partial_t \hat{f} + \frac{\partial}{\partial \mathbf{X}} \cdot \left(\mathbf{V} \hat{f} \right) + \frac{\partial}{\partial \mathbf{X}} \cdot \left(\boldsymbol{\eta} \hat{f} \right) = 0 \qquad \Rightarrow \qquad \partial_t \hat{f} + L \hat{f} + \frac{\partial}{\partial \mathbf{X}} \cdot \left(\boldsymbol{\eta} \hat{f} \right) = 0$$

$$\hat{f}(\mathbf{X}, t) = e^{-Lt} f(\mathbf{X}, 0) - \int_0^t ds\, e^{-L(t-s)} \frac{\partial}{\partial \mathbf{X}} \eta(s) \hat{f}(\mathbf{x}, s)$$

Fokker-Plank equation - 3

Use properties of Gaussian noise to carry out averages

$$\partial_t < \hat{f} > \quad + \quad \frac{\partial}{\partial \mathbf{X}} \cdot \mathbf{V} < \hat{f} > + \frac{\partial}{\partial \mathbf{X}} \cdot < \boldsymbol{\eta}(t) e^{-Lt} f(\mathbf{X}, 0) >$$

$$- \frac{\partial}{\partial \mathbf{X}} \cdot < \boldsymbol{\eta}(t) \int_0^t ds\, e^{-L(t-s)} \frac{\partial}{\partial \mathbf{X}} \boldsymbol{\eta}(s) \hat{f}(\mathbf{X}, s) > = 0$$

$$\partial_t f = -\frac{p}{m} \partial_x f - \partial_p [-U'(x) - \zeta p/m] f + \Delta \partial_p^2 f$$

Fokker-Plank eq. easily generalized to many interacting particles

$$\frac{dp_\alpha}{dt} = -\zeta v_\alpha - \sum_\beta \partial_{x_\alpha} V(x_\alpha - x_\beta) + \eta_\alpha(t)$$

$$\partial_t f_1(1, t) = -v_1 \partial_{x_1} f_1(1) + \zeta \partial_{p_1} v_1 f_1(1) + \Delta \partial_{p_1}^2 f_1(1) + \partial_{p_1} \int d2\, \partial_{x_1} V(x_{12}) f_2(1, 2, t)$$

Fokker-Plank equation - 3

Use properties of Gaussian noise to carry out averages

$$\partial_t < \hat{f} > \quad + \quad \frac{\partial}{\partial \mathbf{X}} \cdot \mathbf{V} < \hat{f} > + \frac{\partial}{\partial \mathbf{X}} \cdot < \boldsymbol{\eta}(t) e^{-Lt} f(\mathbf{X}, 0) >$$
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Smoluchowski equation

1. One obtains a hierarchy of Fokker-Planck equations for $f_1(1)$, $f_2(1,2)$, $f_3(1,2,3)$, ... To proceed we need a closure ansatz. Low density (neglect correlations) $f_2(1,2,t) \simeq f_1(1,t)f_1(2,t)$
2. It is instructive to solve the FP equation by taking moments

$$c(x,t) = \int dp\, f(x,p,t) \qquad \text{concentration of particles}$$
$$J(x,t) = \int dp\, (p/m) f(x,p,t) \qquad \text{density current}$$

Eqs. for the moments obtained by integrating the FP equation.

$$\partial_t c(x,t) = -\partial_x J(x,t)$$
$$\partial_t J(x_1) = -\zeta J(x_1) - \frac{m\Delta}{\zeta}\partial_{x_1} c(x_1) - \int dx_2 [\partial_{x_1} V(x_{12})] c(x_1,t) c(x_2,t)$$

For $t >> \zeta^{-1}$, we eliminate J to obtain a Smoluchowski eq. for c

$$\partial_t c(x_1,t) = D\partial_{x_1}^2 c(x_1,t) + \frac{1}{\zeta}\partial_{x_1}\int_{x_2}[\partial_{x_1} V(x_{12})] c(x_1,t) c(x_2,t)$$

Hydrodynamics

Due to the interaction with the substrate, momentum is not conserved. The only conserved field is the concentration of particles $c(x,t)$. This is the only hydrodynamic field.

To obtain a hydrodynamic equation form the Smoluchowski equation we recall that we are interested in large scales. Assuming the pair potential has a finite range R_0, we consider spatial variation of $c(x,t)$ on length scales $x >> R_0$ and expand in gradients

$$\begin{aligned}\partial_t c(x_1,t) &= D\partial^2_{x_1} c(x_1,t) + \frac{1}{\zeta}\partial_{x_1}\int_{x'} V(x')[\partial_{x'} c(x_1+x',t)]c(x_1,t) \\ &= D\partial^2_{x_1} c(x_1,t) + \frac{1}{\zeta}\partial_{x_1}\int_{x'} V(x')[\partial_{x_1} c(x_1,t) + x'\partial^2_{x_1} c(x_1,t) + ...]c(x_1,t)\end{aligned}$$

The result is the expected diffusion equation, with a microscopic expression for D_{ren} which is renormalized by interactions

$$\partial_t c(x,t) = \partial_x[D_{ren}\partial_x c(x,t)] \simeq D_{ren}\partial^2_x c(x,t)$$

Summary of Tutorial and Plan

Microscopic Langevin dynamics of interacting particles

Approximations: noise average; low density: $f_2(1,2) \simeq f_1(1)f_1(2)$

$\Downarrow$

Fokker Planck equation

$\Downarrow$

Overdamped limit: $t >> 1/\zeta$ Smoluchowski equation

$$\partial_t c(x_1,t) = \partial_{x_1}\left[D\partial_{x_1} c(x_1,t) - \frac{1}{\zeta}\int_{x_2} F(x_{12})c(x_2,t)c(x_1,t\right]$$

Pair interaction $F(x_{12})$:

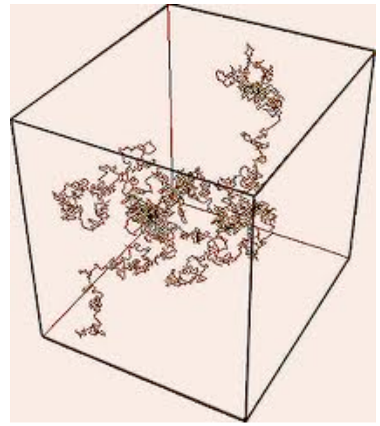
- steric repulsion $\longrightarrow$ SP rods
- short-range active interactions $\longrightarrow$ cross-linkers in motor-filaments mixtures
- medium-mediated hydrodynamic interactions $\longrightarrow$ swimmers

Smoluchowski $\longrightarrow$ Hydrodynamic equations

Diffusion of self-propelled (SP) rod

The center of mass of a Brownian rod performs a random walk

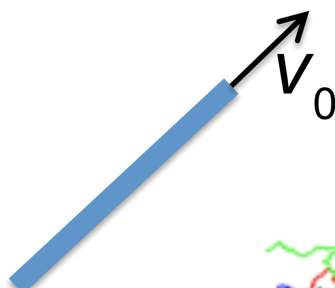
$$\Delta X(t) = \sqrt{\left\langle \left[\Delta \vec{x}(t) \right]^2 \right\rangle} \sim Dt$$

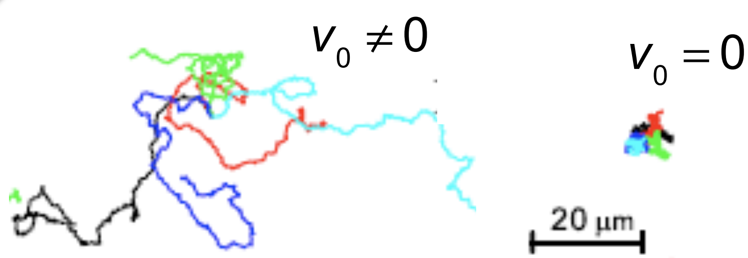


The center of mass of a SP rod performs a directed random walk

$$\sqrt{\left\langle \left[\Delta \vec{x}(t) \right]^2 \right\rangle} \sim \left(D + \frac{v_0^2}{2D_r} \right) t$$

Ballistic motion at speed v_0 randomized by rotational diffusion at rate D_r





Howse et al, PRL 2007

Smoluchowski equation for SP rods

The Smoluchowski equation for $c(\mathbf{r}, \hat{\boldsymbol{\nu}}, t)$ is given by

$$\begin{aligned}\partial_t c + v_0 \partial_{\|} c &= D_R \partial_\theta^2 c + (D_{\|} + D_S)\partial_{\|}^2 c + D_\perp \partial_\perp^2 c \\ &\quad -(I\zeta_R)^{-1}\partial_\theta(\tau_{ex} + \tau_{SP}) - \nabla \cdot \zeta^{-1} \cdot (\mathbf{F}_{ex} + \mathbf{F}_{SP})\end{aligned}$$

$$\partial_{\|} = \hat{\boldsymbol{\nu}} \cdot \boldsymbol{\nabla}$$
$$\boldsymbol{\partial}_\perp = \boldsymbol{\nabla} - \hat{\boldsymbol{\nu}}(\hat{\boldsymbol{\nu}} \cdot \boldsymbol{\nabla})$$

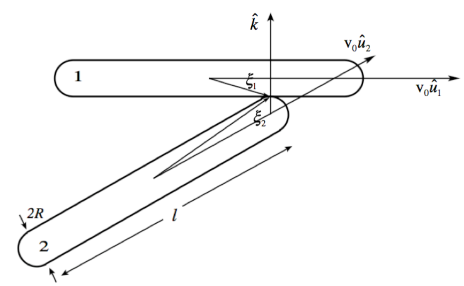
$D_S = v_0^2/\zeta_{\|}$ enhancement of longitudinal diffusion

Torques and forces exchanged upon collision as the sum of Onsager excluded volume terms and contributions from self-propulsion:

$$\tau_{ex} = -\partial_\theta V_{ex}$$
$$\mathbf{F}_{ex} = -\boldsymbol{\nabla} V_{ex}$$

$$V_{ex}(1) = k_B T a c(1,t) \int_{\xi_{12}} \int_{\hat{\boldsymbol{\nu}}_2} |\hat{\boldsymbol{\nu}}_1 \times \hat{\boldsymbol{\nu}}_2| \, c\,(\mathbf{r}_1 + \boldsymbol{\xi}_{12}, \hat{\boldsymbol{\nu}}_2, t)$$
$$\boldsymbol{\xi}_{12} = \boldsymbol{\xi}_1 - \boldsymbol{\xi}_2$$

$$\begin{pmatrix} \mathbf{F}_{SP} \\ \tau_{SP} \end{pmatrix} = v_0^2 \int_{s_1, s_2}' \int_{2, \hat{\mathbf{k}}} \begin{pmatrix} \widehat{\mathbf{k}} \\ \hat{\mathbf{z}} \cdot (\boldsymbol{\xi}_1 \times \widehat{\mathbf{k}}) \end{pmatrix} [\hat{\mathbf{z}} \cdot (\hat{\boldsymbol{\nu}}_1 \times \hat{\boldsymbol{\nu}}_2)]^2$$
$$\times \Theta(-\hat{\boldsymbol{\nu}}_{12} \cdot \widehat{\mathbf{k}}) c(1,t) c(2,t)$$



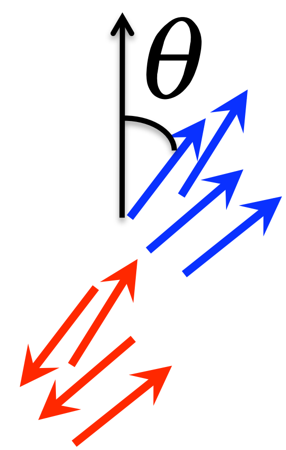
SP terms in Smoluchowski Eq.

- Convective term describes mass flux along the rod's long axis.
- Longitudinal diffusion enhanced by self-propulsion: $D_{||} \to D_{||} + v_0^2/\zeta_{||}$. Longitudinal diffusion of SP rod as persistent random walk with bias $\sim v_0$ towards steps along the rod's long axis.
- The SP contributions to force and torque describe, within mean-field, the additional anisotropic linear and angular momentum transfers during the collision of two SP rods.

  Mean-field Onsager: $\left\langle \frac{\Delta p_{coll}}{\Delta t} \right\rangle \sim \frac{v_{th}}{\tau_{coll}} \sim \frac{\sqrt{k_B T_a}}{\ell/\sqrt{k_B T_a}} \sim \frac{k_B T_a}{\ell}$

  SP rods: $\left\langle \frac{\Delta p_{coll}}{\Delta t} \right\rangle_{SP} \sim \frac{v_0|\hat{\boldsymbol{\nu}}_1 \times \hat{\boldsymbol{\nu}}_2|}{\ell/v_0|\hat{\boldsymbol{\nu}}_1 \times \hat{\boldsymbol{\nu}}_2|} \sim v_0^2|\hat{\boldsymbol{\nu}}_1 \times \hat{\boldsymbol{\nu}}_2|^2$

Hydrodynamics of SP Hard Rods



ρ density

$\vec{\mathrm{P}}$ polarization vector: $|\vec{\mathrm{P}}| \neq 0 \rightarrow$ polar order

$\overleftrightarrow{\mathrm{Q}}$ alignment tensor: $|\overleftrightarrow{\mathrm{Q}}| \neq 0 \rightarrow$ nematic order

$$\partial_t \rho + v_0 \vec{\nabla} \cdot \vec{P} = D\nabla^2 \rho + D_Q \vec{\nabla}\vec{\nabla} : \rho \overleftrightarrow{Q}$$

$$\partial_t \vec{P} + v_0 \vec{\nabla} \cdot \overleftrightarrow{Q} = -D_r \vec{P} + \lambda_1 \vec{P} \cdot \overleftrightarrow{Q} - \lambda_2 \left(\vec{P} \cdot \vec{\nabla}\right) \vec{P} - v_0 \vec{\nabla}\rho + K_P \nabla^2 \vec{P}$$

$$\partial_t \overleftrightarrow{Q} + v_0 \left[\vec{\nabla}\vec{P}\right]^{ST} = -D_r \left(1 - \frac{\rho}{\rho_{IN}}\right) \overleftrightarrow{Q} - \beta Q^2 \overleftrightarrow{Q} + D_Q \left(\vec{\nabla}\vec{\nabla} - \tfrac{1}{2} \overleftrightarrow{1} \nabla^2\right) \rho + K_Q \nabla^2 \overleftrightarrow{Q}$$

No bulk polar (moving) state → ordered state is **nematic**

SP lowers the density of the isotropic-nematic transition

(Baskaran & MCM, 2008)

PRL **96,** 258103 (2006) PHYSICAL REVIEW LETTERS week ending 30 JUNE 2006

Enhanced Ordering of Interacting Filaments by Molecular Motors

Pavel Kraikivski, Reinhard Lipowsky, and Jan Kierfeld

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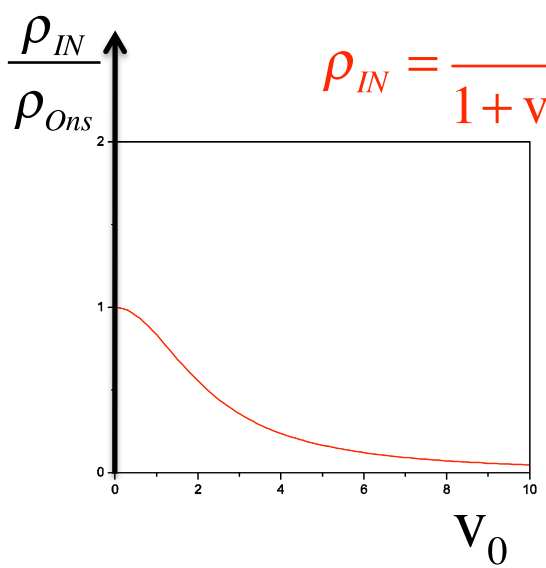
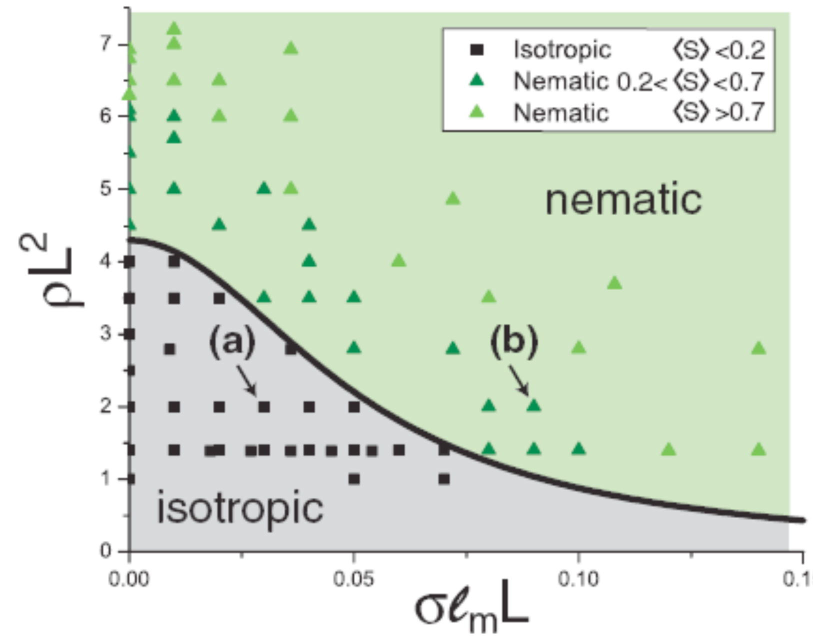
(Received 12 November 2005; published 29 June 2006)

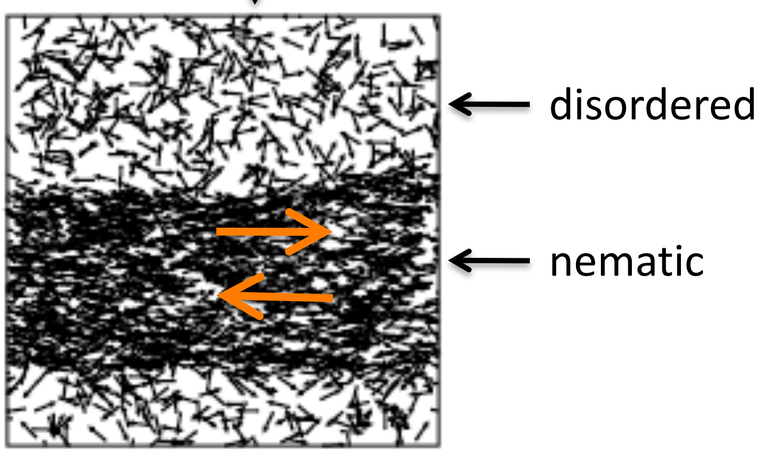


$$\rho_{IN} = \frac{\rho_{Ons}}{1 + v_0^2 / 3k_B T}$$



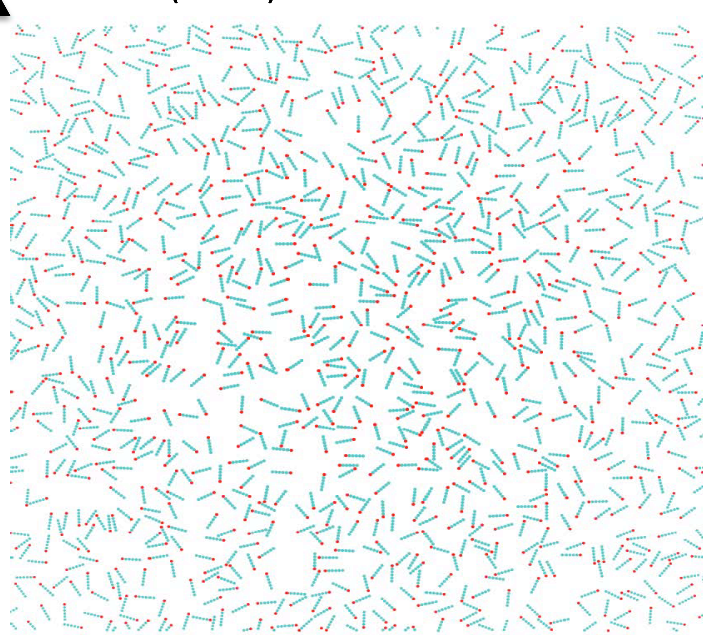
SP hard rods- Results:

- No uniform polar (moving) state, only nematic order (Baskaran & MCM 2008)
- Enhancement of nematic order & longitudinal diffusion (Baskaran & MCM, 2008)
- Uniform nematic state unstable → pattern formation (Baskaran & MCM, 2008)
- Strongly fluctuating nematic phase:
  - Polar "flocks" (Peruani et al,Yang et al.)
  - Nematic bands (Ginelli et al 2010)



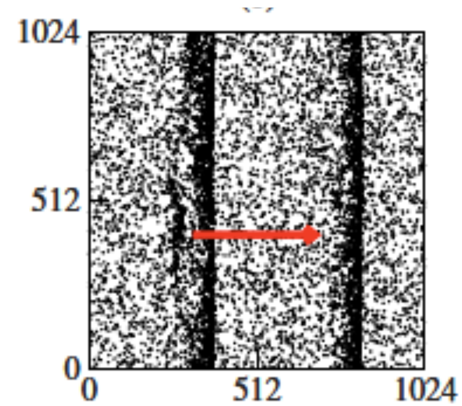
Ginelli, Peruani, Bar, Chate', PRL **104**, 184502 (2010)

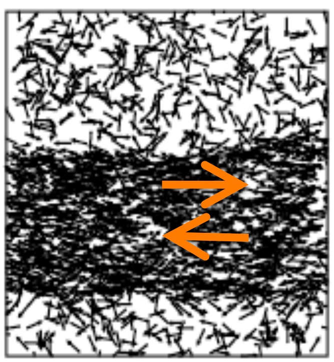
Yang, Marceau & Gompper, PRE **82**, 031904 (2010)



Three "universality" classes?

Active polar = polar particles+aligning interactions (bacteria, birds, motor-fils)
→polar moving state, traveling bands
→LRO in 2d, is the transition first order?





SP rods: polar particles+apolar interactions (myxobacteria, epithelial cells?)
→enhancement of nematic order, stationary bands, polar clusters

Active nematic: apolar particles+apolar interaction (melanocytes, motor-fils,epithelial cells?)

Ubiquitous giant number fluctuations