Active and Driven Soft Matter
Lecture 3: Self-Propelled Hard Rods

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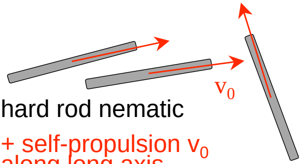
Lecture 1: Table of Contents

Active Hard Rod Nematic

- 2d hard rods
- Excluded volume interaction
- Overdamped dynamics
- Non-thermal white noise

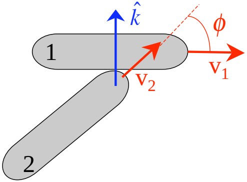
$\Rightarrow$ hard rod nematic

+ self-propulsion v_0 along long axis



1. Start with Langevin dynamics of coupled orientational and translational degrees of freedom plus hard core collisions

$\rightarrow$ SP yields anisotropic enhancement of momentum transferred in a hard core collision



2. **Derive** continuum theory

Plan and Results

- The lecture illustrates how to use the tools of statistical physics to derive hydrodynamics from microscopic dynamics for a minimal model of a self-propelled system.
- Inspired by Vicsek model of SP point particles that align with neighbors according to prescribed rules in the presence of noise. This rule-based model orders in polar (moving) states below a critical value of the noise.
- Hard rods order in nematic states due to steric effects: can excluded volume interactions, plus self-propulsion, yield a polar state?
- **Result**: **no** homogeneous polar state, but other nonequilibrium effects:
  - SP enhances nematic order
  - SP enhances longitudinal diffusion ("persistent" random walk)
  - SP yields propagating sound-like waves in the isotropic state
  - SP destabilizes the nematic state
  - SP+boundary effects can yield a polar state

Langevin dynamics

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

$$m\frac{dv}{dt} = -\zeta v + \eta(t) \qquad \zeta = 6\pi\eta a \text{ friction}$$

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

In this case it is convenient to work with phase-space distribution functions:

$$\hat{f}_N(x_1, p_1, x_2, p_2, ..., x_N, p_N, t) \equiv \hat{f}_N(x_N, p_N, t)$$

These are useful when dealing with both Hamiltonian dynamics and Langevin (stochastic) dynamics.

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

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

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

Conservation law for probability distribution

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

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

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

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

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

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

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

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

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

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

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

Smoluchowski $\rightarrow$ Hydrodynamic equations

SP Rods

The algebra is quite a bit more involved for a number of reasons:

1. translational and rotational degrees of freedom are coupled

$$\frac{\partial \mathbf{v}_\alpha}{\partial t} = v_0 \hat{\boldsymbol{\nu}}_\alpha - \boldsymbol{\zeta}(\hat{\boldsymbol{\nu}}_\alpha) \cdot \mathbf{v}_\alpha - \sum_\beta T(\alpha,\beta)\,\mathbf{v}_\alpha + \boldsymbol{\eta}_\alpha(t)$$

$$\frac{\partial \omega_\alpha}{\partial t} = -\zeta_R \omega_\alpha - \sum_\beta T(\alpha,\beta)\,\omega_\alpha + \eta^R_\alpha(t)$$

where $\langle \eta_{\alpha i}(t)\eta_{\beta j}(t')\rangle = 2k_B T_a\,\zeta_{ij}(\hat{\boldsymbol{\nu}}_\alpha)\delta_{ij}\delta(t-t')$

$$\left\langle \eta^R_\alpha(t)\,\eta^R_\beta(t')\right\rangle = 2k_B T_a\,(\zeta_R/I)\,\delta_{\alpha\beta}\delta(t-t'), \qquad I = \ell^2/12$$

$$\zeta_{ij}(\hat{\boldsymbol{\nu}}_\alpha) = \zeta_{||}\hat{\nu}_{\alpha i}\hat{\nu}_{\alpha j} + \zeta_\perp(\delta_{ij} - \hat{\nu}_{\alpha i}\hat{\nu}_{\alpha j})$$

2. hard core interactions must be treated with care to handle properly the instantaneous momentum transfer
3. coupling of self-propulsion and collisional dynamics yields angular correlations

Smoluchowski equation for SP rods

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

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

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

$D_S = v_0^2/\zeta_\parallel$ enhancement of longitudinal diffusion

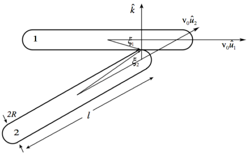
Torques and forces exchanged upon collision as the sum of Onsager excluded volume terms and contributions from self-propulsion:

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

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

$$\boldsymbol{\xi}_{12} = \boldsymbol{\xi}_1 - \boldsymbol{\xi}_2$$

$$\begin{pmatrix} \mathbf{F}_{SP} \\ \tau_{SP} \end{pmatrix} = v_0^2 \int_{s_1, s_2}^{l} \int_{2,\hat{\mathbf{k}}} \begin{pmatrix} \widehat{\mathbf{k}} \\ \hat{\mathbf{z}} \cdot (\boldsymbol{\xi}_1 \times \widehat{\mathbf{k}}) \end{pmatrix} [\hat{\mathbf{z}} \cdot (\hat{\boldsymbol{\nu}}_1 \times \hat{\boldsymbol{\nu}}_2)]^2$$
$$\times \Theta(-\hat{\boldsymbol{\nu}}_{12} \cdot \widehat{\mathbf{k}}) c(1,t) c(2,t)$$



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

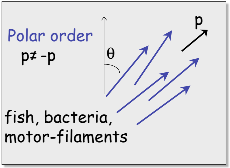
SP rods: $\left\langle \frac{\Delta p_{coll}}{\Delta t} \right\rangle_{SP} \sim \frac{v_0 |\hat{\boldsymbol{\nu}}_1 \times \hat{\boldsymbol{\nu}}_2|}{\ell / v_0 |\hat{\boldsymbol{\nu}}_1 \times \hat{\boldsymbol{\nu}}_2|} \sim v_0^2 |\hat{\boldsymbol{\nu}}_1 \times \hat{\boldsymbol{\nu}}_2|^2$

Hydrodynamics Fields

- Conserved density: $\rho(\mathbf{r}, t) = \int_{\hat{\boldsymbol{\nu}}} c(\mathbf{r}, \hat{\boldsymbol{\nu}}, t)$
- Order parameter fields:

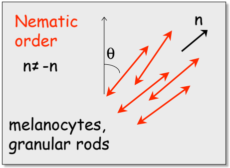
Polarization vector:

$$\mathbf{P}(\mathbf{r}, t) = \int_{\hat{\boldsymbol{\nu}}} \hat{\boldsymbol{\nu}}\, c(\mathbf{r}, \hat{\boldsymbol{\nu}}, t)$$



Nematic alignment tensor:

$$Q_{ij}(\mathbf{r}, t) = \int_{\hat{\boldsymbol{\nu}}} (\hat{\nu}_i \hat{\nu}_j - \tfrac{1}{2}\delta_{ij}) c(\mathbf{r}, \hat{\boldsymbol{\nu}}, t)$$



Hydrodynamics Equations

$$\partial_t \rho + v_0 \nabla \cdot \mathbf{P} = D_\rho \nabla^2 \rho + D_Q \boldsymbol{\nabla}\boldsymbol{\nabla} : \rho \mathbf{Q}$$

$$\begin{aligned}\partial_t \mathbf{P} = -D_R \mathbf{P} \quad + \quad & \lambda \mathbf{P} \cdot \mathbf{Q} - v_0 \boldsymbol{\nabla} \cdot \mathbf{Q} - \lambda_1 (\mathbf{P} \cdot \boldsymbol{\nabla}) \mathbf{P} - \lambda_2 \boldsymbol{\nabla} P^2 - \lambda_3 \mathbf{P} (\boldsymbol{\nabla} \cdot \mathbf{P}) \\ & - \frac{v_0}{2} \boldsymbol{\nabla} \rho + D_{bend} \nabla^2 \mathbf{P} + (D_{splay} - D_{benb}) \boldsymbol{\nabla} (\boldsymbol{\nabla} \cdot \mathbf{P})\end{aligned}$$

$$\begin{aligned}\partial_t \mathbf{Q} = -4 D_R \left(1 - \frac{\rho}{\rho_{IN}}\right) \mathbf{Q} \quad - \quad & v_0 [\boldsymbol{\nabla} \mathbf{P}]^{ST} - \lambda_4 [\mathbf{P} \boldsymbol{\nabla} \mathbf{Q}]^{ST} - \lambda_5 [\mathbf{Q} \boldsymbol{\nabla} \mathbf{P}]^{ST} - \lambda_6 [\boldsymbol{\nabla} \mathbf{P}]^{ST} \\ & + \frac{D_Q}{4} (\boldsymbol{\nabla}\boldsymbol{\nabla} - \frac{1}{2} \mathbf{1}) \rho + D'_Q \nabla^2 \mathbf{Q}\end{aligned}$$

$$[\mathbf{T}]_{ij}^{ST} = \tfrac{1}{2} (T_{ij} + T_{ji} - \tfrac{1}{2} \delta_{ij} T_{kk})$$

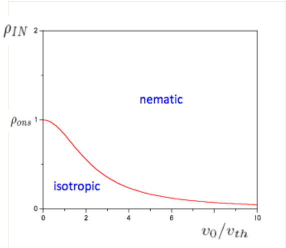
Homogeneous States

Neglecting all gradients, the equations are given by

$$\partial_t \rho = 0$$
$$\partial_t \mathbf{P} = -D_R \mathbf{P} + \lambda \mathbf{P} \cdot \mathbf{Q}$$
$$\partial_t \mathbf{Q} = -4 D_R \left[1 - \rho / \rho_{IN}(v_0)\right] \mathbf{Q}$$

Bulk states:

- Isotropic State: $\rho = \rho_0$, $\mathbf{P} = \mathbf{Q} = 0$
- No bulk uniform polar state: $\mathbf{P} = 0$
- Nematic state $\mathbf{P} = 0$, $\mathbf{Q} \neq 0$ for $\rho > \rho_{IN}$
- SP enhances nematic order: $\rho_{IN} = \frac{\rho_N}{1 + \frac{v_0^2}{5 k_B T}}$ with $\rho_N = 3/(\pi \ell^2)$

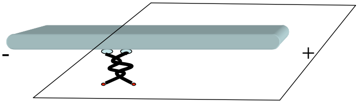


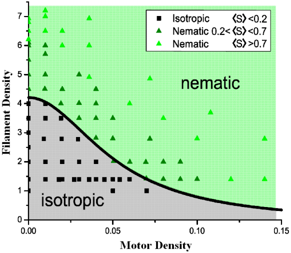
Enhanced Nematic order in Simulations of Actin Motility Assay

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
Max Planck Institute of Colloids and Interfaces, Science Park Golm, 14424 Potsdam, Germany
(Received 12 November 2005; published 29 June 2006)





Hydrodynamic Modes Stability of Bulk States

We examine the dynamics of the fluctuations of the hydrodynamic fields about their mean values and analyze the hydrodynamic modes of the system.

Isotropic state (neglect $\mathbf{Q}$)

$$\rho = \rho_0 + \delta\rho$$
$$\mathbf{P} = \mathbf{0} + \delta\mathbf{P}$$

Linearized equations:

$$\partial_t \delta\rho = D_\rho \nabla^2 \delta\rho + v_0 \rho_0 \boldsymbol{\nabla} \cdot \delta\mathbf{P}$$
$$\partial_t \delta\mathbf{P} = -D_R \delta\mathbf{P} + (v_0/2\rho_0)\boldsymbol{\nabla}\delta\rho$$

Fourier modes:

$$\delta\rho(\mathbf{r}, t) = \sum_{\mathbf{k}} \delta\rho_{\mathbf{k}}(t) e^{i\mathbf{k}\cdot\mathbf{r}} \qquad \delta\rho_{\mathbf{k}}(t) \sim e^{-z(k)t}$$
$$\delta\mathbf{P}(\mathbf{r}, t) = \sum_{\mathbf{k}} \delta\mathbf{P}_{\mathbf{k}}(t) e^{i\mathbf{k}\cdot\mathbf{r}} \qquad \delta\mathbf{P}_{\mathbf{k}}(t) \sim e^{-z(k)t}$$

$$z_\pm = -\frac{1}{2}(D_R + D_\rho k^2) \pm \frac{1}{2}\sqrt{(D_R - D_\rho k^2)^2 - 2v_0^2 k^2}$$

Sound Waves in Isotropic State

Propagating density waves in isotropic state of overdamped SP rods

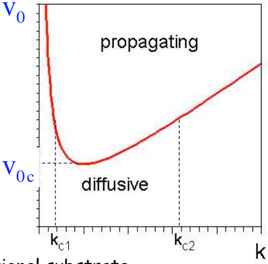
$$\partial_t \delta\rho = D_\rho \nabla^2 \delta\rho + v_0 \rho_0 \vec{\nabla} \cdot \vec{P}$$

$$\partial_t \vec{P} = -D_R \vec{P} + v_0 \vec{\nabla} \frac{\delta\rho}{\rho_0}$$

fluctuations: $\rho = \rho_0 + \delta\rho, \quad \vec{P} = \cancel{\vec{P}_0}^{\,0} + \delta\vec{P}$

Above a critical v_0 the system supports sound-like waves in a range of wavevectors

$$\boxed{v_{0c} \sim \ell D_R}$$

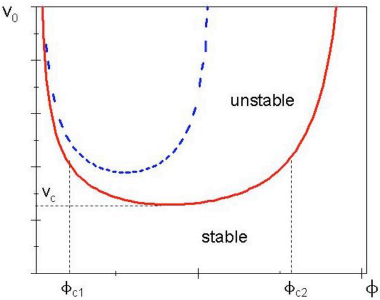


Ramaswamy & Mazenko, 1982: fluid on frictional substrate
--> movie of fluidized rods by Durian's lab

Instability of Nematic State

The nematic state is unstable for $v_0 > v_c(\phi, S)$, as shown in the figure for $S = 1$ (red line) and $S < 1$ (dashed blue line). The instability arises from a subtle interplay of splay and bend deformations.

$cos\phi = \hat{n}_0 \cdot \hat{\mathbf{k}}$
$\phi = 0$ pure bend
$\phi = \pi/2$ pure splay



Enhanced polar order near boundaries

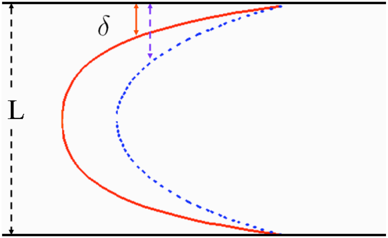
SP can enhance the size of correlated polar regions, as seen in simulations [F. Peruani, A. Deutsch and M. Bär, Phys. Rev. E **74**, 030904 (2006).].

Polarization profile across channel ($P_x(\pm L/2) = P_0$)

$$P_x(y) = P_0 \cosh(y/\delta)/\cosh(L/2\delta)$$

$$\delta = \ell/2\sqrt{5/2 + v_0^2/k_B T}$$

$$\delta(v_0 = 0) \sim \ell$$



Summary and Outlook

- A minimal model of interacting SP hard rods exhibits several novel nonequilibrium phenomena at large scales
  - No bulk polar state
  - enhancement of nematic order
  - enhancement of longitudinal diffusion
  - sound waves in isotropic state
  - enhanced polarization correlations
- We will consider in the last lecture a richer model that incorporates the role of fluid flow.
- References

1. R. Zwanzig, *Nonequilibrium Statistical Mechanics* (Oxford University Press, 2001), Chapters 1 and 2.
2. A. Baskaran and M. C. Marchetti, *Hydrodynamics of Self-Propelled Hard Rods*, Phys. Rev. E **77**, 011920 (2008).
3. A. Baskaran and M. C. Marchetti, *Enhanced Diffusion and Ordering of Self-Propelled Rods*, Phys. Rev. Lett. **101**, 268101 (2008).