Nematic states of active rods: Ordering and instabilities

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Introduction

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PHYSICAL REVIEW LETTERS

7 AUGUST 1995

Novel Type of Phase Transition in a System of Self-Driven Particles

Tamás Vicsek,^{1,2} András Czirók,¹ Eshel Ben-Jacob,³ Inon Cohen,³ and Ofer Shochet³



'Ferrofishes'



Lessons from Vicsek Model

• Large-scale and longtime behavior of the active system could be interesting.

Two active rod systems



V. Narayan et al, Science, (2007).

Plant Cell Cortical Microtubule Array



D.B. Slautterback 1963 JCB

Interphase microtubule asters of mice fibroblast cell

Interphase cortical microtubule array & preprophase band





http://www.maths.bris.ac.uk/~matbl/research/biophys.html

http://biology.anu.edu.au/CMS/FileUploads/file/gunning/

Cytoskeleton Nematics



1. Nucleation and treadmilling of microtubules



S.L. Shaw et al. 2003 Science

2. Zippering and crossover between interacting microtubules



The plant cell, 16, 3274(2004)

Cytoskeleton Nematics

1. Nucleation and treadmilling of microtubules



S.L. Shaw et al. 2003 Science



The plant cell, 16, 3274(2004)

Y. Sumino, et al, Nature, 2012

Basics of microtubule





Plus end dynamics



Minus end





A. Roll-Mecak & R.D. Vale, NATURE 451,363(2008)

'Self-propelled' microtubules



Molecular Biology of the Cell. 4th ed. Alberts B., et al. New York: <u>Garland Science</u>; 2002.

T. Surrey et al. Science, 292, 1167 (2001)

Time

A minimal model for interaction

Kinetic Monte-Carlo simulation model



X. Shi & Y. Ma, PNAS, 107, 11709 (2010)

Parameter description (symbol)	Simulated values
Simulated MT segment length (a)	1 (80 nm)
Simulated time step (7)	1 (0.2 s)
Plus-end GTP-state growing rate (k _{at})	0.3 (120 nm/s)
Plus-end GTP-state shortening rate (k _{st})	0.005 (2 nm/s)
Plus-end GDP-state growing rate (k_{gd})	0.03 (12 nm/s)
Plus-end GDP-state shortening rate (k_{sd})	0.5 (200 nm/s)
Minus-end GDP-state shortening rate (k _{sm})	0.1 (40 nm/s)
Hydrolysis rate of GTP-state unit (k _h)	0.05 (2.5 segments/s)
Nucleation rate (k _n)	0.005 (~4.0 μm ⁻² s ⁻¹)
Maximum MT length (Lm)	50 (4 µm)

Discontinuous isotropic-nematic transition



Dynamic mean-field theory 1

1. The moving of microtubules' center of mass







2. Discrete rate equation

$$\begin{aligned} \frac{\partial f(\mathbf{r},\mathbf{u},l,t)}{\partial t} &= k_p f\left(\mathbf{r} - \frac{a}{2}\mathbf{u},\mathbf{u},l - a,t\right) - k_p f(\mathbf{r},\mathbf{u},l,t) \\ &+ k_{df} f\left(\mathbf{r} + \frac{a}{2}\mathbf{u},\mathbf{u},l + a,t\right) - k_{df} f(\mathbf{r},\mathbf{u},l,t) \\ &+ k_{db} f\left(\mathbf{r} - \frac{a}{2}\mathbf{u},\mathbf{u},l + a,t\right) - k_{db} f(\mathbf{r},\mathbf{u},l,t) \end{aligned}$$

3. Spatially homogeneous condition

$$\frac{\partial f(\mathbf{u},l,t)}{\partial t} = k_p f(\mathbf{u},l-a,t) - k_p f(\mathbf{u},l,t) + k_{df} f(\mathbf{u},l+a,t) - k_{df} f(\mathbf{u},l,t) + k_{db} f(\mathbf{u},l+a,t) - k_{db} f(\mathbf{u},l,t).$$

4. Boundary condition for length

$$\frac{\partial f(\mathbf{u},2a,t)}{\partial t} = k_{ne}(\mathbf{u}) - (k_{df} + k_{db})f(\mathbf{u},2a,t) - k_p(\mathbf{u})f(\mathbf{u},2a,t) + (k_{df} + k_{db})f(\mathbf{u},3a,t),$$
$$\frac{\partial f(\mathbf{u},L,t)}{\partial t} = -(k_{df} + k_{db})f(\mathbf{u},L,t) + k_p(\mathbf{u})f(\mathbf{u},L-a,t),$$

Dynamic mean-field theory 2

Steric interaction hinders polymerization



Steric interaction kernal of a segment with length a/N

$$W(\mathbf{r},\mathbf{r}',\mathbf{u},\mathbf{u}',l,l') = |\mathbf{u}\times\mathbf{u}'| \int_0^{a/N} d\eta \int_{-\frac{l'}{2}}^{\frac{l'}{2}} d\xi \delta \left[\left(\mathbf{r} + \left(\frac{l}{2} + \eta\right)\mathbf{u}\right) - (\mathbf{r}' - \xi\mathbf{u}') \right]$$

Probability of a segment with length a/N intersect with existing microtubule

$$p_r(\mathbf{r},\mathbf{u},l) = \int dl' \int d\mathbf{u}' \int d\mathbf{r}' W(\mathbf{r},\mathbf{r}',\mathbf{u},\mathbf{u}',l,l') f(\mathbf{r}',\mathbf{u}',l')$$

Modified polymerization rate

$$k_p(\mathbf{u}) = k_{p0} \lim_{N \to \infty} \left(1 - p_r(\mathbf{u}) \right)^N = k_{p0} \exp\left(-\sum_{l'=2}^L l' \int d\mathbf{u}' f(\mathbf{u}', l') |\mathbf{u} \times \mathbf{u}'| \right)$$

Steady state solution

1.Self-consistent integral equation

$$f(\mathbf{u},l) = A \exp\left[\Delta G \cdot l - l \sum_{l'}^{L} l' \int d\mathbf{u}' f(\mathbf{u}',l') |\mathbf{u} \times \mathbf{u}'|\right]$$

where $A = k_n \exp(-2\Delta G)/(k_{df} + k_{db})$
 $\Delta G = \ln[k_{p0}/(k_{df} + k_{db})]$

2. Isotropic solution

$$f(\mathbf{u},l) = f_l = Ae^{\Delta G \cdot l - 2f_0 l \langle l \rangle} \quad \text{with} \quad f_0 = \sum_{l=2}^L f_l, \, \langle l \rangle = (\sum_{l=2}^L lf_l) / f_0$$

3. Bifurcation analysis and numerical result

We have $f_0 = \frac{3}{2\langle l^2 \rangle}$ at the phase boundary



Phase behavior of cortical microtubules

Phase maps for controlled microtubule number system

 $f(\mathbf{u},l) = A \exp\left[\Delta G \cdot l - l \sum_{i=1}^{L} l' \int d\mathbf{u}' f(\mathbf{u}',l') |\mathbf{u} \times \mathbf{u}'|\right]$ where A is now determined by $\sum_{l=2}^{L} \int_{0}^{\pi} d\mathbf{u} f(\mathbf{u}, l) = \rho$ 0.117 Polymerization Rate (k_{p0}) 0.114 0.111 CEP 0.108 NII 0.105 0.2 0.4 0.8 0.0 0.6 Microtubule Number Density (ρ) Effective free energy functional for steady state $F\{f(\theta,l)\} = \sum_{l=2}^{L} \int_{0}^{\pi} d\mathbf{u} f(\mathbf{u},l) \ln[L\pi f(\mathbf{u},l)]$ + $\frac{1}{2}\sum_{n} ll' \int_0^{\pi} \int_0^{\pi} d\mathbf{u}_1 d\mathbf{u}_2 f(\mathbf{u}_1, l) f(\mathbf{u}_2, l') |\mathbf{u}_1 \times \mathbf{u}_2|$ $-\Delta G \sum_{l=2}^{L} l \int_{0}^{\pi} d\mathbf{u} f(\mathbf{u}, l) + \lambda \left(\sum_{l=2}^{L} \int_{0}^{\pi} d\mathbf{u} f(\mathbf{u}, l) - \rho \right)$

Simulation results



Transition properties across phase boundaries







Band formation







Driven granular rods



V. Narayan et al, Science, (2007).



Nematic State



Orientational order No position order

$$Q_{\alpha\beta} \equiv S(\hat{n}_{\alpha}\hat{n}_{\beta} - \delta_{\alpha\beta}/2) = \int \mathrm{d}\mathbf{u}(u_{\alpha}u_{\beta} - \delta_{\alpha\beta}/2)f(\mathbf{u})/\rho$$

Nematic State



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Curvature induced particle flows in active nematics

• Active flows:

$$J_i = -\alpha \partial_j \rho(\mathbf{r}) Q_{ij}(\mathbf{r}) \qquad J_y = -\partial_x \delta n_y$$

Topological defects



 $\oint_{\Gamma} \frac{\mathrm{d}\theta}{\mathrm{d}s} \mathrm{d}s = 2\pi k_{\mathrm{d}}$

P. M. Chaikin & T. C. Lubensky, Principle of condensed matter

C. Marchetti et al. RMP, 2013



R. Kemkemer, Eur. Phys. J. E 2000





Topological defects





V. Narayan et al, Science 2007

Topological defects







T. Sanchez et al, Nature 2013

Hydrodynamic model with media fluids



T. Sanchez et al, Nature 2013

L. Giomi et al. PRL, 2013

$$\frac{Dc}{Dt} = \partial_i [D_{ij}\partial_j c + \alpha_1 c^2 \partial_j Q_{ij}],$$

$$\rho \frac{Dv_i}{Dt} = \eta \nabla^2 v_i - \partial_i p + \partial_j \sigma_{ij}, \qquad \overline{\sigma_{ij}^a = \alpha_2 c^2 Q_{ij}},$$

$$\frac{DQ_{ij}}{Dt} = \lambda Su_{ij} + Q_{ik}\omega_{kj} - \omega_{ik}Q_{kj} + \gamma^{-1}H_{ij}$$



S. P. Thampi et al. PRL, 2013 S. P. Thampi et al. arXiv:1312.4836

Simulation model for granular rods

Kinetic Monte Carlo model of driven hard ellipse

 $\Delta \mathbf{r'}_j^n = 2\nu_0 h_j^n \mathbf{u}_j^n \eta_j^n$



V. Narayan et al, Science, (2007).



Breakdown of nematic order



g₂(**r**) correlation



Dynamics of topological defects

Active unbinding of topological defects pair



• Collision and annihilation of defects



Dynamics of topological defects

Active unbinding of topological defects pair



• Collision and annihilation of defects



Annihilation

Dynamics of topological defects

Active unbinding of topological defects pair



• Collision and annihilation of defects



Super-diffusivity



Racing of defects





Racing of defects





Polarity and flows







Collective motion in active nematics



Giant number fluctuations

$$\Delta N = \sqrt{\langle N \rangle + \rho_0^2 \int_A d\mathbf{r}_1 \int_A d\mathbf{r}_2 [g(|\mathbf{r}_1 - \mathbf{r}_2|) - 1]},$$











Enhanced ordering effects





Enhanced ordering effects



Collision induced rotations



Collision induced rotations



 $\partial_t f_{\pm} + k(f_{\pm} - f_{\mp}) \pm \nabla \cdot (\mathbf{v} f_{\pm}) = D_{\mathrm{r}} \mathscr{R}^2 f_{\pm} - \mathscr{R}(\omega_{\pm} f_{\pm})$

$$\partial_t f_{\pm} + k(f_{\pm} - f_{\mp}) \pm \nabla \cdot (\mathbf{v} f_{\pm}) = D_{\mathrm{r}} \mathscr{R}^2 f_{\pm} - \mathscr{R}(\omega_{\pm} f_{\pm})$$

• Total number distribution: $f(\mathbf{r}, \mathbf{u}) = f_+(\mathbf{r}, \mathbf{u}) + f_-(\mathbf{r}, \mathbf{u})$

 $\partial_t f(\mathbf{r}, \mathbf{u}) + \nabla \cdot [\mathbf{v} f_{\mathrm{m}}(\mathbf{r}, \mathbf{u})] + \mathscr{R}[\omega_+(\mathbf{r}, \mathbf{u}) f_+(\mathbf{r}, \mathbf{u}) + \omega_-(\mathbf{r}, \mathbf{u}) f_-(\mathbf{r}, \mathbf{u})] = D_{\mathrm{r}} \mathscr{R}^2 f(\mathbf{r}, \mathbf{u})$

$$\begin{split} \partial_t f_{\mathrm{m}}(\mathbf{r},\mathbf{u}) + \nabla \cdot \left[\mathbf{v}f(\mathbf{r},\mathbf{u})\right] + \mathscr{R}[\omega_+(\mathbf{r},\mathbf{u})f_+(\mathbf{r},\mathbf{u}) - \omega_-(\mathbf{r},\mathbf{u})f_-(\mathbf{r},\mathbf{u})] = \\ &- 2k f_{\mathrm{m}}(\mathbf{r},\mathbf{u}) + D_{\mathrm{r}}\mathscr{R}^2 f_{\mathrm{m}}(\mathbf{r},\mathbf{u}). \end{split}$$

$$\partial_t f_{\pm} + k(f_{\pm} - f_{\mp}) \pm \nabla \cdot (\mathbf{v} f_{\pm}) = D_{\mathbf{r}} \mathscr{R}^2 f_{\pm} - \mathscr{R}(\omega_{\pm} f_{\pm})$$

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 $f_{\mathrm{m}}(\mathbf{r},\mathbf{u}) = f_{+}(\mathbf{r},\mathbf{u}) - f_{-}(\mathbf{r},\mathbf{u})$

• Homogeneous condition: $\partial_t f(\mathbf{u}) = -\sigma_r v \mathscr{R}[f(\mathbf{u}) \mathscr{R}(W(\mathbf{u}))] + D_r \mathscr{R}^2 f(\mathbf{u}),$ $W(\mathbf{u}) = \int d\mathbf{u}' |\mathbf{u} \cdot \mathbf{u}'| f(\mathbf{u}')$

$$\partial_t f_{\pm} + k(f_{\pm} - f_{\mp}) \pm \nabla \cdot (\mathbf{v} f_{\pm}) = D_{\mathrm{r}} \mathscr{R}^2 f_{\pm} - \mathscr{R}(\omega_{\pm} f_{\pm})$$

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- Homogeneous condition: $\partial_t f(\mathbf{u}) = -\sigma_r v \mathscr{R}[f(\mathbf{u}) \mathscr{R}(W(\mathbf{u}))] + D_r \mathscr{R}^2 f(\mathbf{u}),$ $W(\mathbf{u}) = \int d\mathbf{u}' |\mathbf{u} \cdot \mathbf{u}'| f(\mathbf{u}')$
- Linear instability for isotropic state: $\partial_t S = (-4D_r + \frac{8\sigma_r v}{3\pi}\rho)S.$
- Critical density $\rho > D_{\rm r} \frac{3\pi}{2\sigma_{\rm r} v}$



$$\partial_t \delta n_y = \left(\frac{v^2 \rho}{4k} + \frac{\sigma_r v \rho^2}{3\pi} + \frac{4\sigma_r v \rho^2}{45\pi} - \frac{\sigma_r v \rho^2 (v+k)}{8k} - \frac{4\sigma_r v^2 \rho^2}{3\pi k}\right) \partial_x^2 \delta n_y + \left(\frac{v^2 \rho}{4k} + \frac{2\sigma_r v \rho^2}{15\pi}\right) \partial_y^2 \delta n_y$$

• Linear instability $\left[\rho > \rho^\star = \frac{90\pi v}{\sigma_r [(45\pi - 152)k + (45\pi + 240)v]}\right] \left[v/k > \frac{152/15 - 3\pi}{16 + 3\pi}\right]$



Regulation of collective motion through topological defects



Conclusions









Thank you for your attention!