THE ENIGMATIC ACTIVE NEMATIC

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Homi Bhabha Chair, Tata Education and Development Trust

OUTLINE

- Introduction
  - systems; aims; framework; early results
- Active nematics I: linear theory
  - fluctuation spectrum; stability from activity
- Active nematics II: topological defects
  - +1/2 is motile; unbinding transition; reentrance
- Conclusion

INTRODUCTION

systems of interest

millipedes: Surajit Dhara, U of Hyderabad

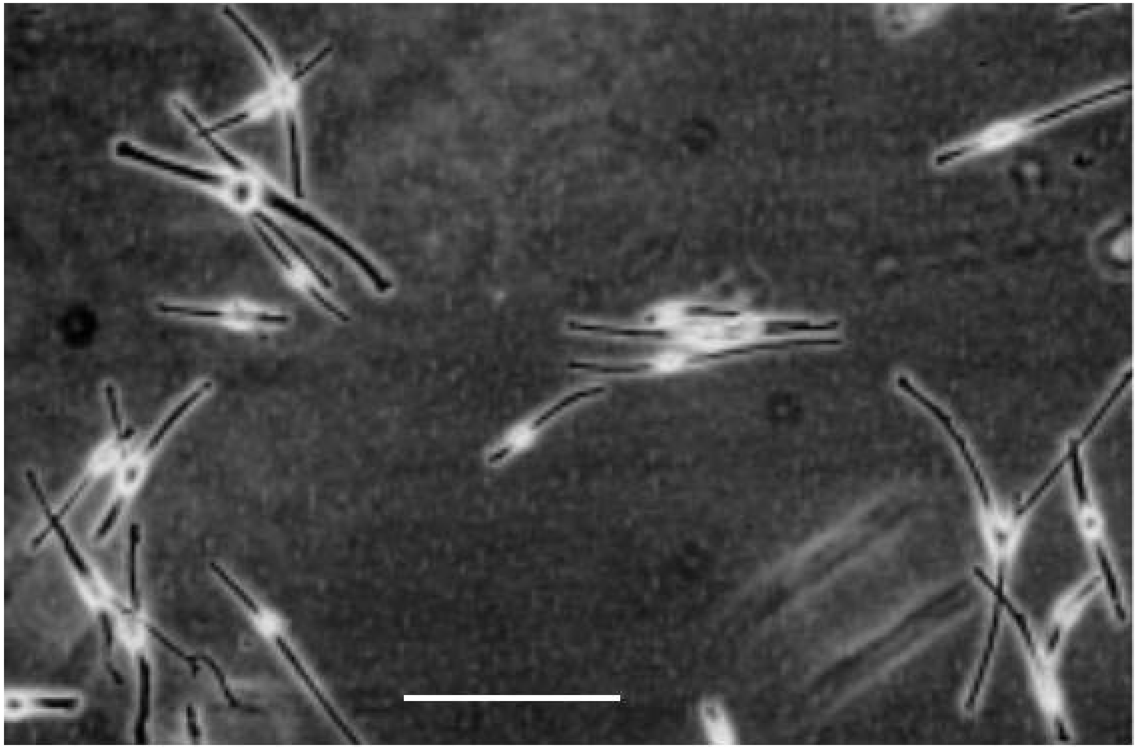
/home/sriram/talks/activemattertalks/current/mynas_rakesh_sharma_watch?v=nffdc9sLYnY.mp4

polar self-driven particles

E coli from Howard Berg's webpage http://www.rowland.harvard.edu/labs/bacteria/movies/ecoli.php

Nitin Kumar's self-propelled rods

systems of interest

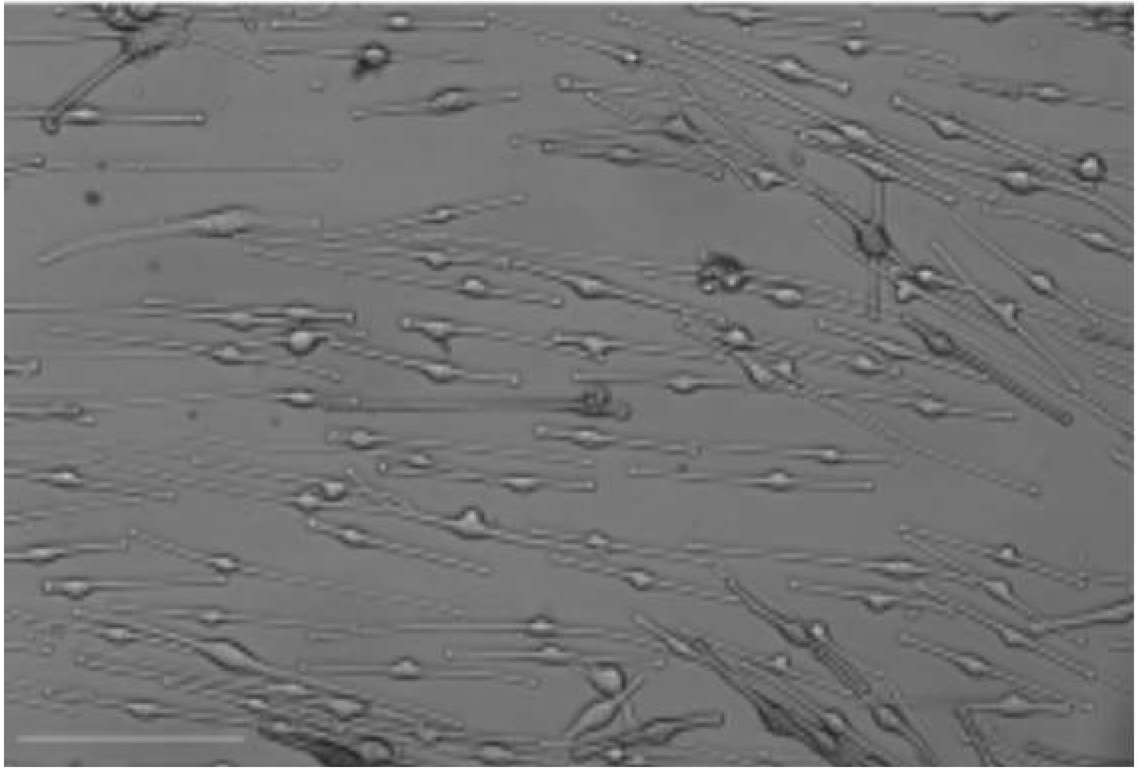


apolar:
self-driven,
pulsating, but
going nowhere

Human melanocytes on a plastic surface. The bar represents 100 µm: (a) melanocytes spread at low cell density. Small sized clusters with oriented cells are formed.

Kemkemer, R., Teichgräber, V., Schrank-Kaufmann, S. et al. Eur. Phys. J. E (2000) 3: 101. https://doi.org/10.1007/s101890070023

systems of interest

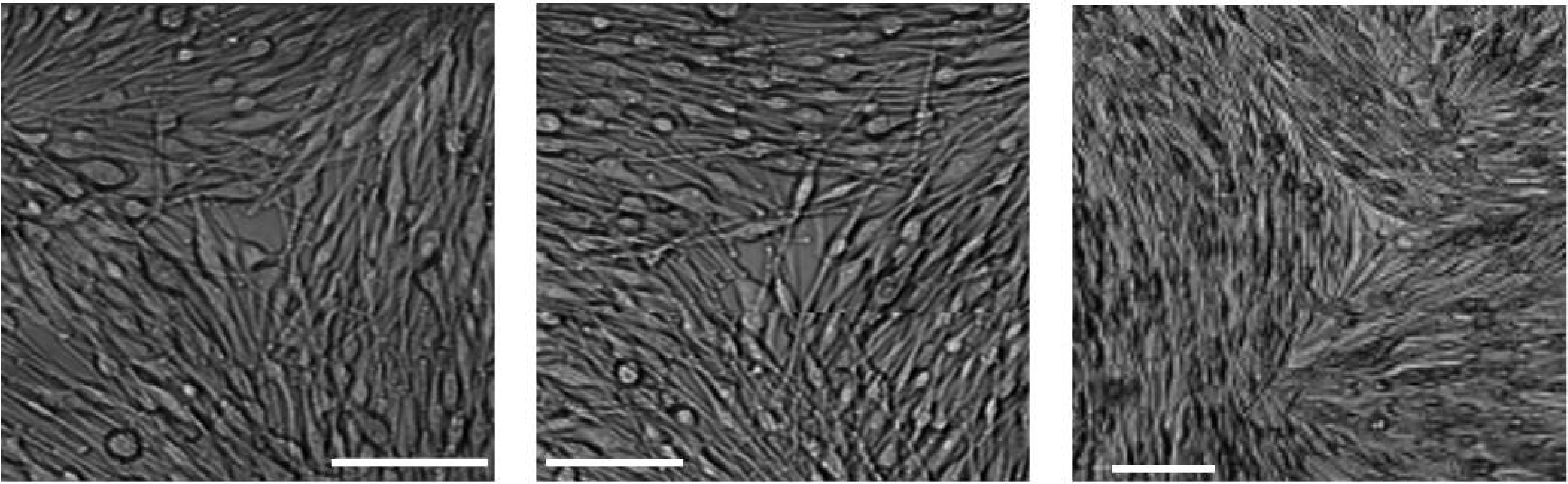


apolar:
self-driven,
pulsating, but
going nowhere

Human melanocytes on a plastic surface. The bar represents 100 μm: (b) At high cell density the cell density becomes more uniform and the cells are oriented over large distances.

Kemkemer, R., Teichgräber, V., Schrank-Kaufmann, S. et al. Eur. Phys. J. E (2000) 3: 101. https://doi.org/10.1007/s101890070023

systems of interest

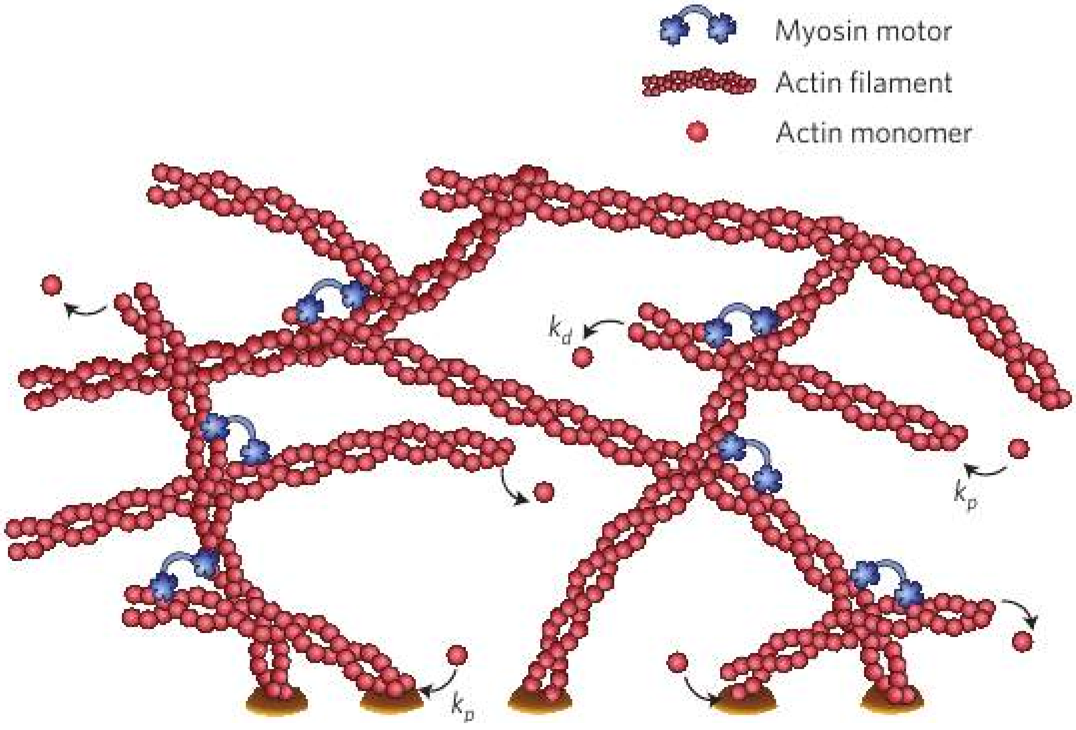


Kemkemer, R., Teichgräber, V., Schrank-Kaufmann, S. et al. Eur. Phys. J. E (2000) 3: 101. https://doi.org/10.1007/s101890070023

Winding number -1/2: nematic, not vector order

A m = −1/2 disclination is shown for melanocytes. The bar is 100 μm. Different possibilities are shown: (a) the core of the disclination is an area free of cells. (b) The core of the disclination is an area with isotropically distributed cell. (c) The core of the disclination is occupied by a star-shaped cell. The cells which form the nematoid fluid are in an elongated bipolar state.

systems of interest



Inside one cell: the cytoskeleton + motors + ATP

J. Prost, F. Jülicher and J-F. Joanny, Nat Phys 2015

INTRODUCTION
systems of interest

- A recurring and recursive theme
  - organised group of multicellular organisms: flock
  - organised collection of cells: colony/tissue/organism
  - organised collection of active components: cell
  - or even the nucleus

- Minimal realizations
  - purified cell extracts; reconstituted bio systems
  - active colloids, vibrated grains, `bots

- A machine in which each part is a machine*

*Leibniz, quoted by Needleman & Dogic

Active matter: definition

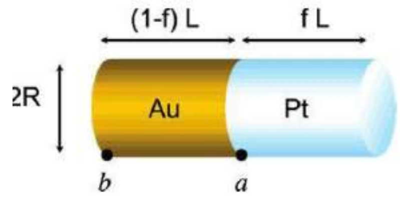
- Active particles are alive, or “alive”
  - living systems and their components
  - each constituent has dissipative Time’s Arrow
  - steadily transduces free energy to movement
  - detailed balance homogeneously broken
  - collectively: active matter
  - transient information: sensing and signalling
  - heritable information: self-replication
  - information on long timescales: evolution

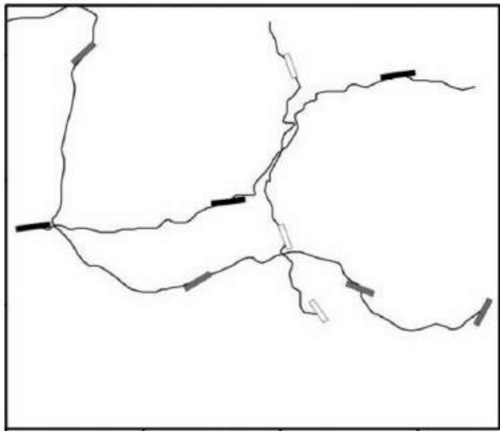
SR J Stat Mech 2017
Marchetti, Joanny, SR, Liverpool, Prost, Rao, Simha, *Rev. Mod. Phys.* **85** (2013) 1143-1189
Prost, Jülicher, Joanny, *Nat Phys* Feb 2015
SR: *Annu. Rev. Condens. Matt. Phys.* **1** (2010) 323
Toner, Tu, SR: *Ann. Phys.* **318** (2005) 170

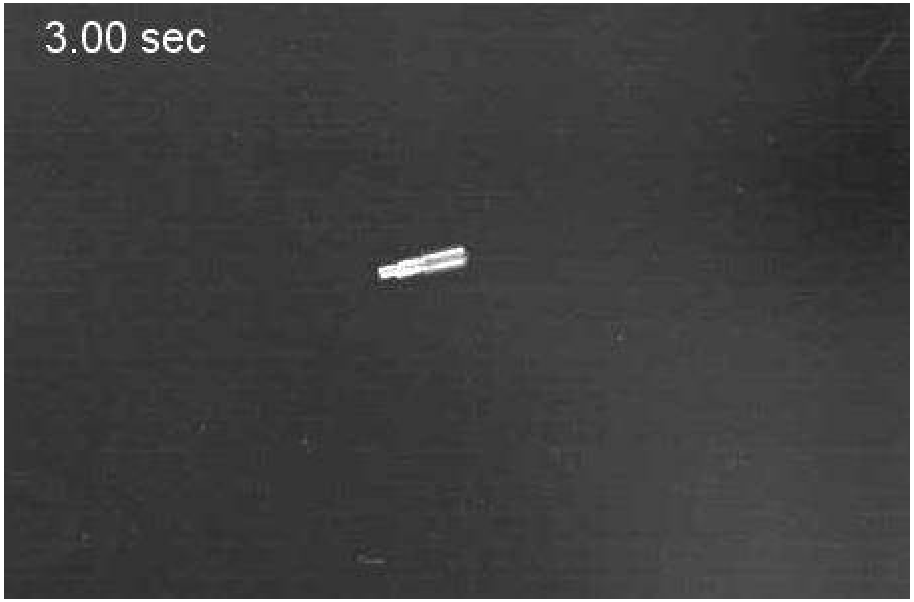
So:
motile creatures
living tissue
membranes + pumps
cytoskeleton + motors
....
but also:

Nonliving active matter

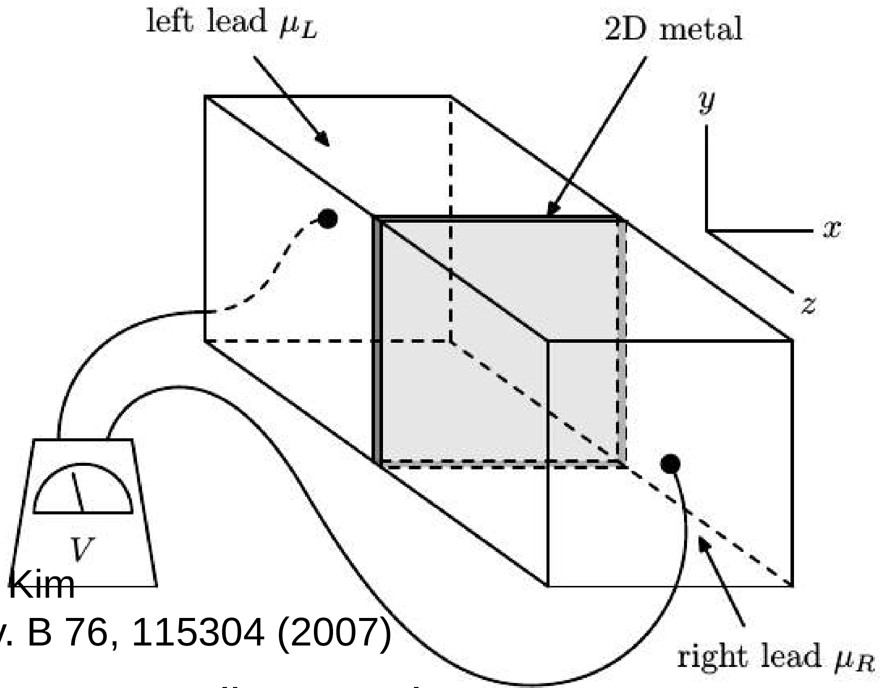
Catalytic particle in reactant bath
Sen, Mallouk, ... 2004; Golestanian et al. 2005
taxis: Saha et al. 2014







Motile brass rod
Kumar et al. 2011 - ....



Takei and Kim
Phys. Rev. B 76, 115304 (2007)

Active quantum matter? Alicea et al. 2006 2DEG + µwave

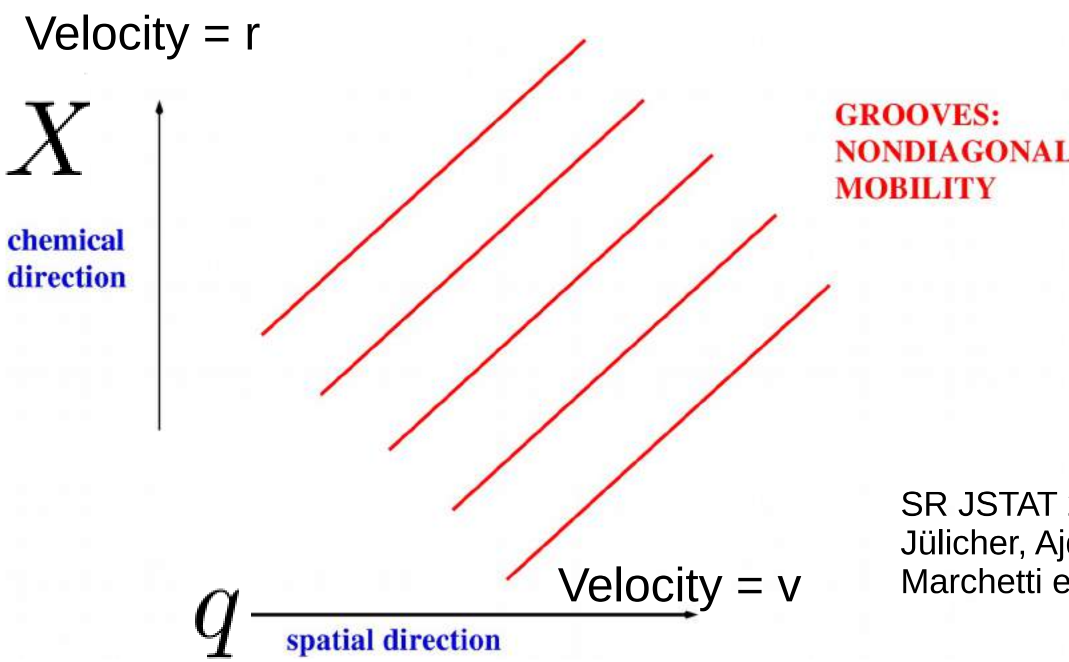
INTRODUCTION
aims

- Understand living stuff as condensed matter

- New physics, of course: powered particles
  - maintained energy *throughput*, not *budget*
  - each constituent carries dissipative Time's Arrow

- Physics in biology: information + mechanics
  - success of active matter: focus on mechanics
  - privileged role for motility, contractility
  - interactions local in spacetime
  - emphasise collective properties
  - focus on steady states: defer growth, selection….

INTRODUCTION
framework



SR JSTAT 2017
Jülicher, Ajdari, Prost RMP Colloq 1993
Marchetti et al. RMP 2013

Motor: catalyst for fuel breakdown

Include chemical direction in configuration space

Driving force $\Delta\mu = \mu_{\mathrm{reactant}} - \mu_{\mathrm{product}}$ in *chemical* direction

Mobility nondiagonal: vel = Mob*Force has *spatial* component

Use this to understand “new” terms, ruled out in equilibrium dynamics?

From Langevin equations to active dynamics

Temperature T; effective Hamiltonian $H(q,p,X,\Pi)$

q (time-rev even), p (odd); X, Π: extra coord, momentum

Off-diagonal q-dependent Onsager coefficients

$$\begin{aligned}
\dot{q} &= \partial_p H \\
\dot{p} + \Gamma_{11}\partial_p H + \Gamma_{12}(q)\partial_\Pi H &= -\partial_q H + \eta \\
\dot{\Pi} + \Gamma_{21}(q)\partial_p H + \Gamma_{22}\partial_\Pi H &= -\partial_X H + \xi \\
\dot{X} &= \partial_\Pi H
\end{aligned}$$

SR JSTAT 2017

$$\text{noises } \eta, \xi \quad \langle \eta(0)\xi(t)\rangle = 2k_B T\Gamma_{12}(q)\delta(t)$$

From Langevin equations to active dynamics

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\cancel{\dot{\Pi}} + \Gamma_{21}(q)\partial_p H + \Gamma_{22}\partial_\Pi H &= -\partial_X H + \xi \\
\dot{X} &= \partial_\Pi H
\end{aligned}$$

eliminate $\dot{X}$ from the p equation

noises η, ξ $\quad \langle \eta(0)\xi(t)\rangle = 2k_B T \Gamma_{12}(q)\delta(t)$

SR JSTAT 2017

From Langevin equations to active dynamics

$$\boxed{\begin{aligned} \dot{q} &= \partial_p H \\ \dot{p} + \Gamma \partial_p H - \frac{\Gamma_{12}(q)}{\Gamma_{22}} \partial_X H &= -\partial_q H + f \end{aligned}}$$

$$\dot{X} + \frac{\Gamma_{12}(q)}{\Gamma_{22}} \partial_p H = -\frac{1}{\Gamma_{22}} \partial_X H + \frac{\xi}{\Gamma_{22}}$$

$f \equiv \eta - (\Gamma_{12}/\Gamma_{22})\xi$ has variance $\propto$ $\Gamma \equiv \Gamma_{11} - \Gamma_{12}^2(q)/\Gamma_{22}$

$$\text{Equilibrium: } \partial_X H = 0$$ simplest

$$\text{Active? Hold } -\partial_X H \equiv -\Delta\mu \neq 0 \text{ fixed}$$

From Langevin equations to active dynamics

$$\dot{q} = \partial_p H$$

$$\dot{p} + \Gamma \partial_p H - \boxed{\frac{\Gamma_{12}(q)}{\Gamma_{22}} \Delta\mu} = -\partial_q H + f$$

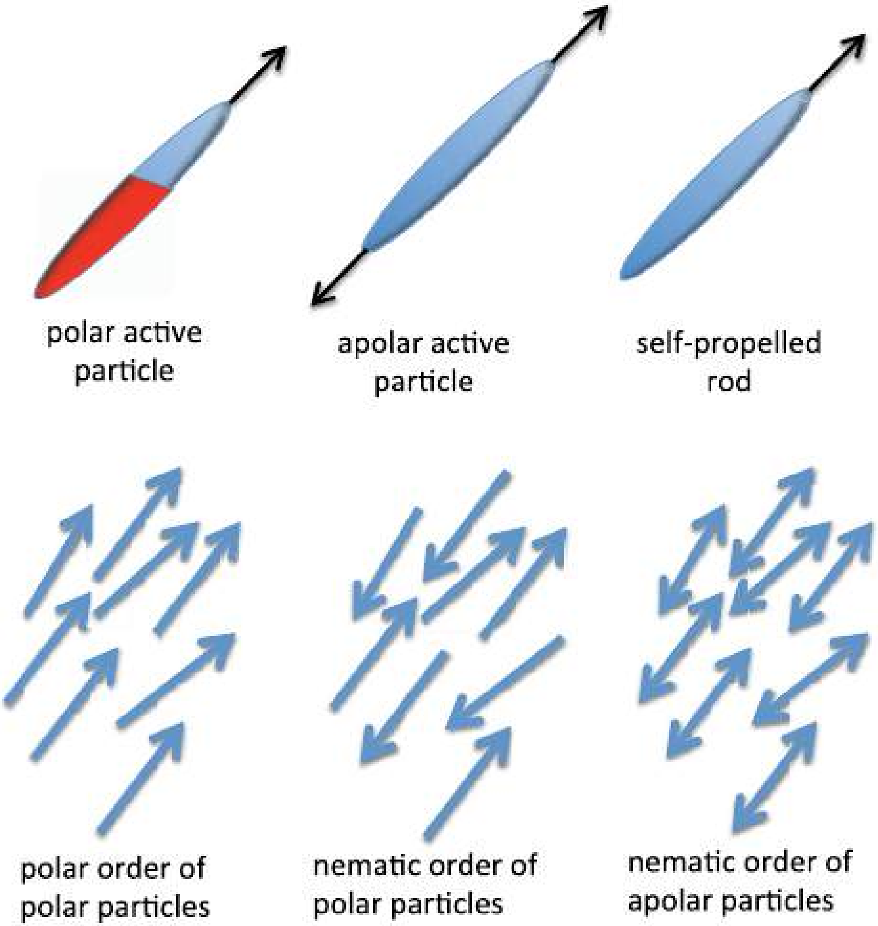
"New" terms, ruled out in equilibrium dynamics.
In general can't hide by redefining H, temperature....

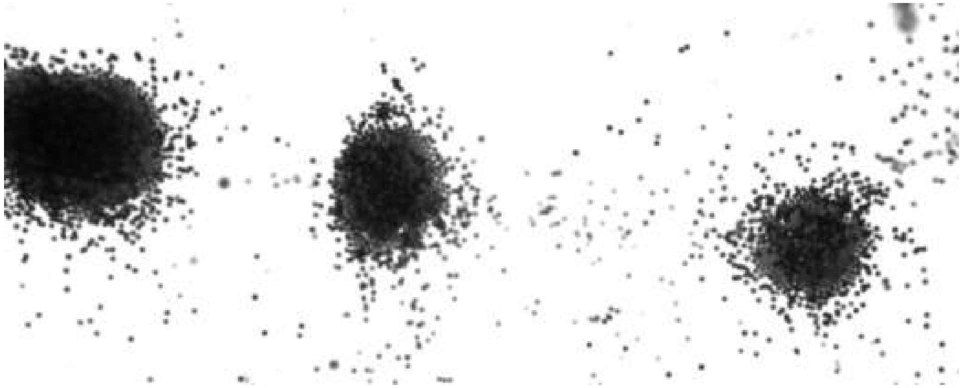
$$\dot{q} + \Gamma^{-1} \partial_q H = \boxed{\frac{\Delta\mu}{\Gamma_{22}\Gamma} \Gamma_{12}(q)} + \Gamma^{-1} f$$

No inertia: q-only equation of motion

Build all(?) active-matter dynamics this way (SR JSTAT 2017, Dadhichi, Maitra SR 2018)

Types of particles and order: examples





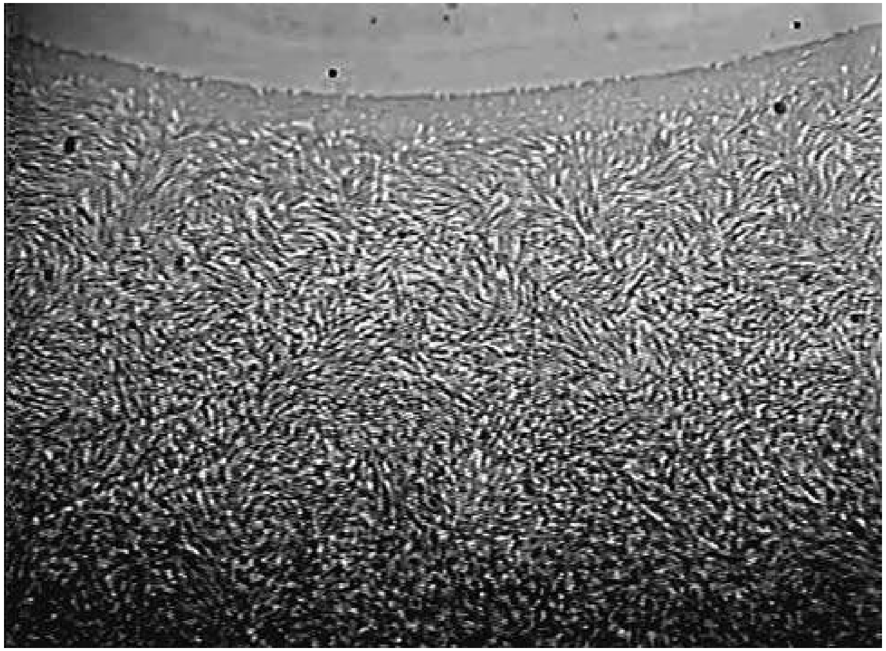
Scalar active matter
Chemically propelled droplets
S Thutupalli NCBS

headless "apolar" active particles

Vijay Narayan & N Menon 2007

Dynamical regimes

Wet: suspended in a fluid



Dry: with a passive momentum sink

DARIUSZ PACIOREK/GETTY https://www.wired.com/2013/03/powers-of-swarms/

Cisneros et al. Exp Fluids (2007) **43**:737–753

INTRODUCTION
early results

Q = orientation tensor (no polarity, only axis)

Flow carries, rotates and aligns orientation

Orientation distortions generate flow, particle currents

Active stress $\propto$ **Q**; current $\propto$ div **Q**

Simha and SR 2002; Simha, SR, Toner 2003, Hatwalne *et al.* 2004
Kruse, Juelicher, Joanny, Prost, Voituriez, Sekimoto 2004

$\Delta\mu$

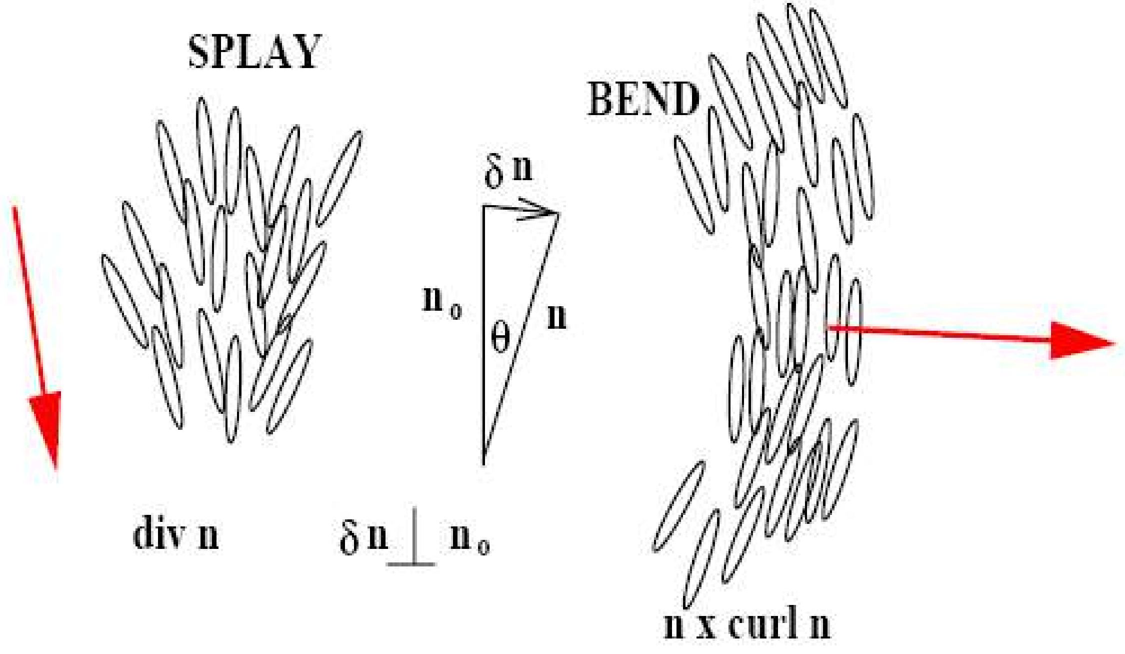
Many consequences & exptal confirmation
For example:

Convective instability by active stress

By B. A. Finlayson† and L. E. Scriven

Motion that sets in suddenly and spontaneously in a previously still material, *without the intervention of outside forces*, is a dramatic kind of conversion of internal energy to kinetic energy. When the ensuing motion is smoothly circulatory and the material itself appears to be homogeneous, devoid of structure on the scale of the motion, the nature of the engine at work challenges understanding. There are indications that such engines operate at the cellular level in living systems, if not yet anywhere else. We are launching here a search for the types of material behaviour required for self-starting, continuous mechanochemistry in mechanically isolated

ACTIVE NEMATICS I: linear theory
fluctuation spectrum



SR, Simha, Toner 2003

ASYMMETRY LEADS TO CURRENT

$$J_x \propto \partial_z \theta \qquad J_z \propto \partial_x \theta$$

Calculating number fluctuations

Langevin equations for concentration c and angle θ fields →

SR, Simha, Toner 2003

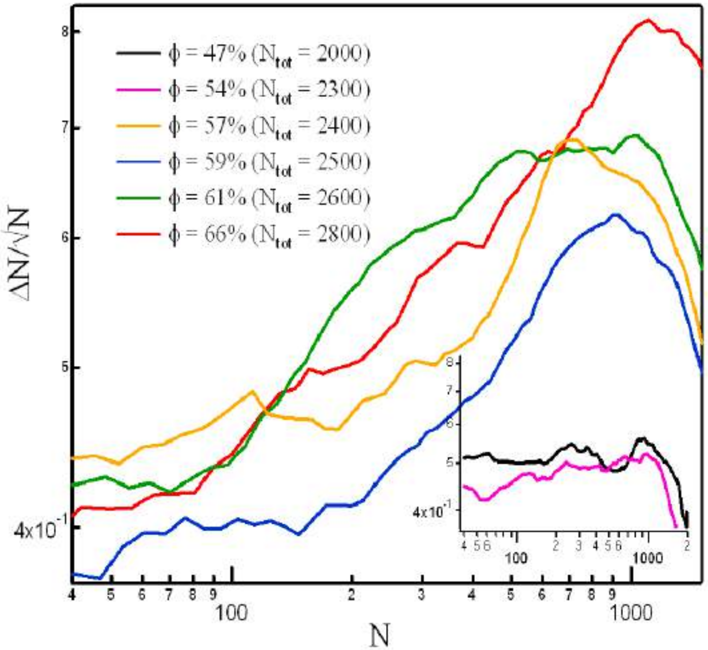
At wavevector q: $\langle|\theta_q|^2\rangle \sim 1/q^2$
nematic turbidity

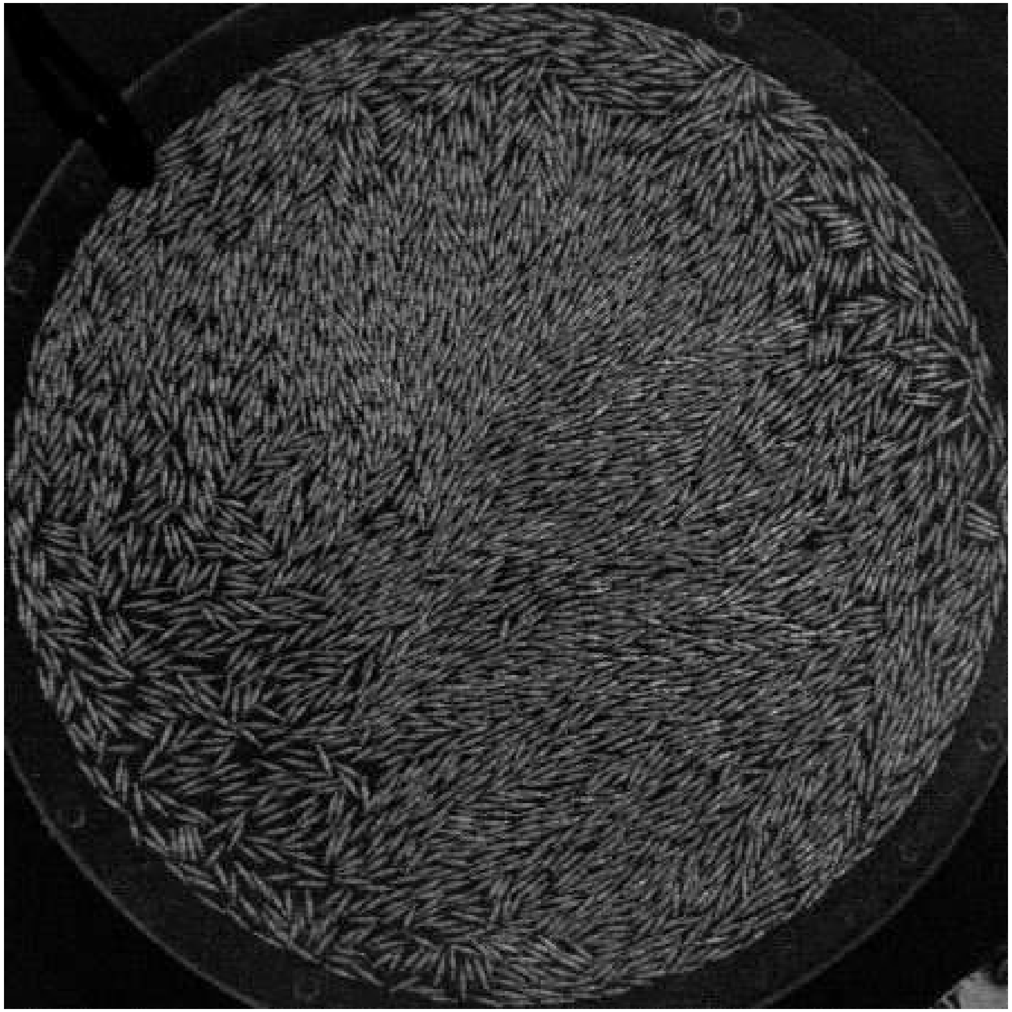
Diffusive current $J \sim \mathrm{grad}\, c$

Active current $J_x \propto \partial_z \theta$ $J_z \propto \partial_x \theta$

Concentration fluctuations also ~ $1/q^2$

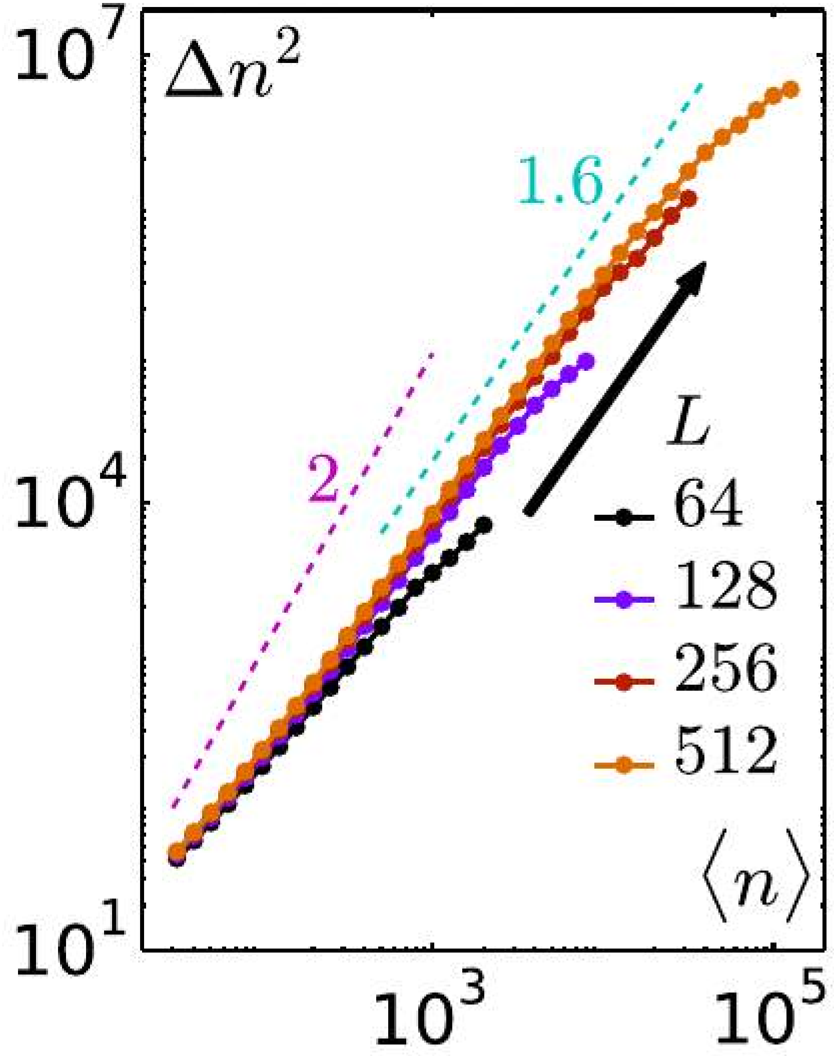
and nonlinearities marginally irrelevant





Experiments: giant number fluctuations
in a nonliving active nematic
V Narayan et al 2007

Computer experiments

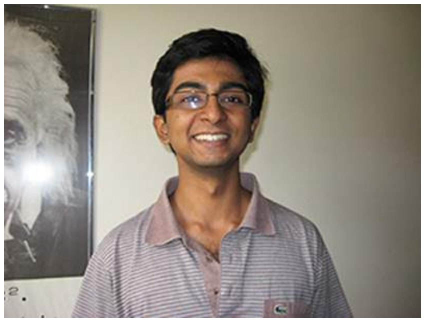


Ngo et al PRL 2014
Vicsek-style model
$\Delta n \sim n^a$, $1/2 < a < 1$

What's wrong with the linear theory?

A partial resolution
quasi-long-range order

Suraj Shankar, SR, M C Marchetti PRE 2018



Active current ~ div Q

Magnitude of Q ~ $L^{-\eta(\Delta)}$

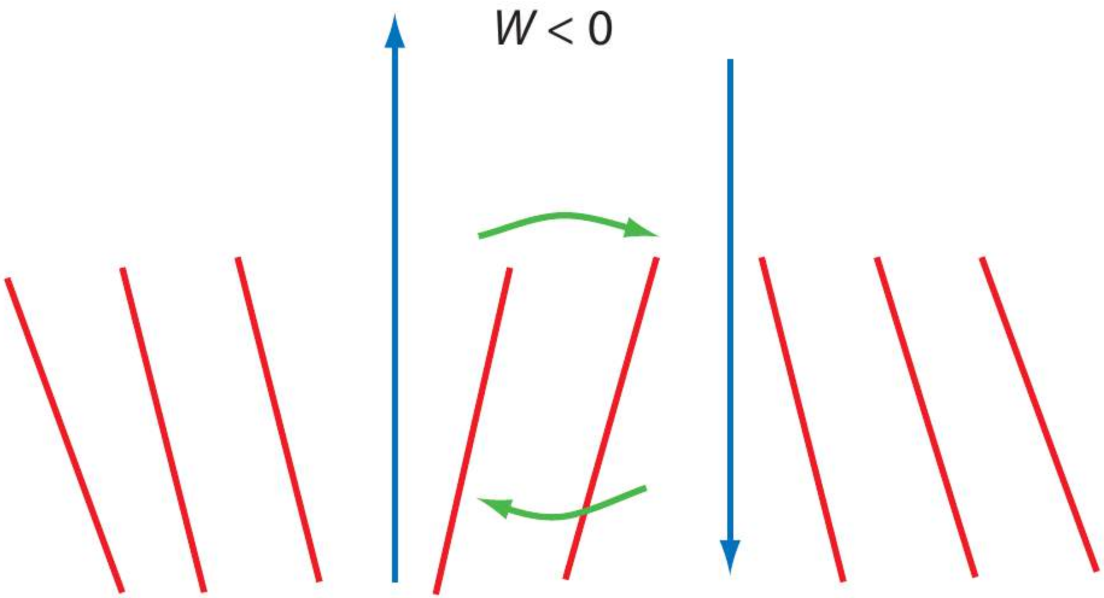
$$\Delta N \sim N^{1-\eta(\Delta)/2}$$

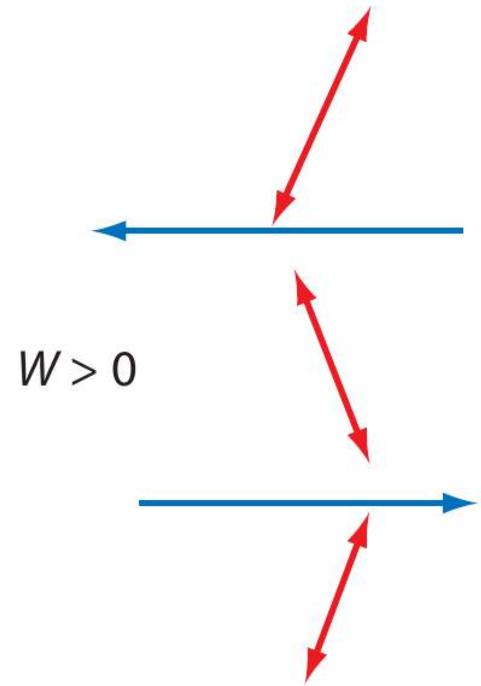
Number fluctuations weakened by quasi-long-range order of nematic

$\eta(\Delta)$ nonuniversal, Δ = noise strength

ACTIVE NEMATICS I: linear theory
instability

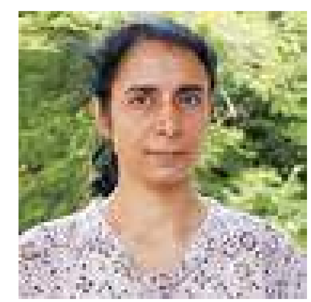
Bulk fluid, ignore inertia: unstable without threshold





growth-rate $\rightarrow W/\eta \neq 0$ as wavenumber $q \rightarrow 0$

viscosity ÷ active stress: a single timescale

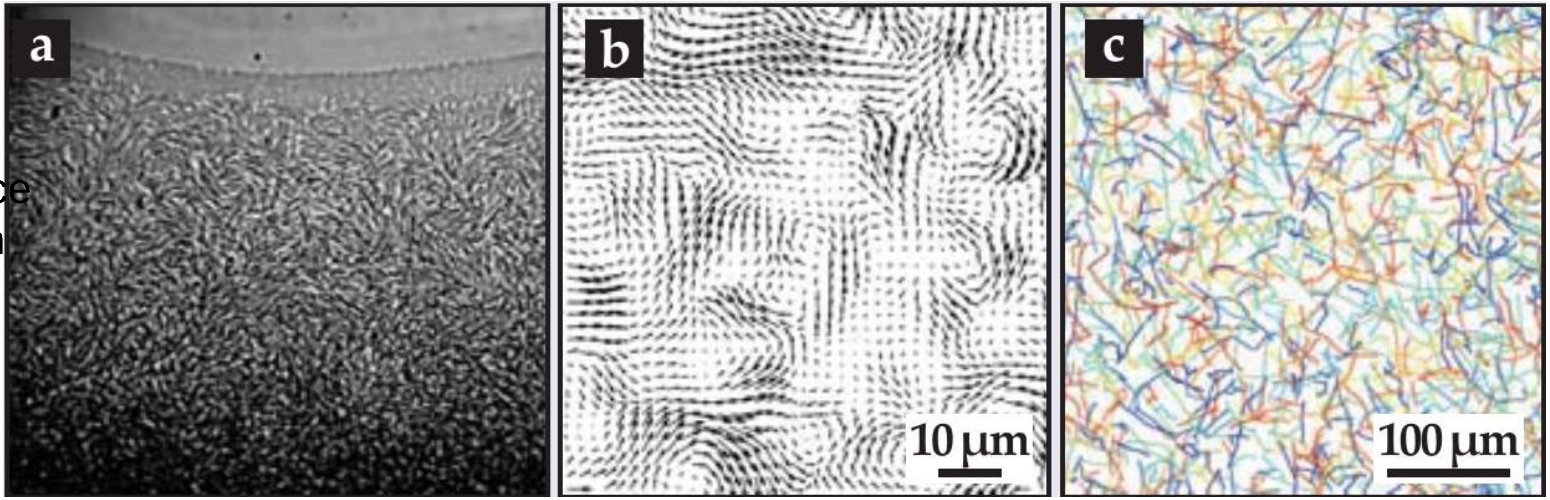


Simha & SR PRL 2002, Voituriez et al 2005
SR & Rao NJP 2007
Giomi, Marchetti, Liverpool 2008

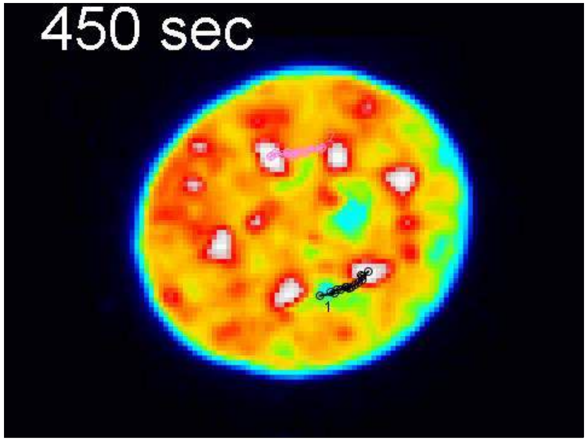
Chatterjee, Perlekar, Simha, SR 2018
Stokesian: self-propelling speed *can* stabilise!
Large scales: need polarity + anomalously high stiffness

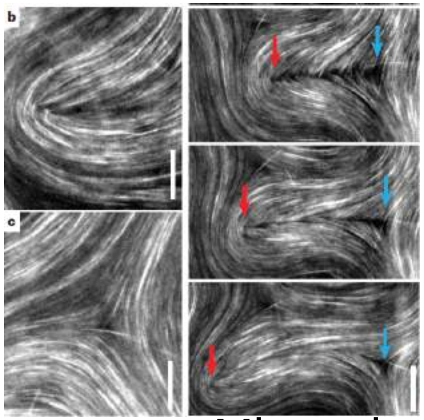
Evidence for the generic instability

Bacterial turbulence
Lauga & Goldstein
Phys Today 2012



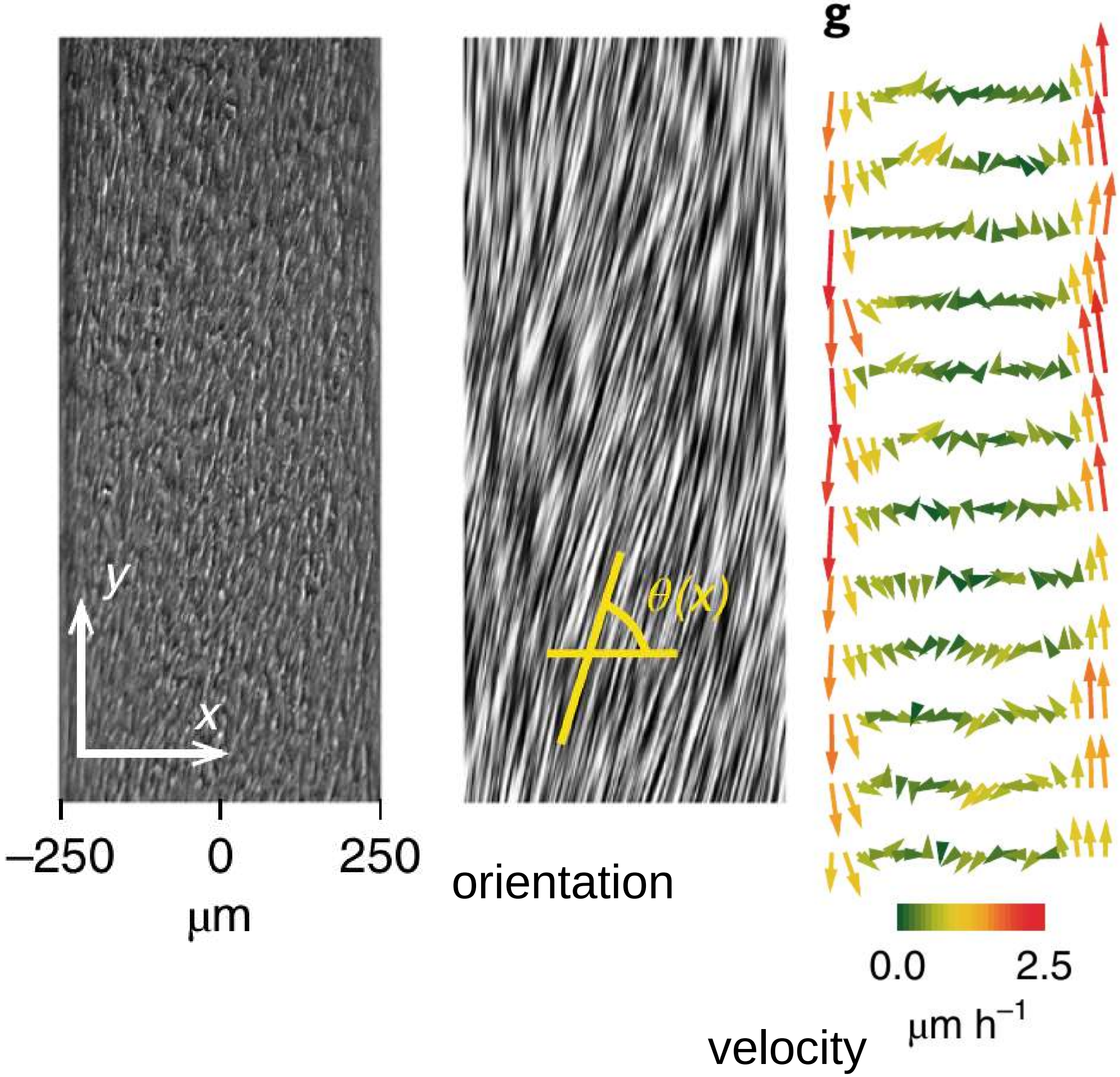
nuclear rotation
Kumar, Maitra... 2014





Microtubules + motors
Self-stirring fluid
Dogic 2013

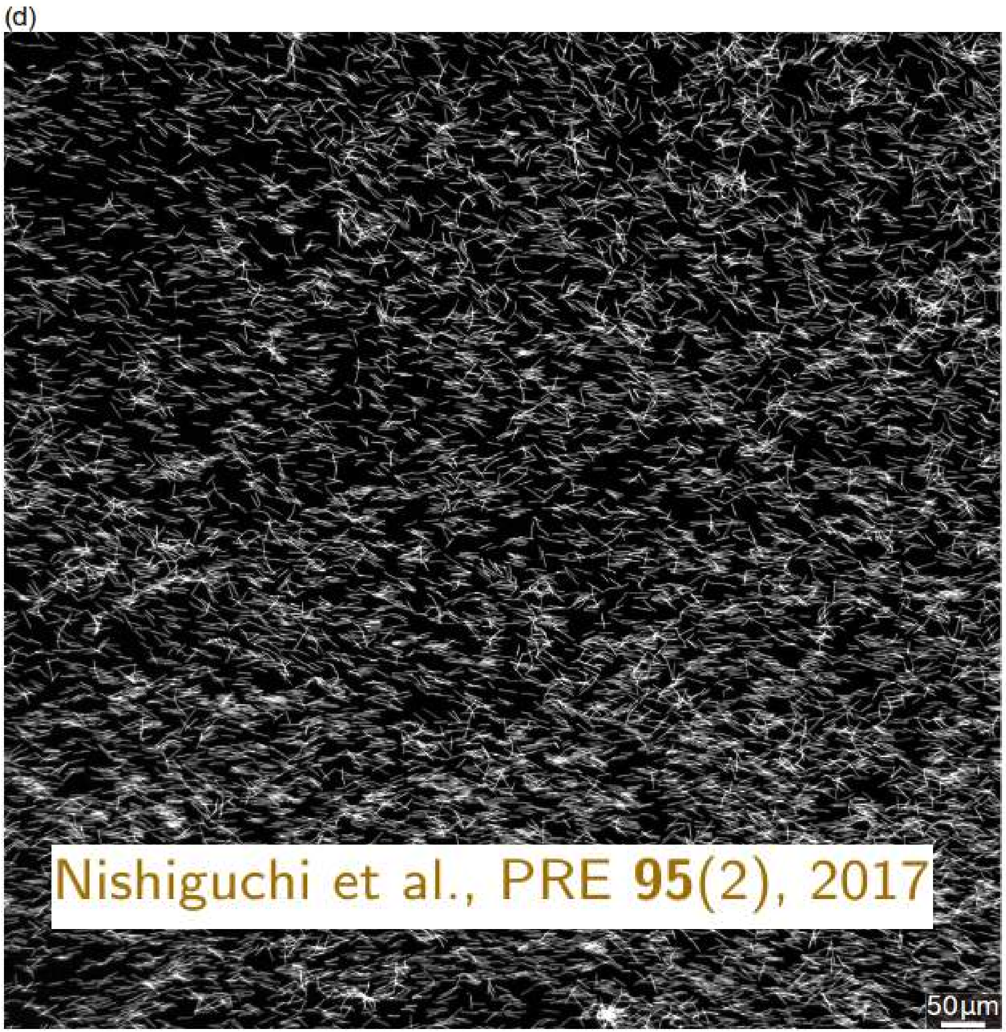
Spontaneous flow instability in a nematic epithelium



detailed confirmation
flow, orientation profile
strip geometry
Duclos et al NPhys 2018

Also: F Sagues 2018
liquid crystal + bacteria
See onset, instability growth,
Single timescale

Unreasonably stable active nematics?

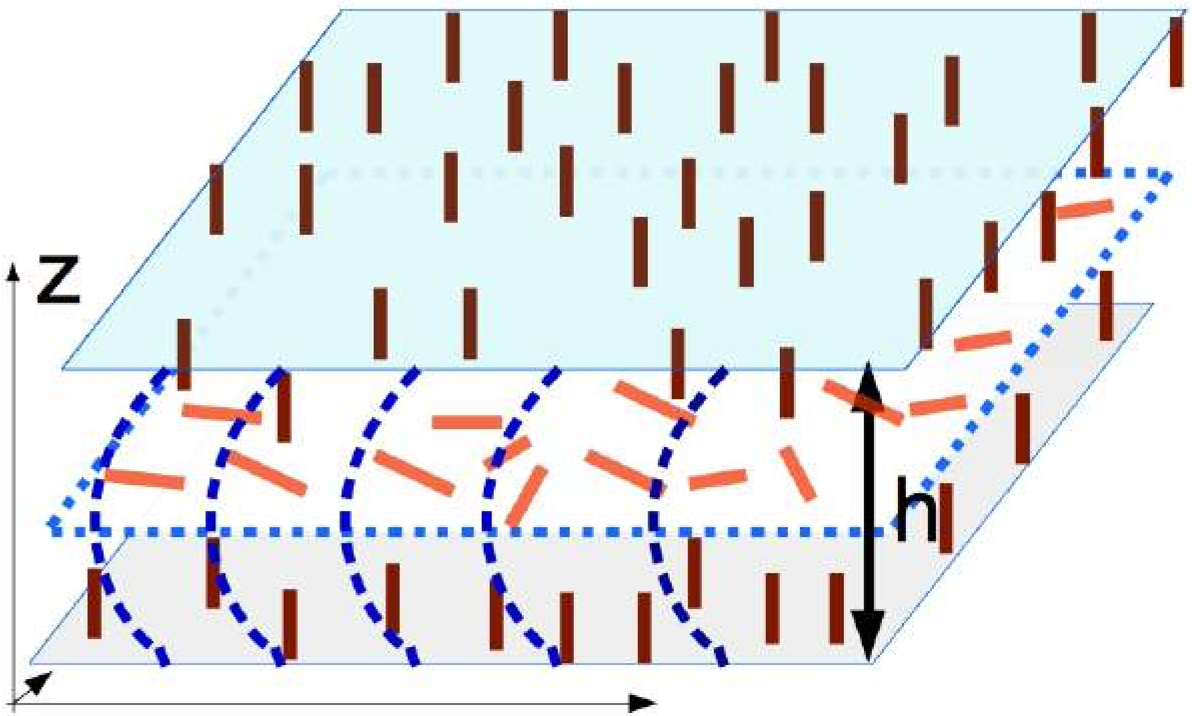


Non-tumbling bacteria: should undergo generic instability easily
Are some active nematics immune to instability?

STABILITY FROM ACTIVE FORCES

Ananyo Maitra
Pragya Srivastava
Cristina Marchetti
Juho Lintuvuori
SR
Martin Lenz

arXiv:1711.02407
PNAS June 2018



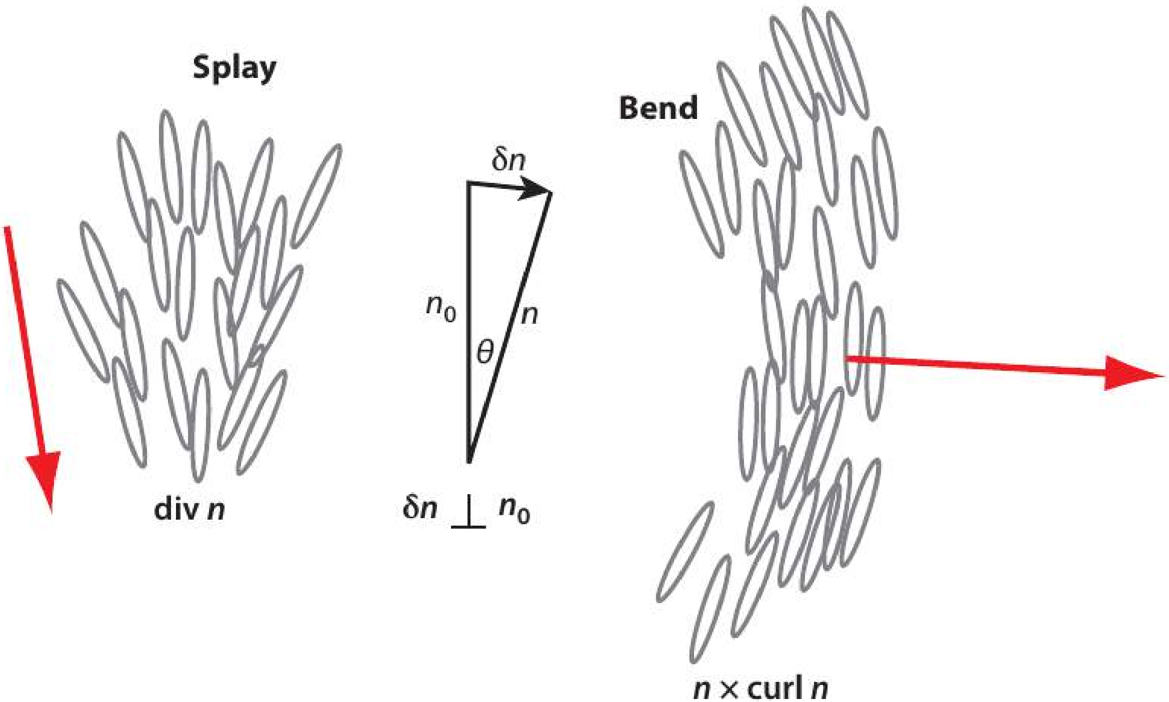
K = Frank elastic constant of underlying liq crystal

Length scale $\xi = (K/W)^{1/2}$; stable if $h < \xi$

Fix h, increase activity W: diffusive instability?

- No: much more interesting

Confined active nematics



Orientation θ
concentration c
velocity field v

free-energy functional

$$\mathcal{H} = \int d^2\mathbf{r} \left[\frac{K}{2} (\nabla\theta)^2 + g(c) \right]$$

confined active nematics

$$\dot{\theta} = \frac{1-\lambda}{2}\partial_x v_y - \frac{1+\lambda}{2}\partial_y v_x - \Gamma_\theta \frac{\delta \mathcal{H}}{\delta \theta}$$

$|\lambda| > 1$ flow-aligning, < 1 flow-tumbling

$$\Gamma \mathbf{v} = -\nabla \Pi + \mathbf{f}^p + \mathbf{f}^a$$

2d pressure Passive Active

$$\nabla \cdot \mathbf{v} = 0$$

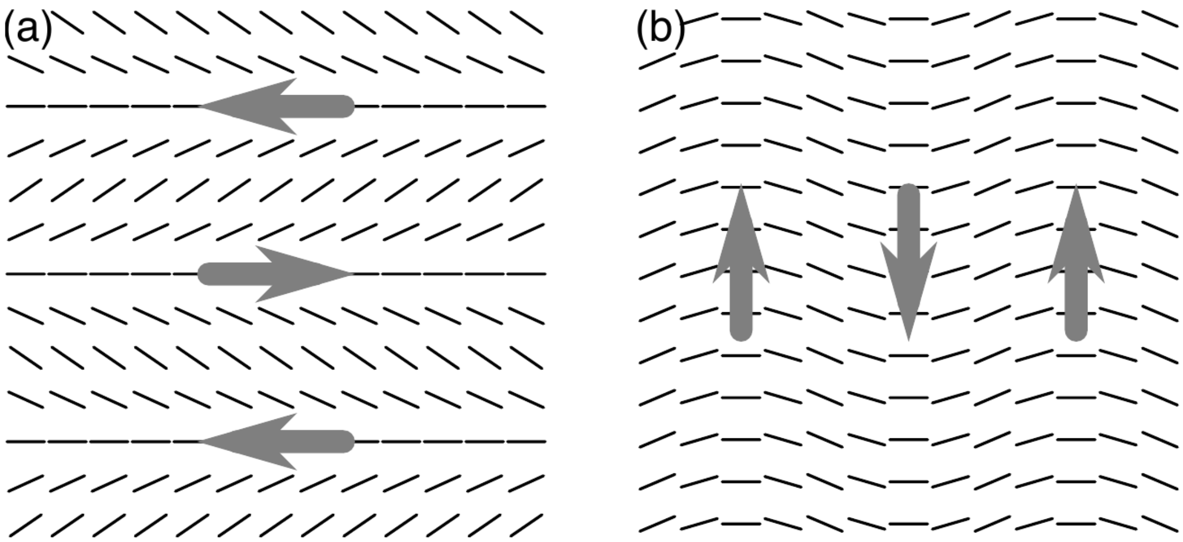
Solve for v, get effective equations for θ

Need force densities f^p, f^a

Force densities

passive

$$\mathbf{f}^p = -\frac{1+\lambda}{2}\partial_y\left(\frac{\delta\mathcal{H}}{\delta\theta}\right)\hat{\mathbf{x}} + \frac{1-\lambda}{2}\partial_x\left(\frac{\delta\mathcal{H}}{\delta\theta}\right)\hat{\mathbf{y}}$$

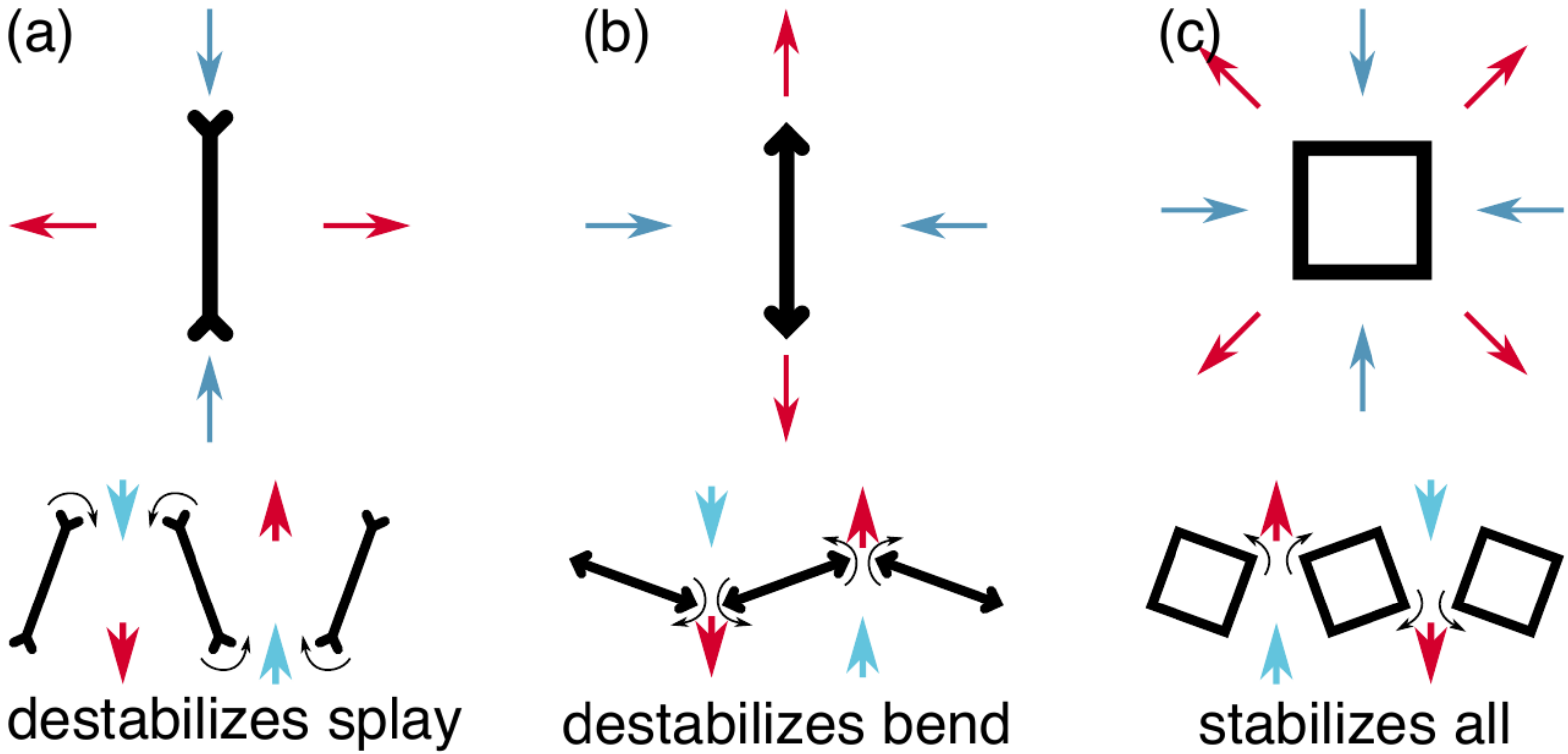


active

$$f_x^a = -(\zeta_1+\zeta_2)\Delta\mu\,\partial_y\theta$$

$$f_y^a = -(\zeta_1-\zeta_2)\Delta\mu\,\partial_x\theta$$

Splay ≠ bend


(a)
(b)
(c)
destabilizes splay
destabilizes bend
stabilizes all

Consequence: effective θ dynamics

$$\partial_t \theta_{\mathbf{q}} \;=\; -D(\phi) q^2 \theta_{\mathbf{q}}$$

$$D(\phi) = \Gamma_\theta K + \frac{\Delta\mu}{2\Gamma}(1 - \lambda\cos 2\phi)(-\zeta_1 \cos 2\phi + \zeta_2)$$

Without ζ_2 instability inevitable at large $\Delta\mu$

Not any more!

$|\lambda| < 1$ (flow-tumbling): large +ve ζ_2 always stable

In more detail:

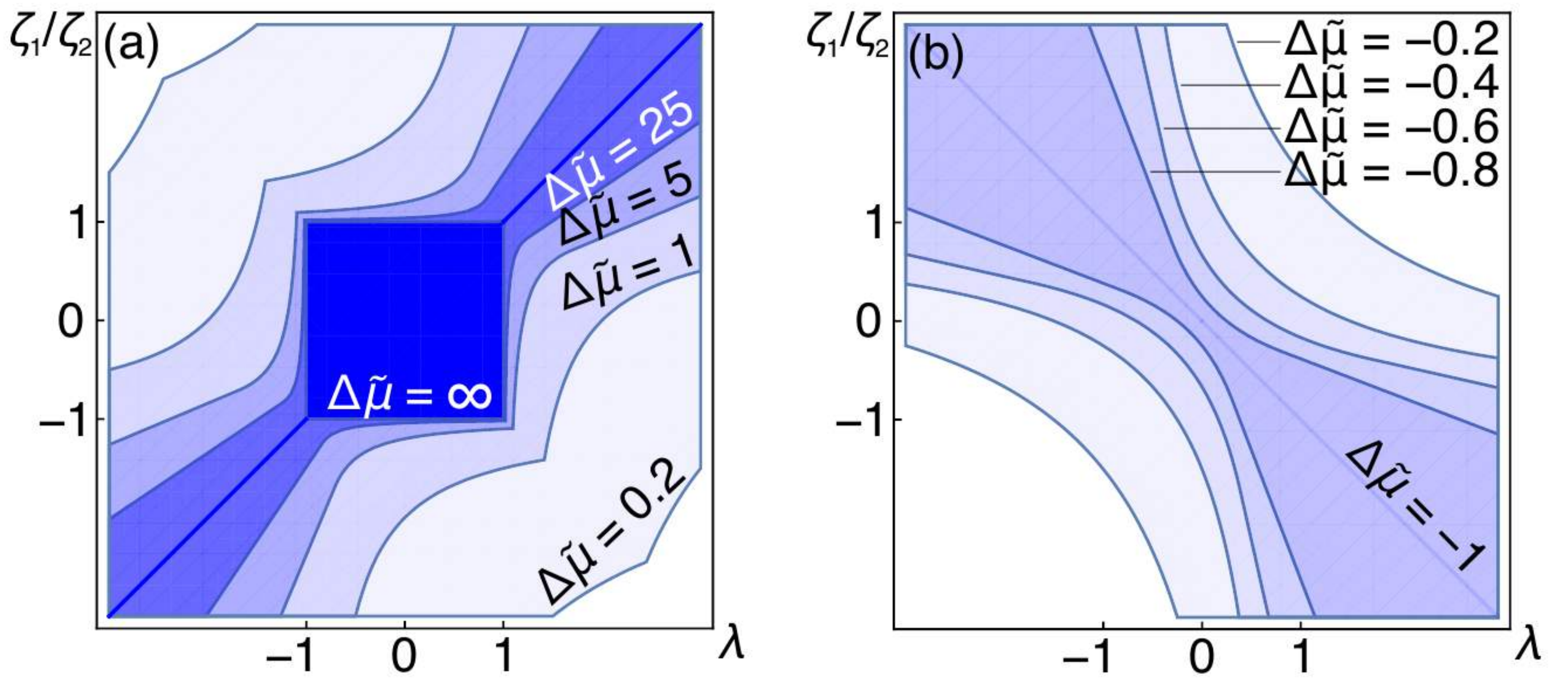
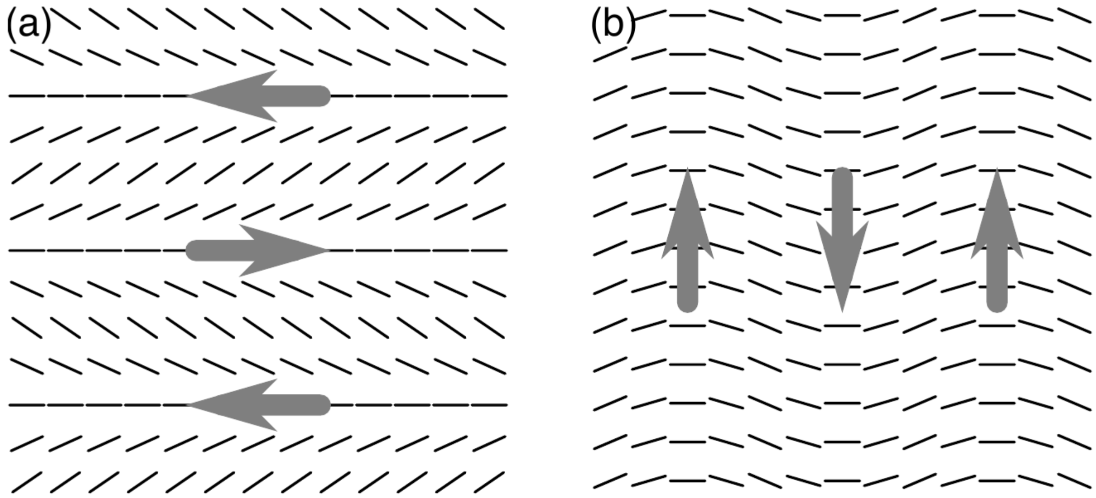


FIG. 2: Regions of stability of the ordered phase as a function of the flow-alignment parameter λ, the ratio ζ_1/ζ_2 of the old and new active forces and the overall magnitude of activity relative to passive friction $\Delta\tilde{\mu} = \zeta_2\Delta\mu/2K\Gamma\Gamma_\theta$. (a) For $\Delta\tilde{\mu} > 0$, the region of linear stability of the ordered phase (shades of blue) shrinks with increasing activity, yet the central dark blue square is stable for arbitrary high activity. (b) For $\Delta\tilde{\mu} < 0$, stability is abolished for large enough activity, namely $\Delta\tilde{\mu} < -1$.

Understanding the active force density



$$-\zeta_1 \Delta\mu \nabla \cdot \mathbf{Q} - 2\zeta_2 \Delta\mu \mathbf{Q} \cdot (\nabla \cdot \mathbf{Q})$$

Independent active force for $\mathbf{n}(\nabla \cdot \mathbf{n})$ and $\mathbf{n} \cdot \nabla \mathbf{n}$

cf flexoelectricity: Lavrentovich, Prost & Marcerou, Meyer

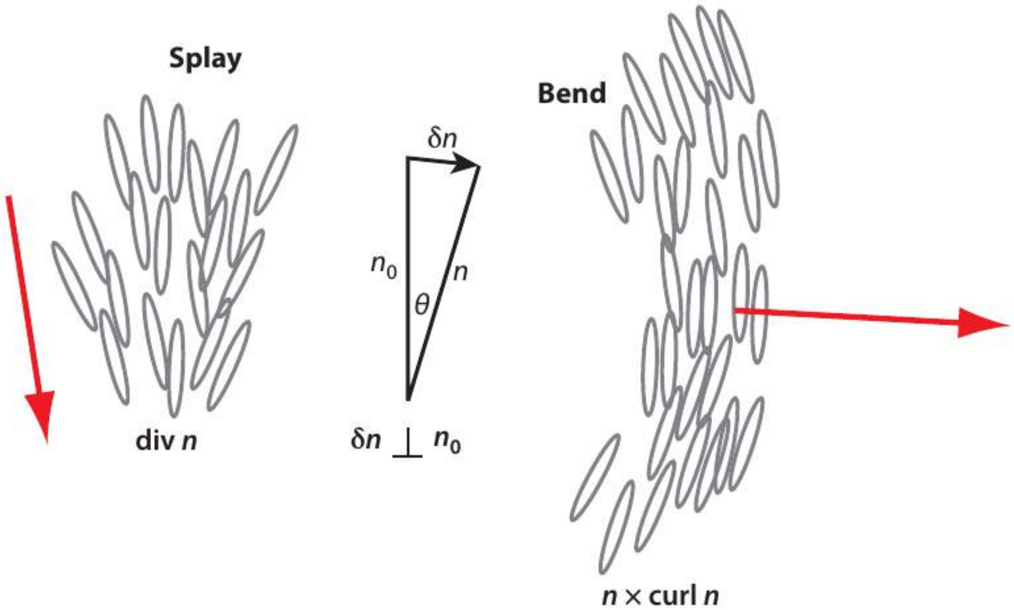
Note: not momentum-conserving, OK on substrate, can derive from 3D hydro

polar case different: Nambu-Goldstone mode gets hydro “mass”; Maitra et al in prep

ACTIVE NEMATICS II
topological defects

Nematic: apolar, goes nowhere on average
But curvature → current

Shankar, Marchetti, SR, Bowick, arXiv 2018



Q = local alignment tensor

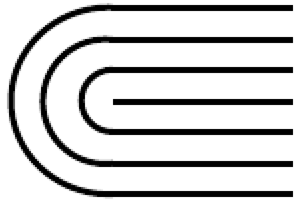
Gradients of **Q**; curvature

Div **Q**: vector

Active: local current ~ div **Q**

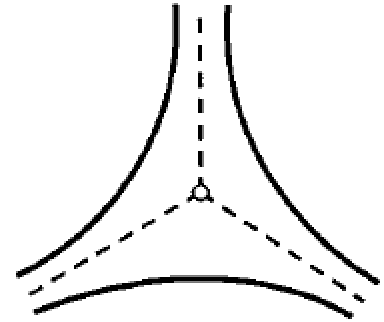
SR, Simha, Toner 2003

Topological defects in a nematic



$$m = \frac{1}{2}, \quad \phi_0 = 0$$

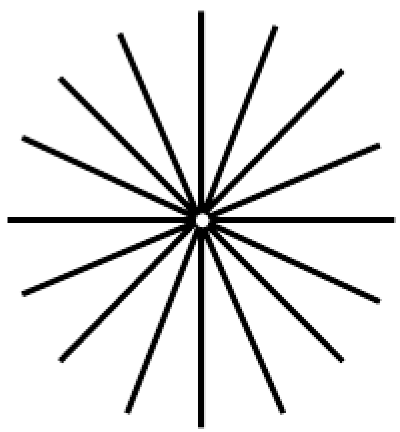
(a)



$$m = -\frac{1}{2}, \quad \phi_0 = 0$$

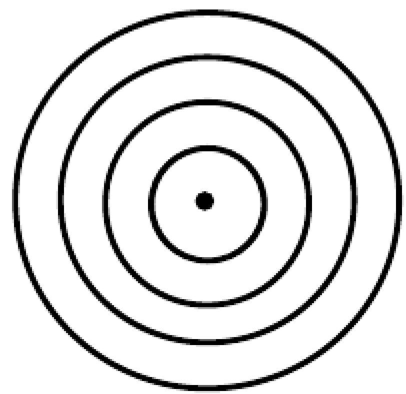
(b)

Kemkemer, R., Teichgräber, V., Schrank-Kaufmann, S. et al. Eur. Phys. J. E (2000) 3: 101. https://doi.org/10.1007/s101890070023



$$m = 1, \quad \phi_0 = 0$$

(c)

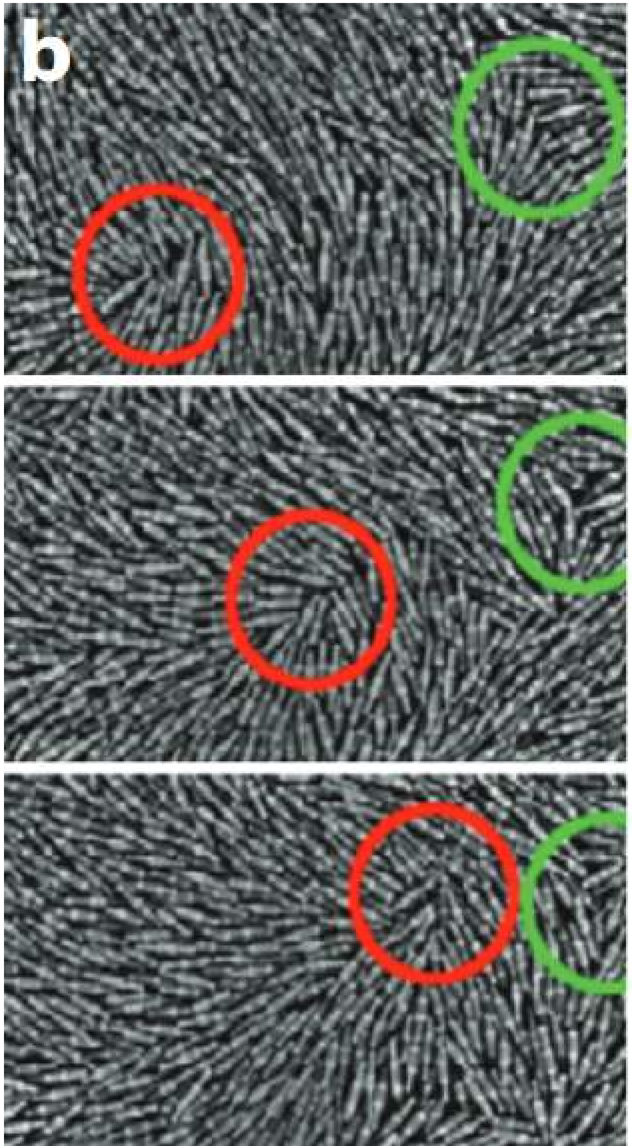


$$m = 1, \quad \phi_0 = \frac{\pi}{2}$$

(d)

Defect unbinding in active nematics

Suraj Shankar, M C Marchetti, SR, MJ Bowick



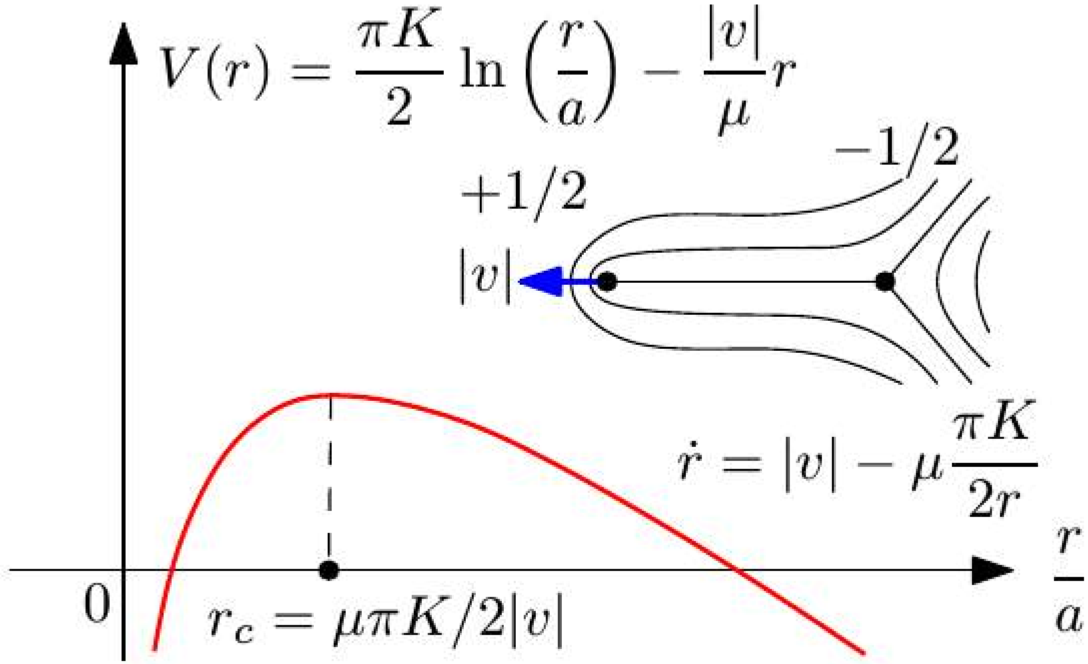
The symmetry of the field around the strength -1/2 defect will result in no net motion, while the curvature around the +1/2 defect has a well-defined polarity and hence should move in the direction of its “nose” as shown in the figure.
V Narayan et al., Science **317** (2007) 105

motile +1/2 defect, static -1/2 defect

Defects as particles:
+1/2 motile, -1/2 not
+1/2 velocity ~ divQ
Giomi, Bowick, Ma, Marchetti PRL 2013
Thampi, Golestanian, Yeomans PRL 2014
DeCamp et al NMat 2015 ....

Defect unbinding in active nematics

Shankar
et al. arXiv 2018



Recall equil BKT transition: but +1/2 defect is motile!

Like insulator in a field? Finite barrier?

Active nematic order always destroyed?

But active nematics exist!

Bertin et al., NJP **15**(8), 2013; Ngo et al., PRL **113**(3), 2014

Shi et al., NJP **16**(3), 2014 $\cdots$

Langevin equations for +/- 1/2 defects: positions and polarization

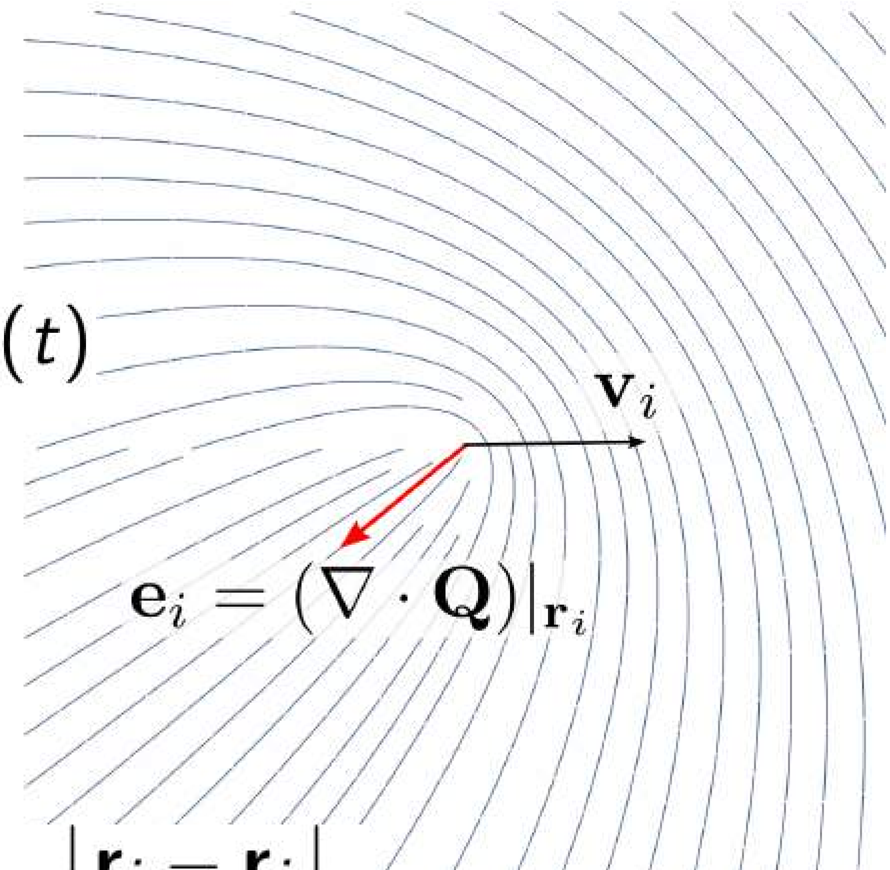
Shankar et al. arXiv 2018:

From active nematic dynamics

+1/2 self-velocity ∝ polarization

$$\dot{\mathbf{r}}_i^+ = v\mathbf{e}_i - \mu \nabla_{\mathbf{r}_i}\mathcal{U} + \sqrt{2\mu T}\,\boldsymbol{\xi}_i(t)$$

$$\dot{\mathbf{r}}_i^- = -\mu \nabla_{\mathbf{r}_i}\mathcal{U} + \sqrt{2\mu T}\,\boldsymbol{\xi}_i(t)$$



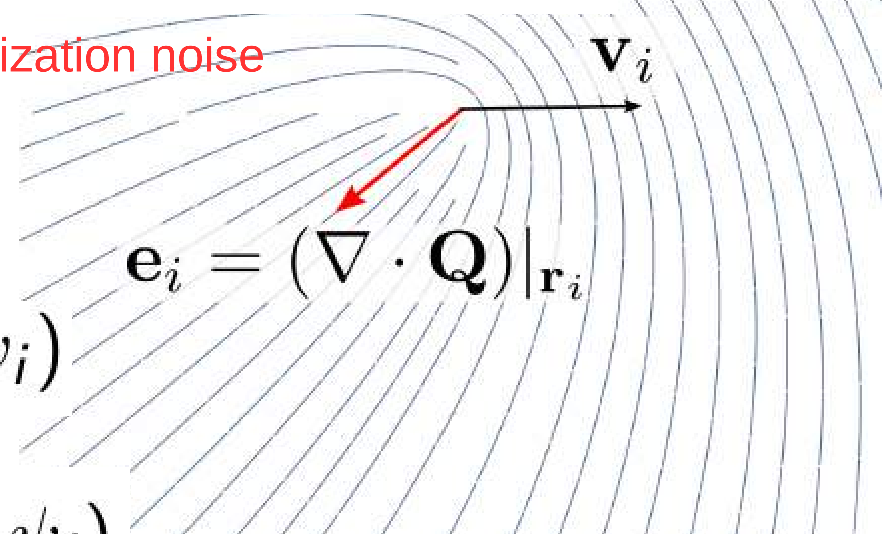
$$\mathcal{U} = -2\pi K \sum_{i \neq j} q_i q_j \ln \left| \frac{\mathbf{r}_i - \mathbf{r}_j}{a} \right|$$

Langevin equations for +/- 1/2 defects: positions and polarization

Shankar et al. arXiv 2018:

$$\dot{\mathbf{e}}_i = -\frac{\mu\gamma}{8K}\left(\mathbf{1} + 4\hat{\mathbf{e}}_i\hat{\mathbf{e}}_i\right)\cdot\left[\mu\mathbf{e}_i|\nabla_i\mathcal{U}|^2 - v|\mathbf{e}_i|^2\nabla_i\mathcal{U}\right] + \sqrt{2D_R\epsilon}\cdot\mathbf{e}_i\eta_i(t) + \boldsymbol{\nu}_i(t)$$

Angular white noise   polarization noise



$$\mathbf{e}_i = |\mathbf{e}_i|(\cos\theta_i, \sin\theta_i)$$

$$\mathbf{F}_i \equiv -\nabla_i\mathcal{U} = |\mathbf{F}_i|(\cos\psi_i, \sin\psi_i)$$

$$\partial_t\theta_i = v|\mathbf{F}_i| \times \text{const. } \sin(\theta_i - \psi_i)$$

Alignment torque: v<0: alignment; v>0: anti-alignment

Langevin equations for +/- 1/2 defects: positions and polarization

Shankar et al. arXiv 2018:

Fokker-Planck steady state, single +/- 1/2 pair, small-activity expansion

$$\rho_{ss}(r) \propto e^{-\mathcal{U}_{\rm eff}(r)/T}$$

$$\mathcal{U}_{\rm eff}(r) = \frac{\pi K}{2} \ln\left(\frac{r}{a}\right) - \frac{\bar{v}^2}{2} \ln\left(1 + \frac{r^2}{r_*^2}\right) + \mathcal{O}(v^4)$$

$$|v|/D_R \ll \mu K/|v|$$

$r_* \sim \sqrt{\mu K/D_R}$

$\bar{v}^2 \sim v^2/(\mu D_R)$

Rotational diffusion dominates
+1/2 can't escape
Active nematic survives

Langevin equations for +/- 1/2 defects: positions and polarization

Shankar et al. arXiv 2018:

$$\mathcal{U}_{\mathrm{eff}}(\mathbf{r}) \simeq (\pi K_{\mathrm{eff}}/2)\ln(r/a)$$

$$K_{\mathrm{eff}}(v) = K - (2\bar{v}^2/\pi)$$

$\Rightarrow T_{BKT}(v) < T_{BKT}(v=0)$

$K_{eff} = 0 \Leftrightarrow$ persistence length of +1/2 motion = location of barrier

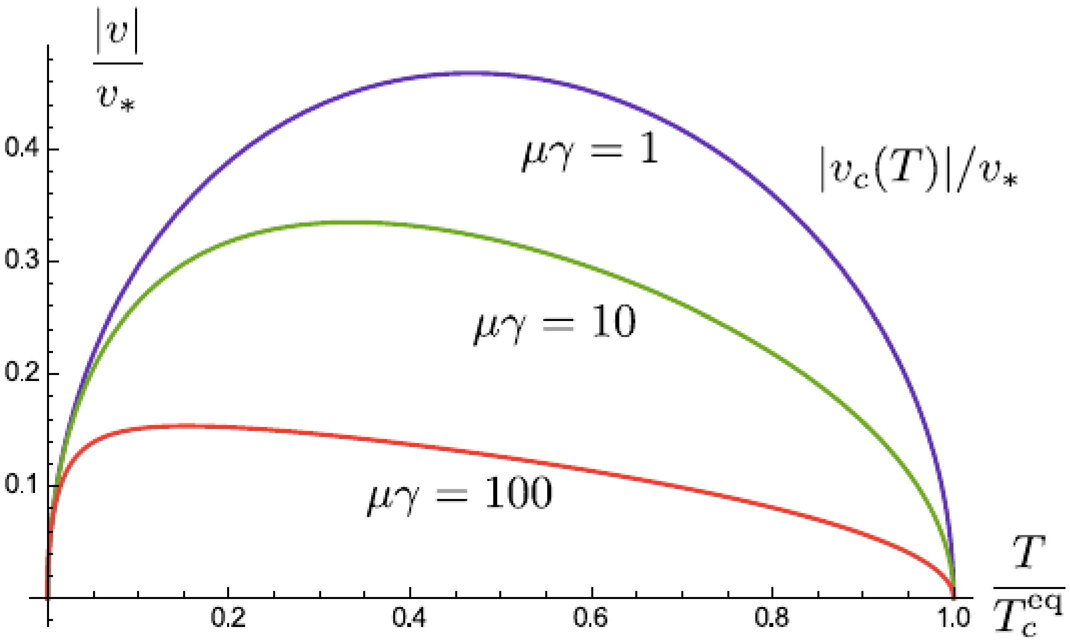
Threshold activity

$$|v_c| = \sqrt{\frac{2\mu K D_R}{[1+\mu\gamma(3T/4K)]}}$$

Re-entrance!

Shankar et al. arXiv 2018:

Threshold activity



$$\frac{|v_c(T)|}{v_*} = \sqrt{\frac{16\ \tilde{T}(1-\tilde{T})}{\pi\left[1+(3\pi/32)\mu\gamma\tilde{T}\right]}}$$

At high T: conventional defect unbinding wins

At low enough T, D_R goes to zero, i.e., persistence length grows

Directed motion of +1/2 wins, defects liberated, order destroyed

(A Maitra)

Conclusion

- Active matter
  - natural language to describe living materials
  - statistical mechanics: new regime, new framework
  - liquid crystal physics with a difference
  - successes in cell & tissue biology
  - many open directions in theory and experiment
- Active nematics
  - nonuniversal density fluctuation spectrum
  - can escape the “inevitable” instability
  - defect liberation à la Berezenskii, Kosterlitz, Thouless
    - nematic order survives motile +1/2
    - melted at high and low T: reentrance