Dynamics, Entropy Production & Defects in Active Matter

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Homi Bhabha Chair, Tata Education and Development Trust

ICTS Entropy School Sep 2018

Outline

- Systems & phenomena
- Framework
- Entropy production
- Flocking, condensation, trapping
- Defect unbinding: an energy–entropy story
- Summary

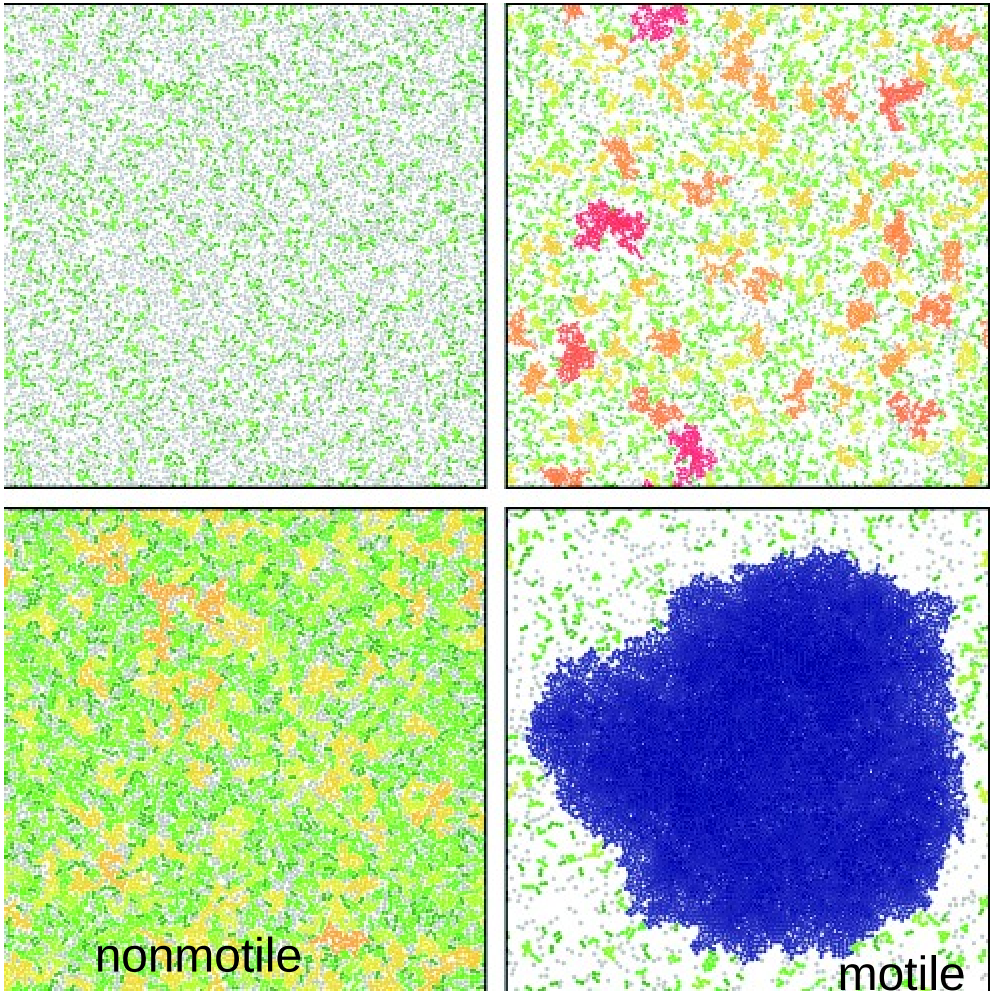
Systems and phenomema

Millipede Flock (S Dhara, U of Hyderabad)

Persistent motion → condensation without attraction

Low conc

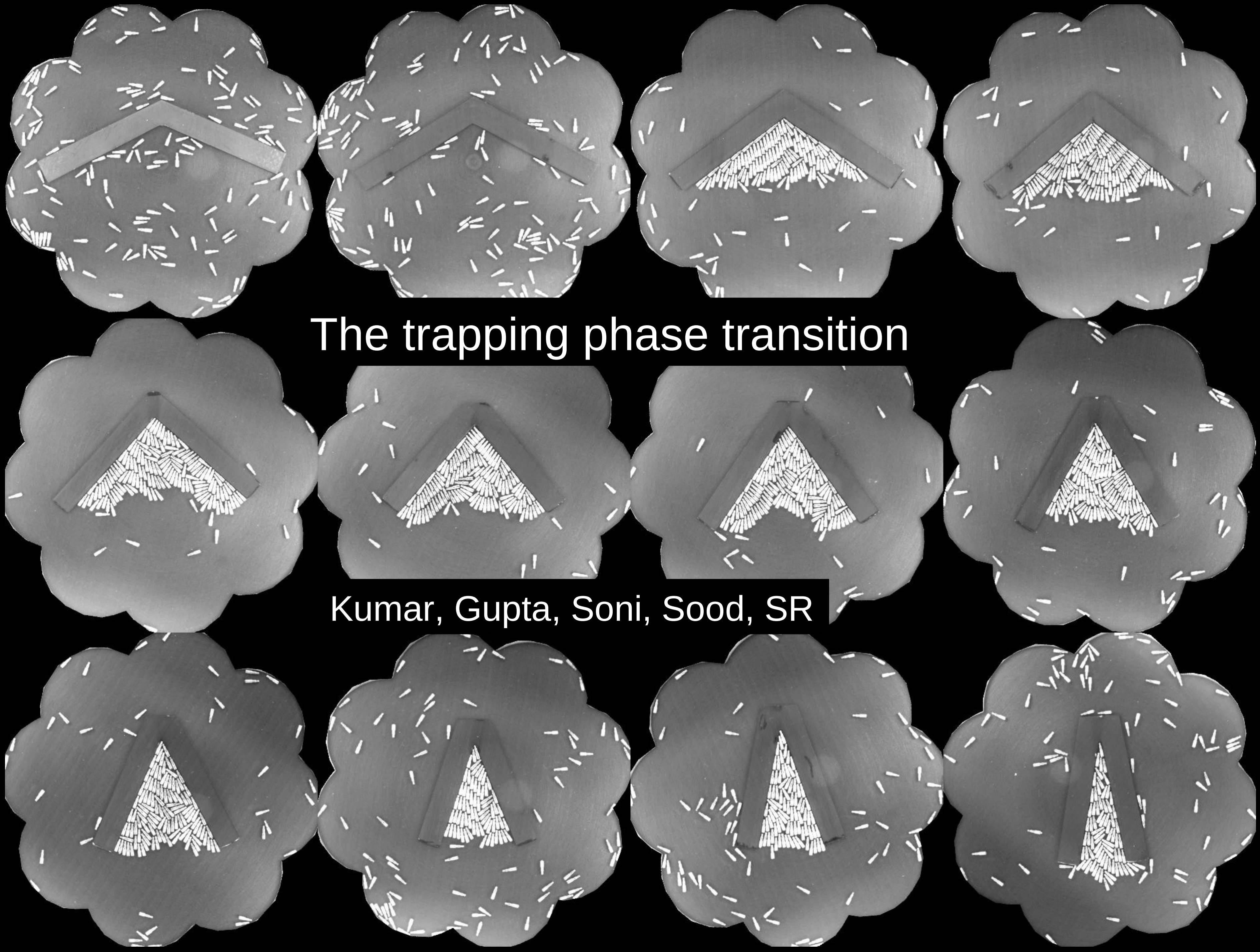
High conc



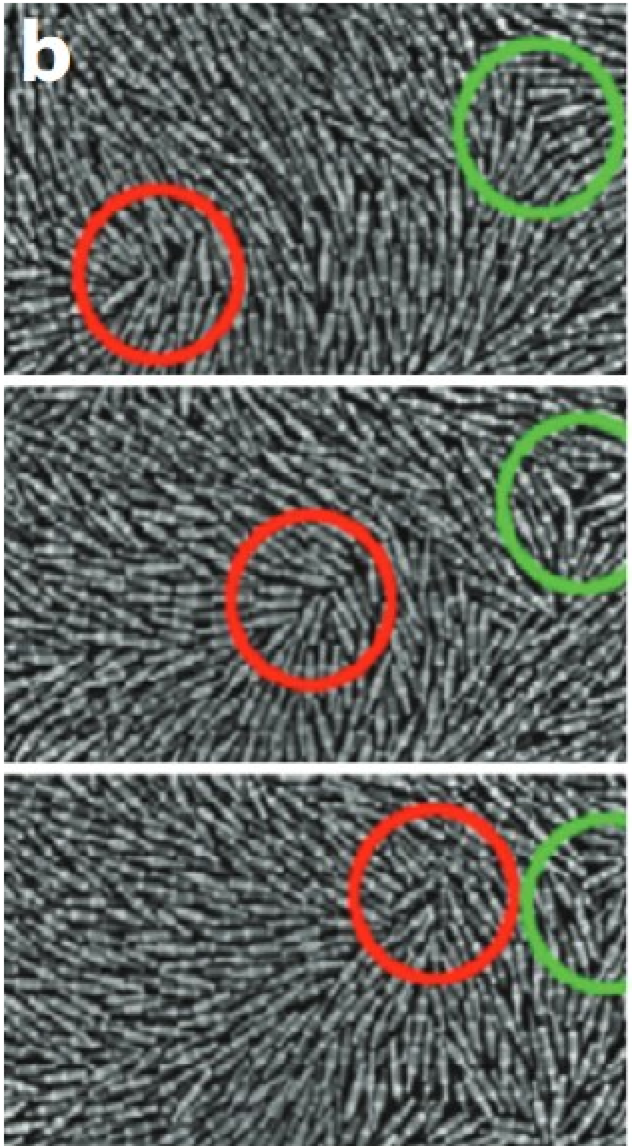
Motility-induced phase separation

Non-aligning SPPs: Fily & Marchetti; Redner, Hagan, Baskaran; Tailleur & Cates;

SP rods: S Weitz, A Deutsch, F Peruani


The trapping phase transition
Kumar, Gupta, Soni, Sood, SR

Self-propelled defects



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 ....

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
  - mutation: evolution

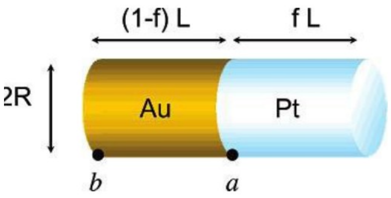
SR J Stat Mech 2017

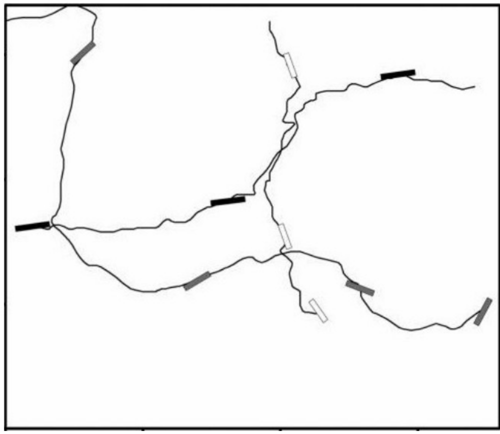
Marchetti, Joanny, SR, Liverpool, Prost, Rao, Simha, *Rev. Mod. Phys.* **85** (2013) 1143-1189
Prost, Jülicher, Joanny, *Nat Phys* Feb 2015
SR: *Annu. Rev. Condens. Matt. Phys.* **1** (2010) 323
Toner, Tu, SR: *Ann. Phys.* **318** (2005) 170

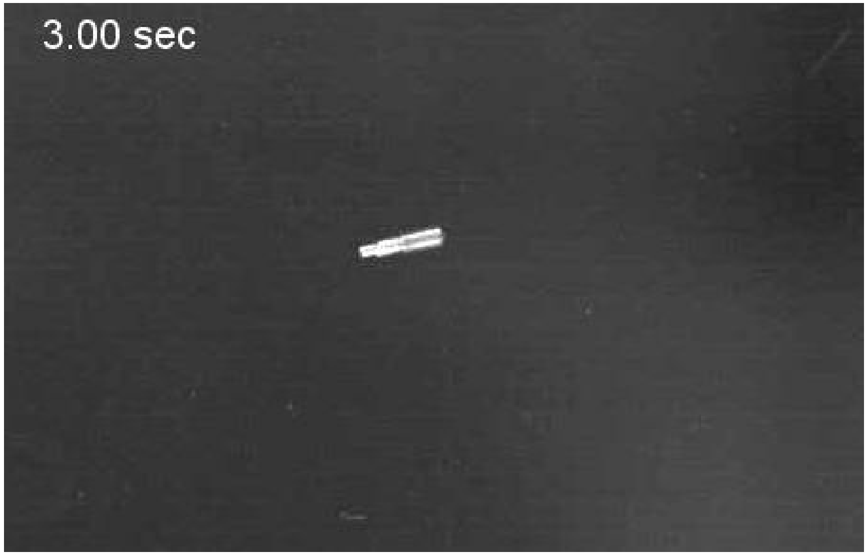
So:
motile creatures
living tissue
membranes + pumps
cytoskeleton + motors
....
but also:

Active matter: nonliving examples

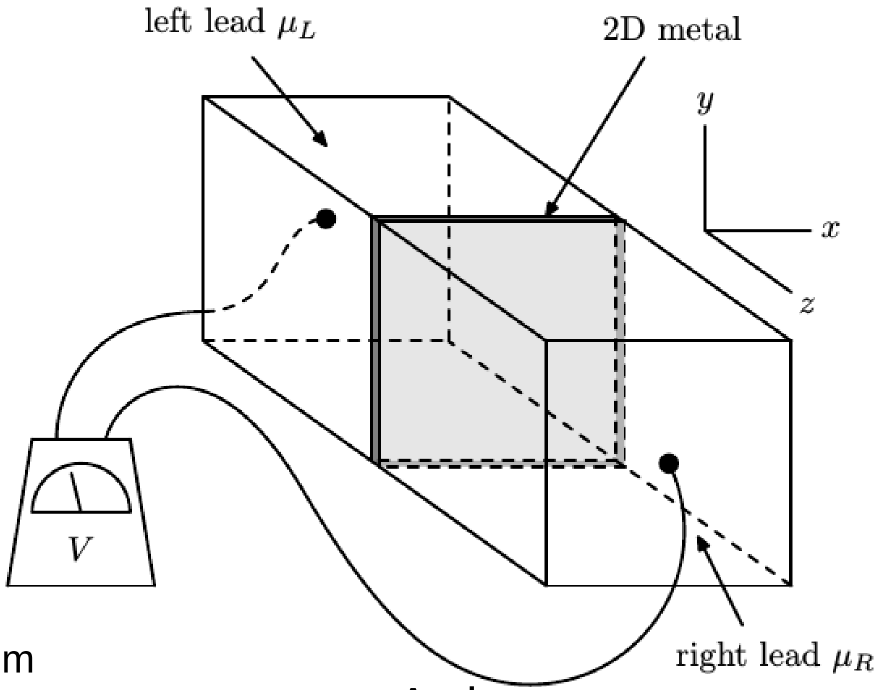
Catalytic particle in reactant bath
Golestanian et al., Paxton et al., Saha et al.







Motile brass rod
Kumar et al. PRL 2011



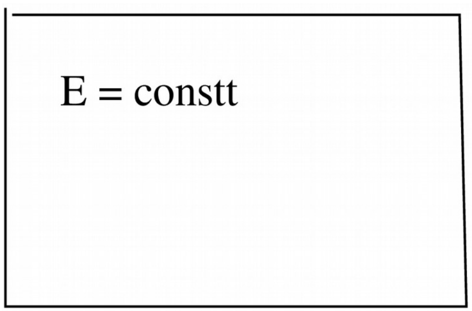
Takei and Kim
Phys. Rev. B 76, 115304 (2007)

Active quantum matter?

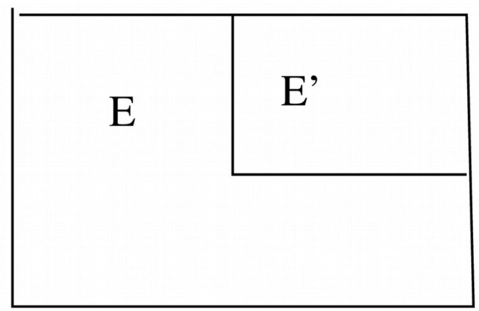
INTRODUCTION

framework

Thermal equilibrium: “closed” systems



E = constt

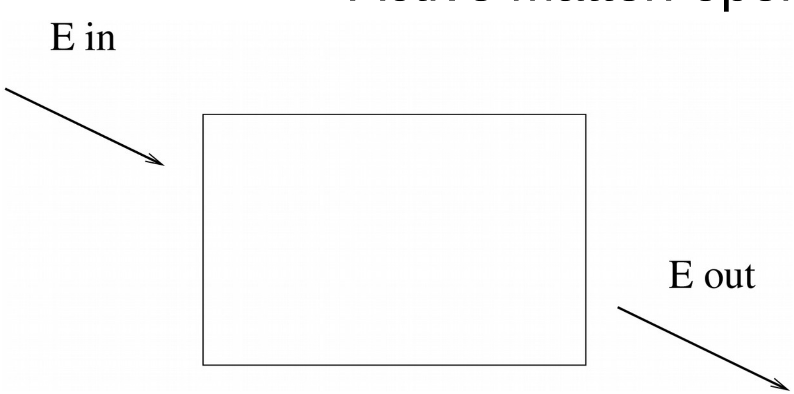


E + E’ = constt
Temperature of subsystem = constt

$t \leftrightarrow -t$

Physics students know the rules

Active matter: open systems (& questions)



- running engine + fuel
- living organism + food

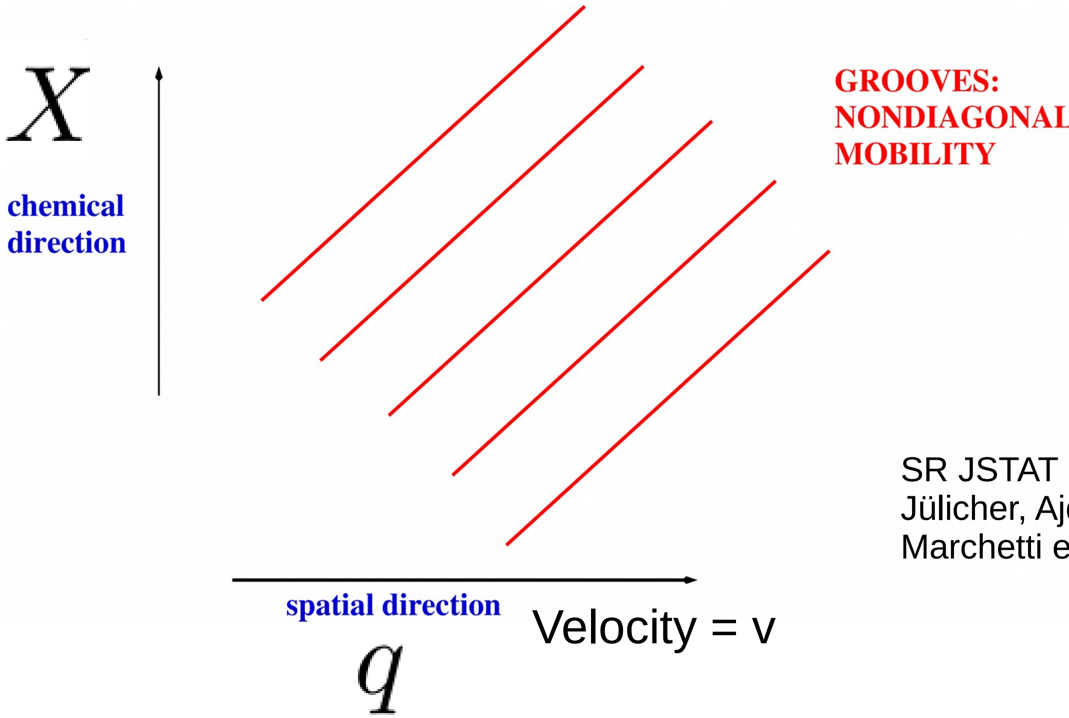
~~$t \leftrightarrow -t$~~

Physics students don’t know the rules

INTRODUCTION

framework

Velocity = r



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

Motor: catalyst for fuel breakdown; 2d configuration space

Driving force $Dm = m_{reactant} - m_{product}$ 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

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

$$\dot{p} + \Gamma_{11}\partial_p H + \underline{\Gamma_{12}(q)}\partial_\Pi H = -\partial_q H + \eta$$

$$\dot{\Pi} + \underline{\Gamma_{21}(q)}\partial_p H + \Gamma_{22}\partial_\Pi H = -\partial_X H + \xi$$

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

$$\dot{X} = \partial_\Pi H$$

SR JSTAT 2017

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

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SR JSTAT 2017

From Langevin equations to active dynamics

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

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

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

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

Active? Hold $-\partial_X H \equiv -\Delta\mu \neq 0$ 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

Framework

example: active interface

$$q \to h(\mathbf{x}, t) = \text{height field of interface}$$

$$\text{Invariance: } h \to h + \text{constant } \textbf{but not } h \to -h$$

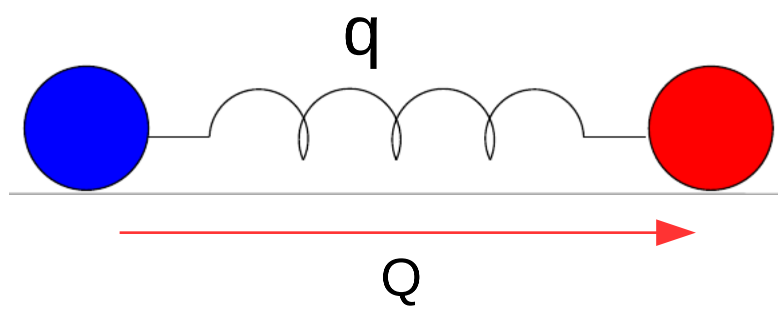
$$\dot{h} + \frac{1}{\zeta}\frac{\delta H}{\delta h} = \frac{\Delta\mu}{\Gamma_{22}\Gamma}\Gamma_{12}(h, \nabla h, \ldots) + \sqrt{\frac{2k_B T}{\zeta}} f$$

$$\text{Symmetries} \to \Gamma_{12} = \text{constt} + (\nabla h)^2$$

KPZ equation

ABP or AOUP from dimer + chemistry

LP Dadhichi
A Maitra
SR 2018



KV Kumar
M Rao
A Baule
SR 2008

Joint & relative (q,p) & (Q,P); "chemical" (X,Π)

$$\dot{p} + \gamma_{11}\partial_p H + \gamma_{12}(Q)\partial_\Pi H = -\partial_q H + \eta$$

$$\dot{\Pi} + \gamma_{21}(Q)\partial_p H + \gamma_{22}\partial_\Pi H = -\partial_X H + \xi$$

$$\dot{P} + \Gamma_{11}\partial_P H = -\partial_Q H + \bar{\eta}$$

ABP or AOUP from dimer + chemistry

$$\dot{q} + \frac{\gamma_{22}}{\mathcal{D}}\partial_q H = \boxed{\frac{\gamma_{12}(Q)}{\mathcal{D}}\Delta\mu} + \frac{\gamma_{22}}{\mathcal{D}}\eta - \frac{\gamma_{12}(Q)}{\mathcal{D}}\xi$$

$$\dot{Q} + \frac{1}{\Gamma_{11}}\partial_Q H = \bar{\eta}/\Gamma_{11}$$

$$\mathcal{D} = \gamma_{11}\gamma_{22} - \gamma_{12}(Q)^2$$

Choosing $\gamma_{12}/\mathcal{D} \propto Q+$ h.o. propels particle along Q

$$H \sim -Q \cdot Q + (Q \cdot Q)^2$$

Propulsion speed $\sim |q| \simeq$ const: Active Brownian Particle ABP

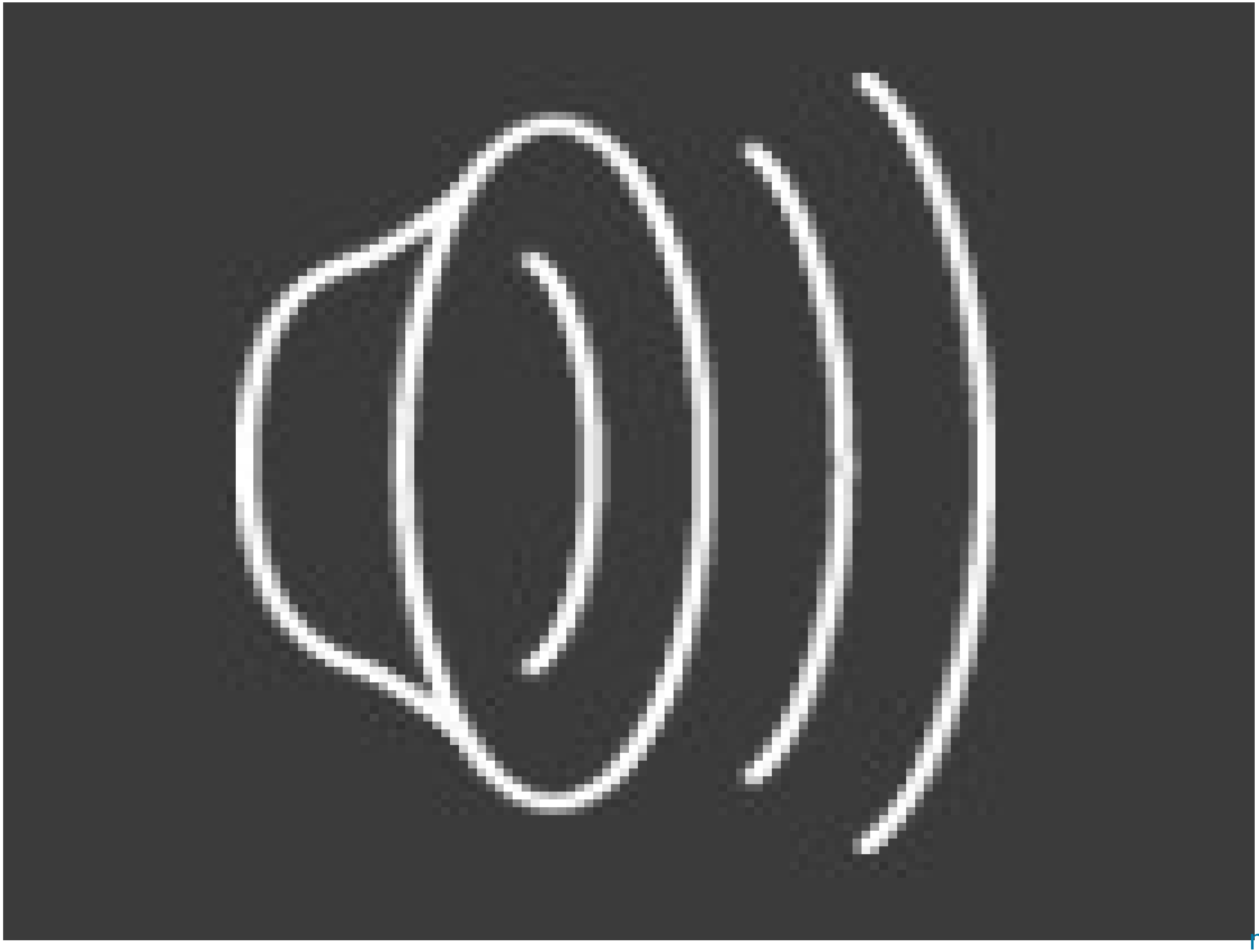
H harmonically binds Q

$\Delta\mu$ term $\sim$ coloured noise: Active Ornstein-Uhlenbeck Particle AOUP

Notice translation diffusion in q equation.

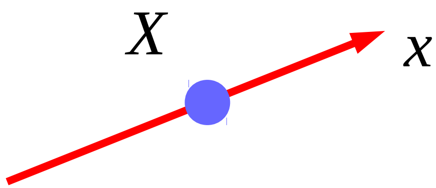
Brownian inchworm

K Vijay Kumar
M Rao
SR 2008



many animals

Entropy production of active dimer



$$v = \gamma_{12}\Delta\mu/\gamma_{22}$$

For a potential harmonic in X, $\partial H/\partial X = kX$

$$\sigma = \frac{v^2}{\gamma_{11} + \gamma_{33}k}$$

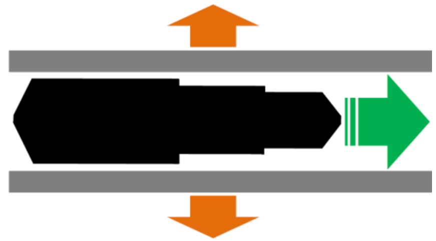
Without x reversal

$$\sigma = \frac{v^2 k \gamma_{33}}{\gamma_{11}(\gamma_{11} + \gamma_{33}k)}$$

With x reversal

Dadhichi, Maitra, SR 2018: Harada-Sasa relates our nonzero σ to Fodor et al's 0

A single active particle



active, apolar, non-motile, in a groove

active, polar, motile, in a groove

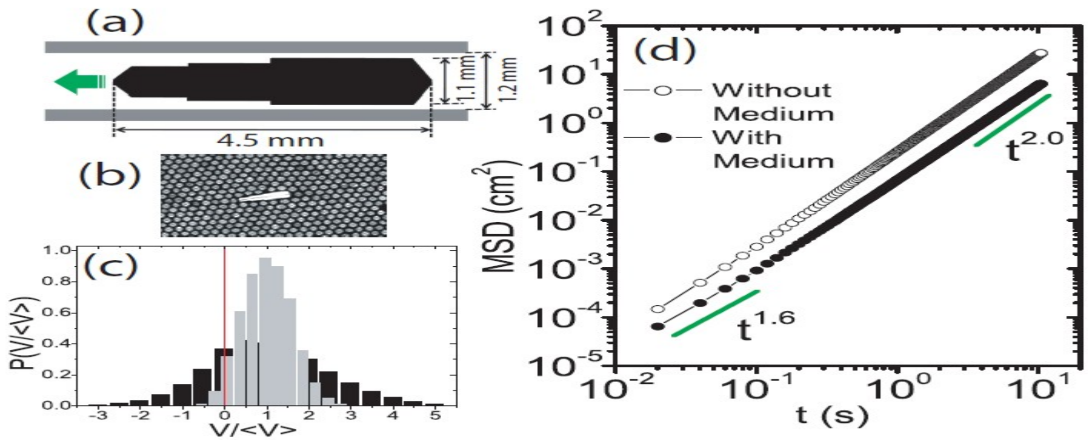
Vijay Narayan, PhD thesis, IISc 2008

one motile rod in a sea of bead
s

Nitin Kumar, A K Sood, SR 2011

Vijay Narayan, Narayanan Menon, Nitin Kumar, Ajay Sood

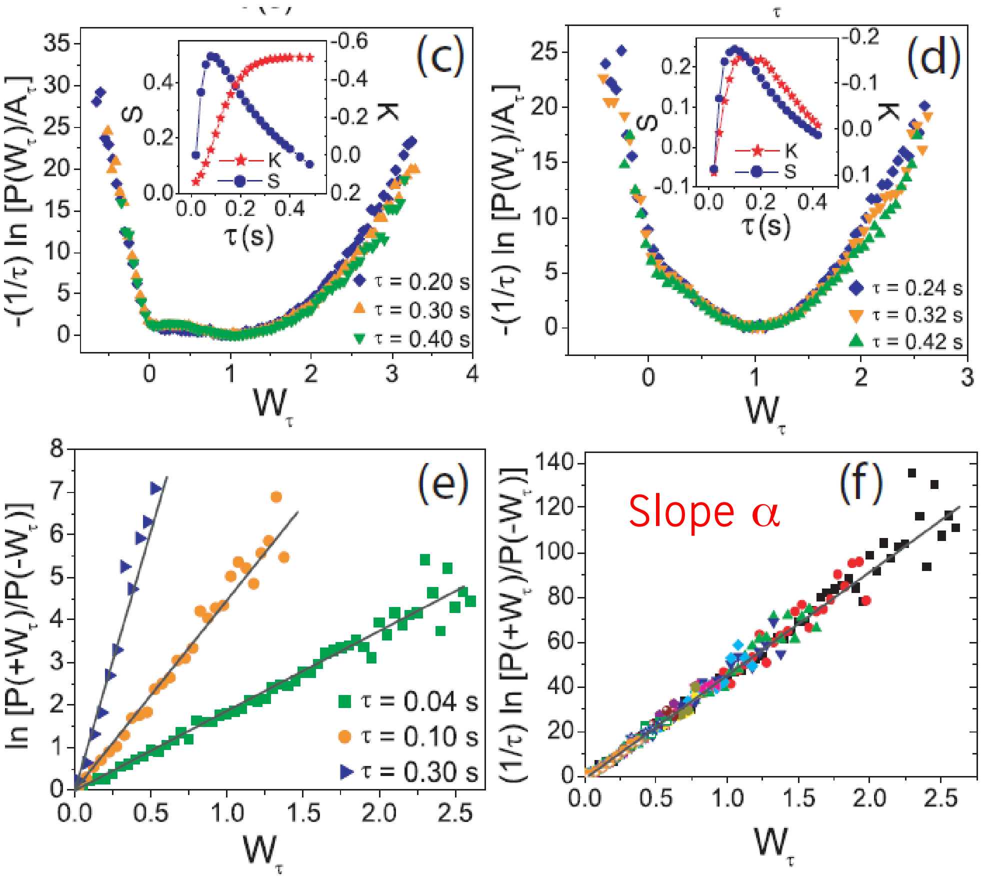
Fluctuation relations in active matter



Polar rod
self-propelled
through bead-bed
Nitin Kumar, A K Sood, SR
PRL 2011

An imitation self-propelled system: laboratory for exploring stat-mech of active matter

Symmetry properties of the large−deviation function of the velocity: a new "fluctuation relation"



$$V(t) \equiv \mathbf{v}(t)\cdot\hat{\mathbf{n}}(t)$$

$$W_\tau(t) = (1/\tau)\int_t^{t+\tau}[V(t')/\langle V\rangle]\,dt'$$

$$F(W_\tau) \equiv \lim_{\tau\to\infty}(-1/\tau)\ln P(W_\tau)$$

$$F(W_\tau) - F(-W_\tau) \propto W_\tau$$

Nitin Kumar, A K Sood, SR
PRL 2011

Notable features

Large deviation function F: statistics of extremes

Central Limit Theorem: behaviour near minimum of F

Experiments:

- Strongly non-Gaussian
- Antisymmetric part linear
- kink at zero argument
- Slope a: relative persistence rates of + and - motion

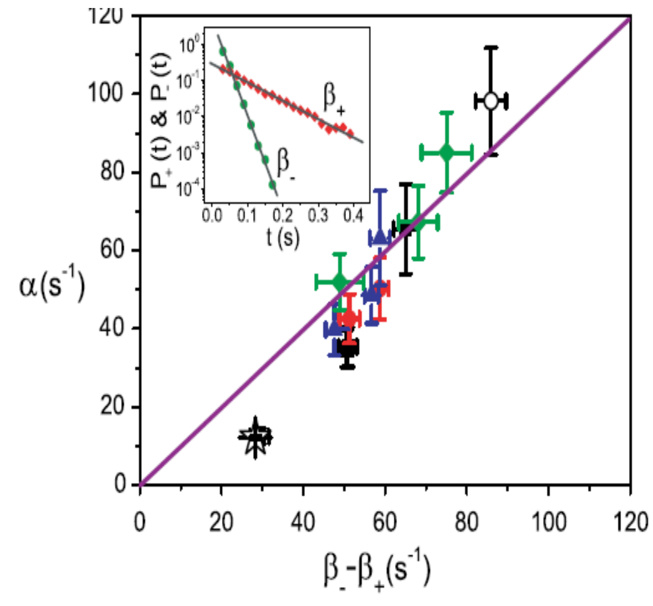
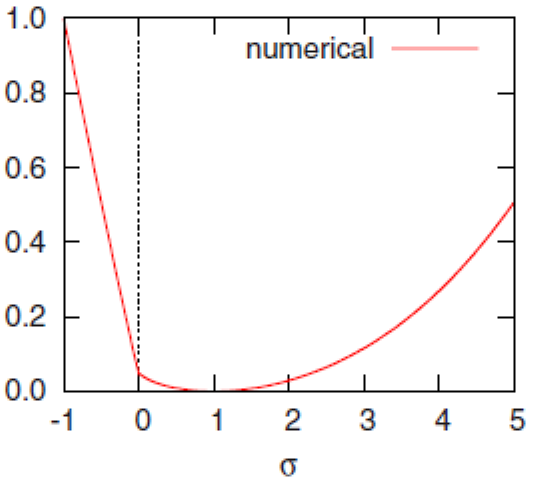


FIG. 4 (color online). Analogue of phase-space contraction rate α vs $\beta_- - \beta_+$, the difference in persistence rates of negative and positive velocities. Solid squares: $\Phi = 0.83$ ($\Gamma =$

Large−deviation function: theory

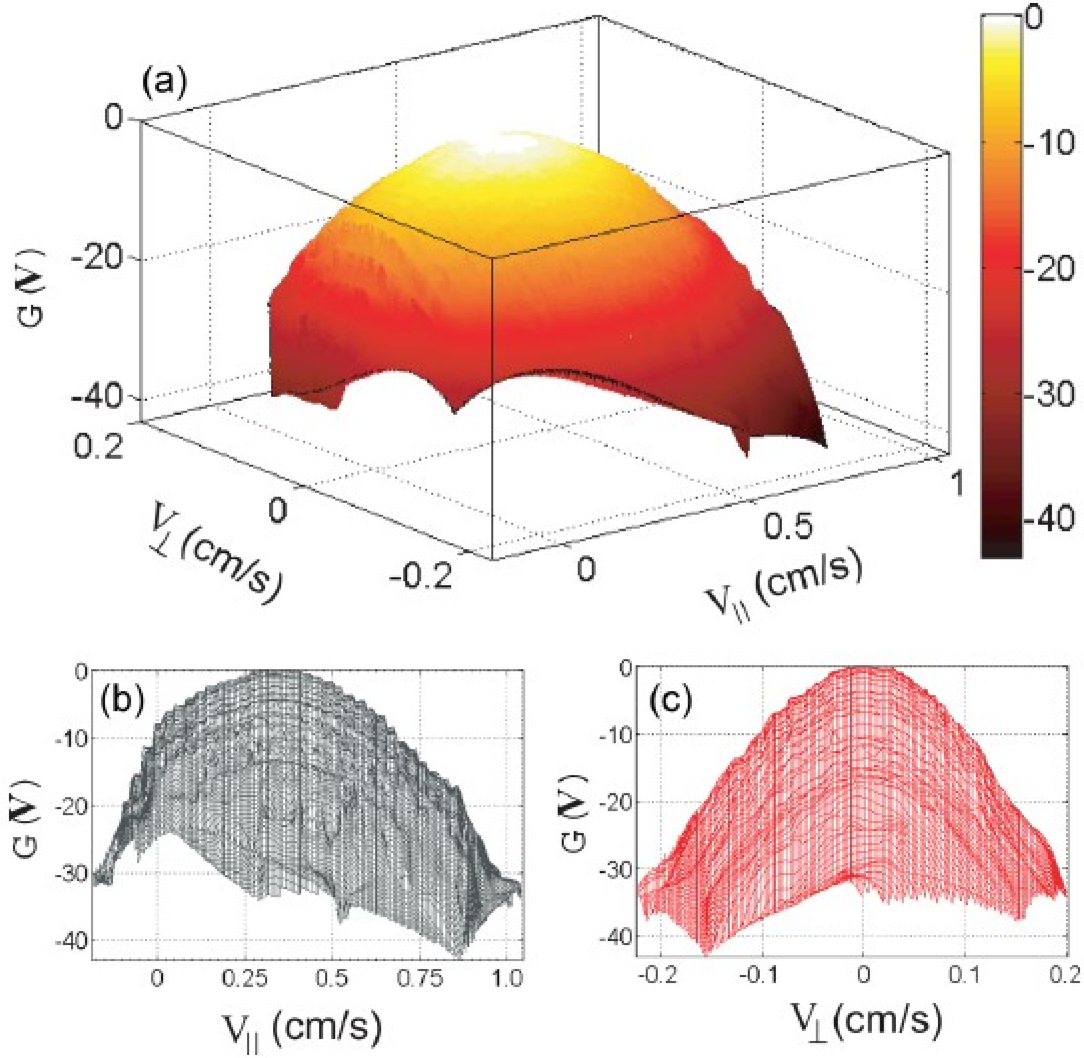
Mehl et al. Phys Rev E **78** (2008) 011123

- Brownian particle: periodic potential + constant force
- pronounced deviations from Gaussian behavior
- characteristic kink at zero entropy production



Large−deviation function for velocity vector $\mathbf{V}$

Kumar, Soni, SR, Sood PRE 2015



Non-paraboloid

Strong asymmetry along $V_{||}$

Anisotropically isometric fluctuation relation

Kumar, Soni, SR, Sood PRE 2015

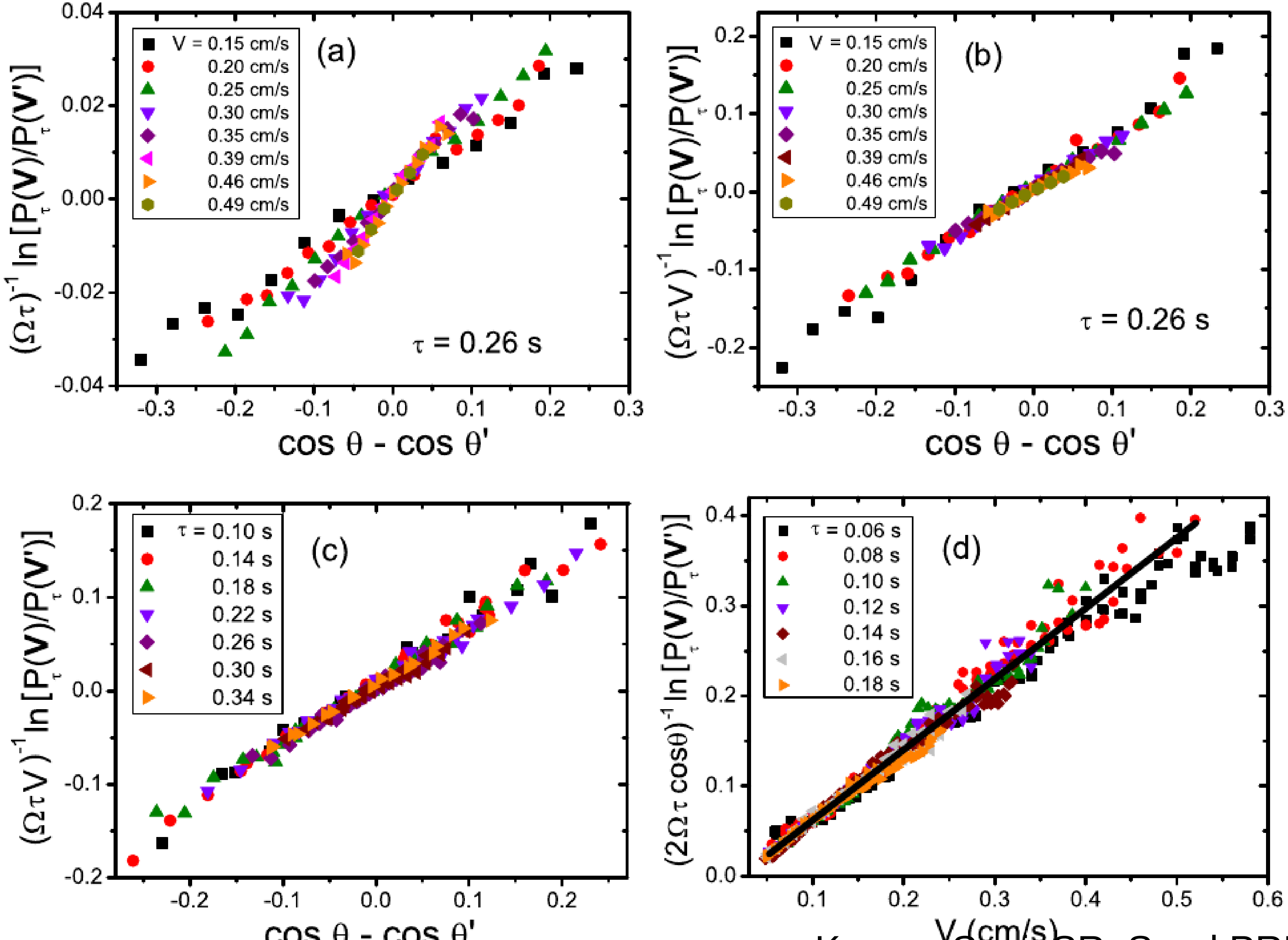
D = diffusivity tensor

Velocity vectors **V**, **V**' with

$$\mathbf{V}^T \mathbf{D}^{-1} \mathbf{V} = \mathbf{V}'^T \mathbf{D}^{-1} \mathbf{V}'$$

$$\lim_{\tau \to \infty} \frac{1}{\tau} \ln \frac{P_\tau(\mathbf{V}_\tau = \mathbf{V})}{P_\tau(\mathbf{V}_\tau = \mathbf{V}')} = \boldsymbol{\epsilon} \cdot (\mathbf{V} - \mathbf{V}')$$

Hurtado et al. PNAS 2011, Villavicencio-Sanchez et al. EPL 2014



Kumar, Soni, SR, Sood PRE 2015

FIG. 2. (Color online) (a) A typical plot of $(\Omega\tau)^{-1}\ln[P_\tau(\mathbf{V})/P_\tau(\mathbf{V}')]$ vs $\cos\theta - \cos\theta'$ over various constant-velocity contours for $\tau = 0.26$ s showing a linear trend for all V. (b) Data scaling of $(\Omega\tau V)^{-1}\ln[P_\tau(\mathbf{V})/P_\tau(\mathbf{V}')]$ vs $\cos\theta - \cos\theta'$. (c) Scaling of $(\Omega\tau V)^{-1}\ln[P_\tau(\mathbf{V})/P_\tau(\mathbf{V}')]$ with τ variation. Here each τ line contains all the V values as in (b). (d) Plot of $(2\Omega\tau\cos\theta)^{-1}\ln[P_\tau(\mathbf{V})/P_\tau(\mathbf{V}')]$ vs V for various τ for the special case when $\theta - \theta' = 180^\circ$. Here θ varies between -30° to 30° in steps of 10° for all τ.

Nonliving dry active matter

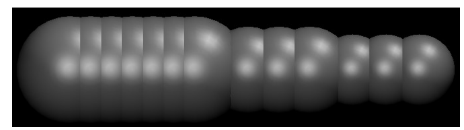
apolar medium, motile topological defect

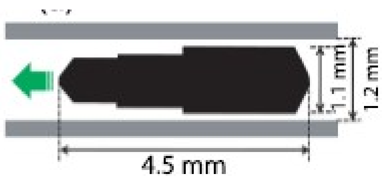
Vijay Narayan

Nitin Kumar

Ajay Sood

Narayanan Menon





Granular dynamics simulations: Harsh Soni

active, apolar, non-motile, in a groove

Confined quasi-2d geometry

+ aluminium beads 0.8 diameter

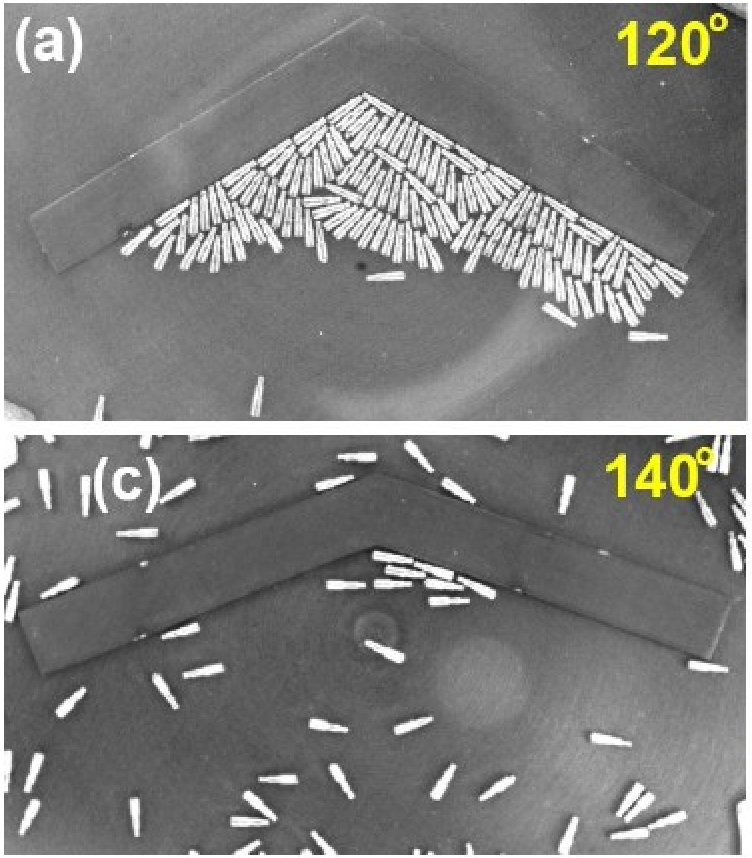
active, polar, motile, in a groove

one motile rod in a sea of bead
s

Active nematic: Narayan, SR, Menon Science 2007
Large deviations, flocking: Kumar, Soni, Sood, SR PRL 2011, PRE 2014, Nat Comm 2014 & in prep
Trapping: Kumar, Gupta, Soni, SR, Sood arXiv 2018

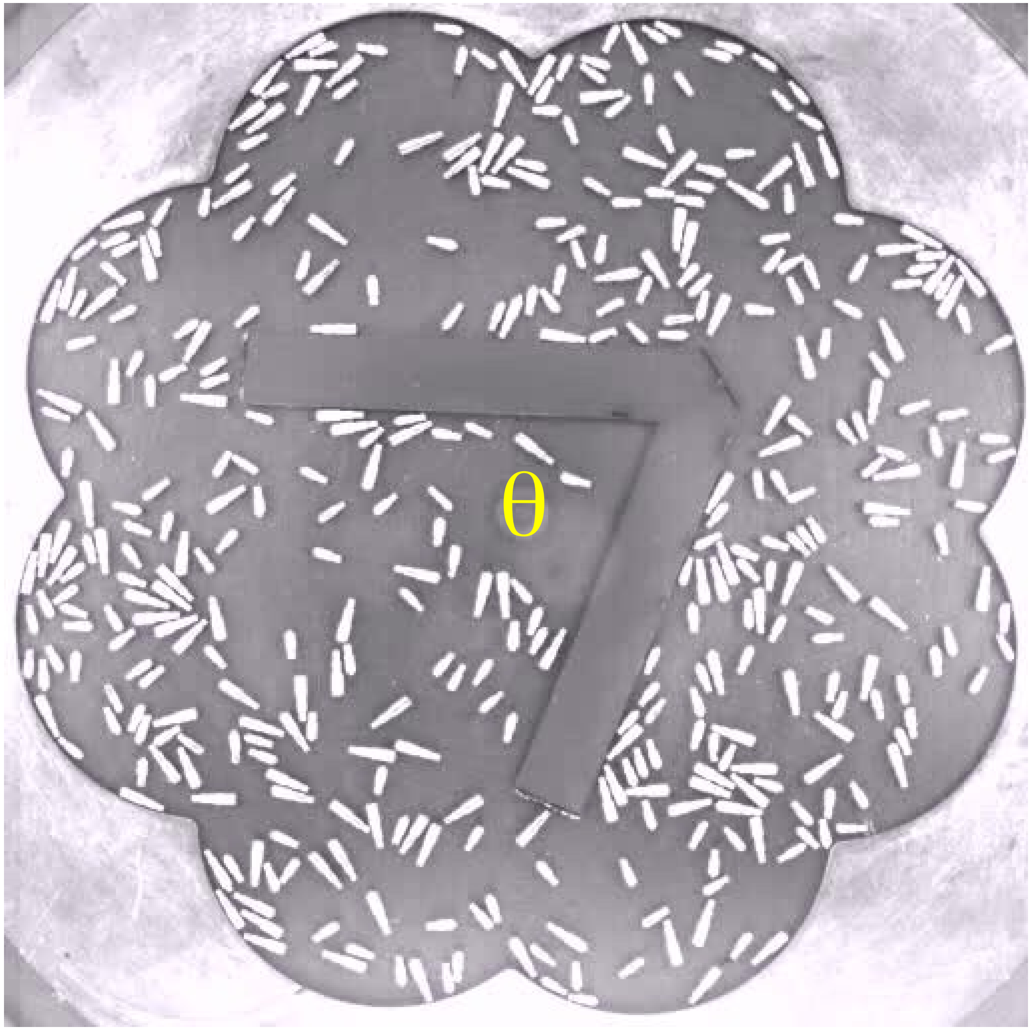
Trapping active liquid crystals

N Kumar, R K Gupta, H Soni, S Ramaswamy, A.K. Sood arXiv:1803.02278



Rahul Gupta
TCIS, TIFR Hyderabad

The trap



Flower geometry
Dauchot group

$L = 10\ell \simeq 4.5$ cm with $20° \leq \theta \leq 160°$ in steps of $10°$

Mechanically faithful simulations

Rahul Gupta & Harsh Soni

Rod = tapered sphere array

Newtonian rigid body dynamics

Friction μ restitution e

Base, lid vertically vibrated

Rotational diffusion: random angular velocity, $\omega = \varepsilon v_{rel}$

$\varepsilon = \pm 0.01$ (prob 1/2), at each rod-base or rod-lid collision

(reproduces experimental angular diffusion)

μ & e

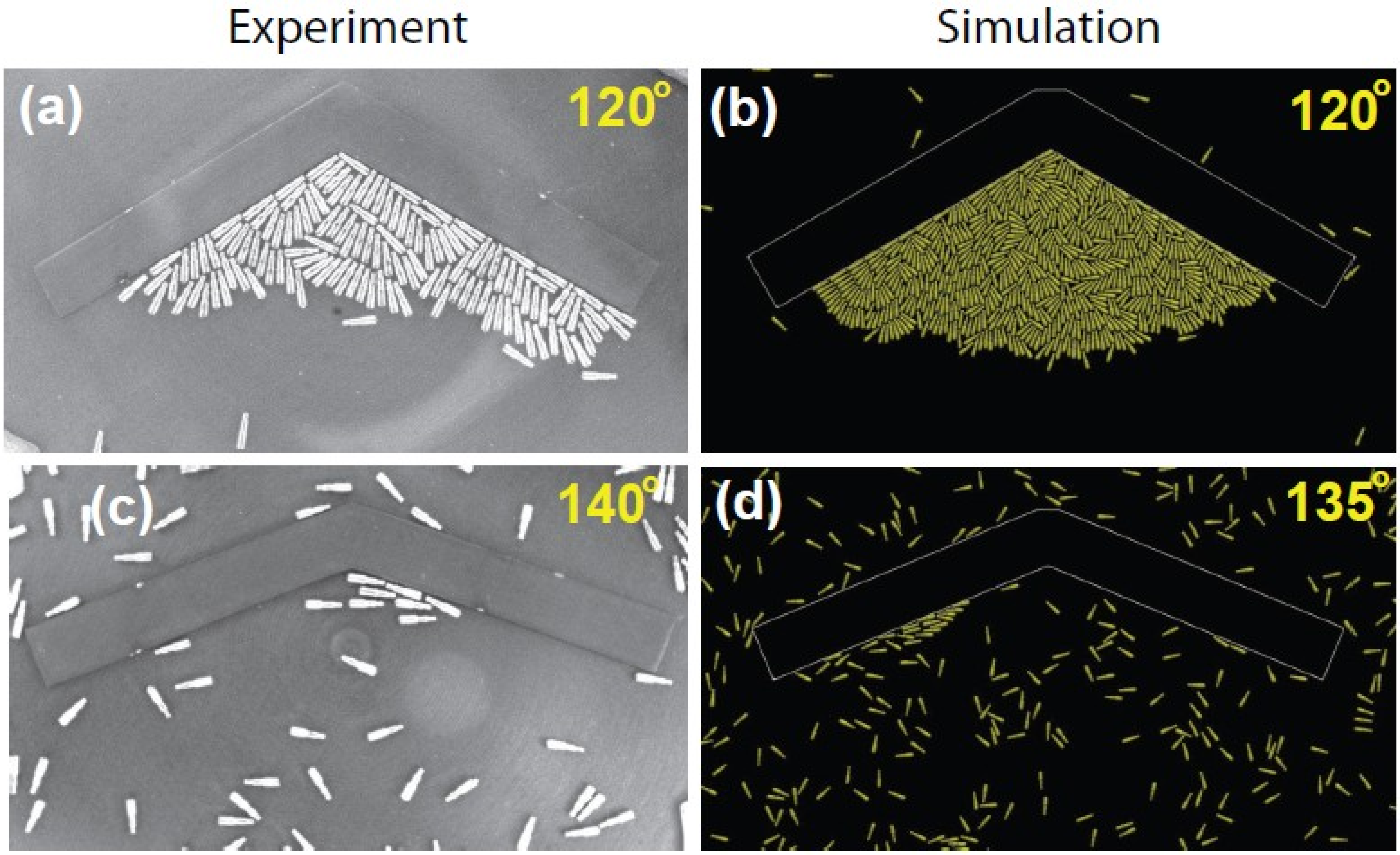
0.05 & 0.3 particle-particle

0.03 & 0.1 rod-base

0.01 & 0.1 rod-lid

0.03 & 0.65 particle-V

Trapped and untrapped states

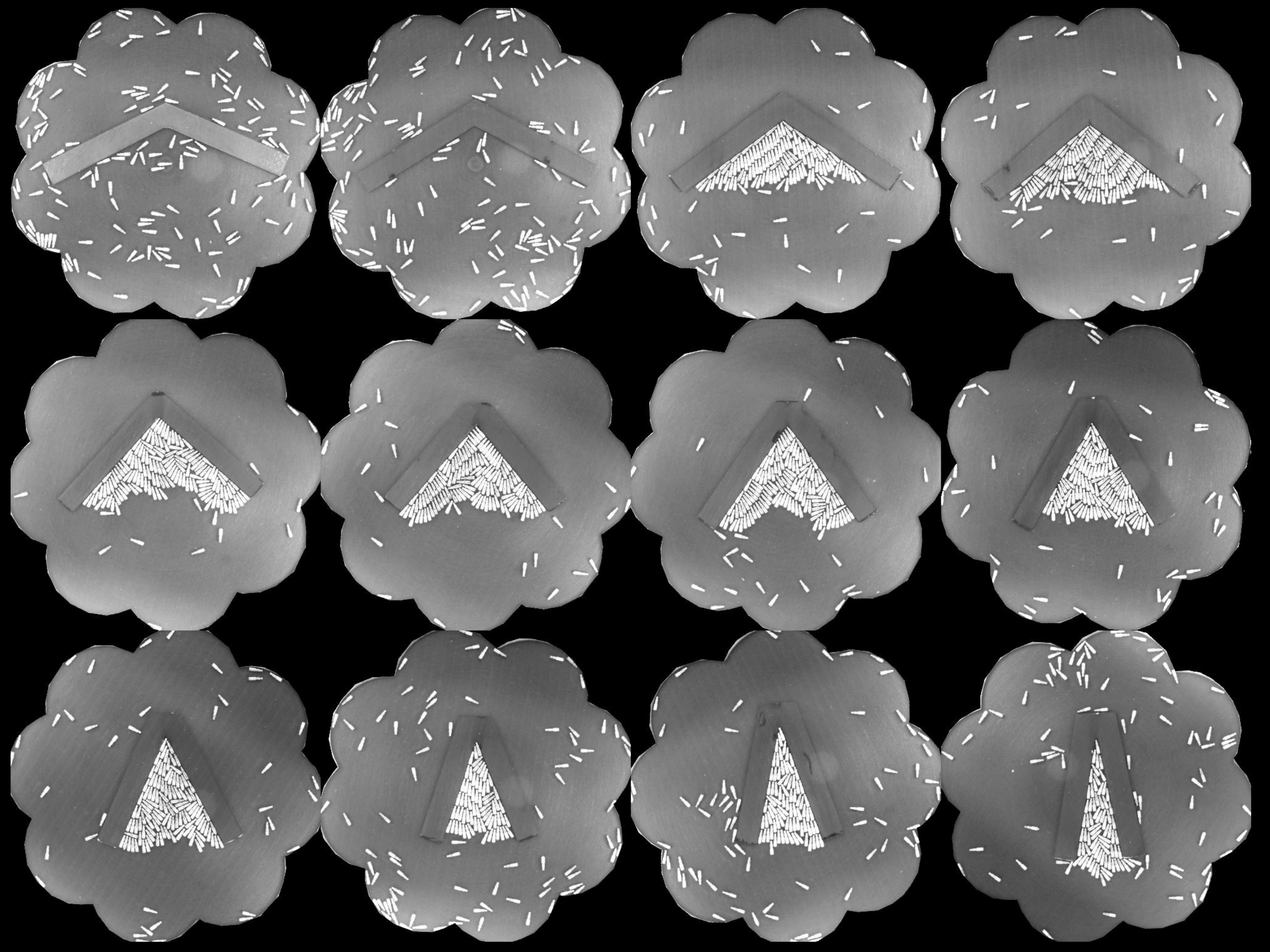


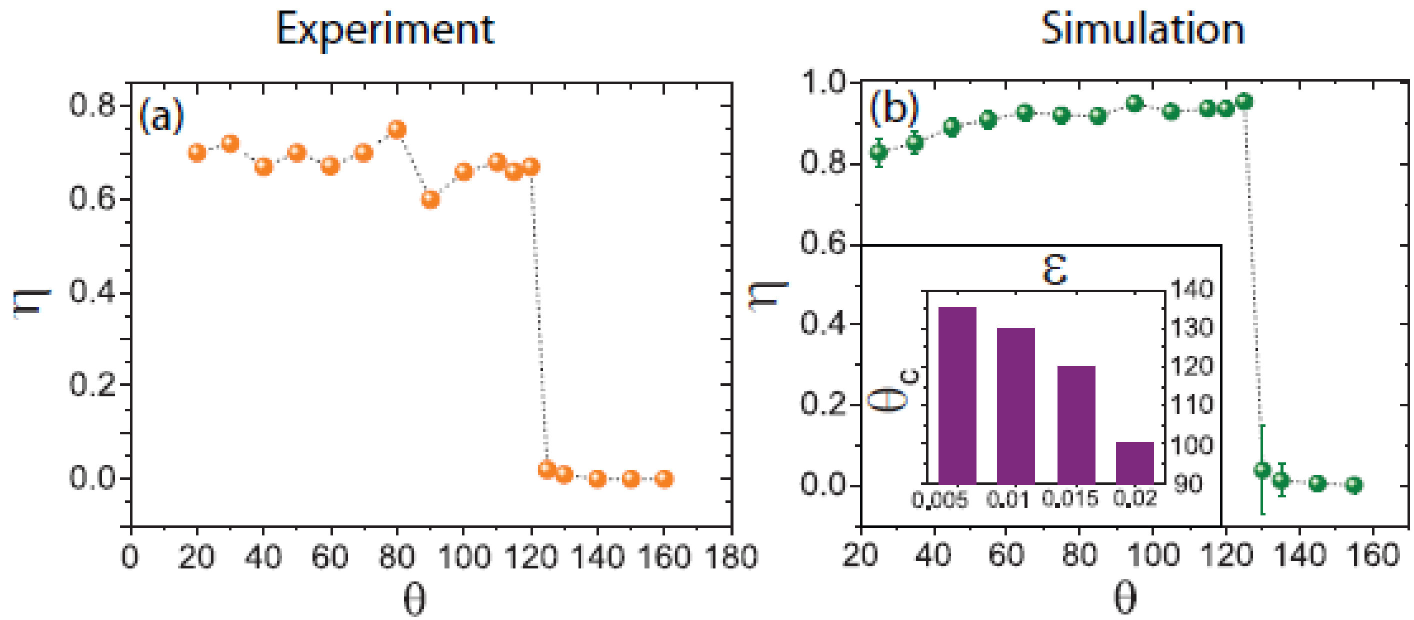
Trapping kinetics: experiments

Single particle /home/sriram/talks/activemattertalks/current/aps2016/nitin15Mar16/SM 6.avi

Collective trapped and untrapped states

transient trapping





INSET: trapping threshold angle decreases as noise increases

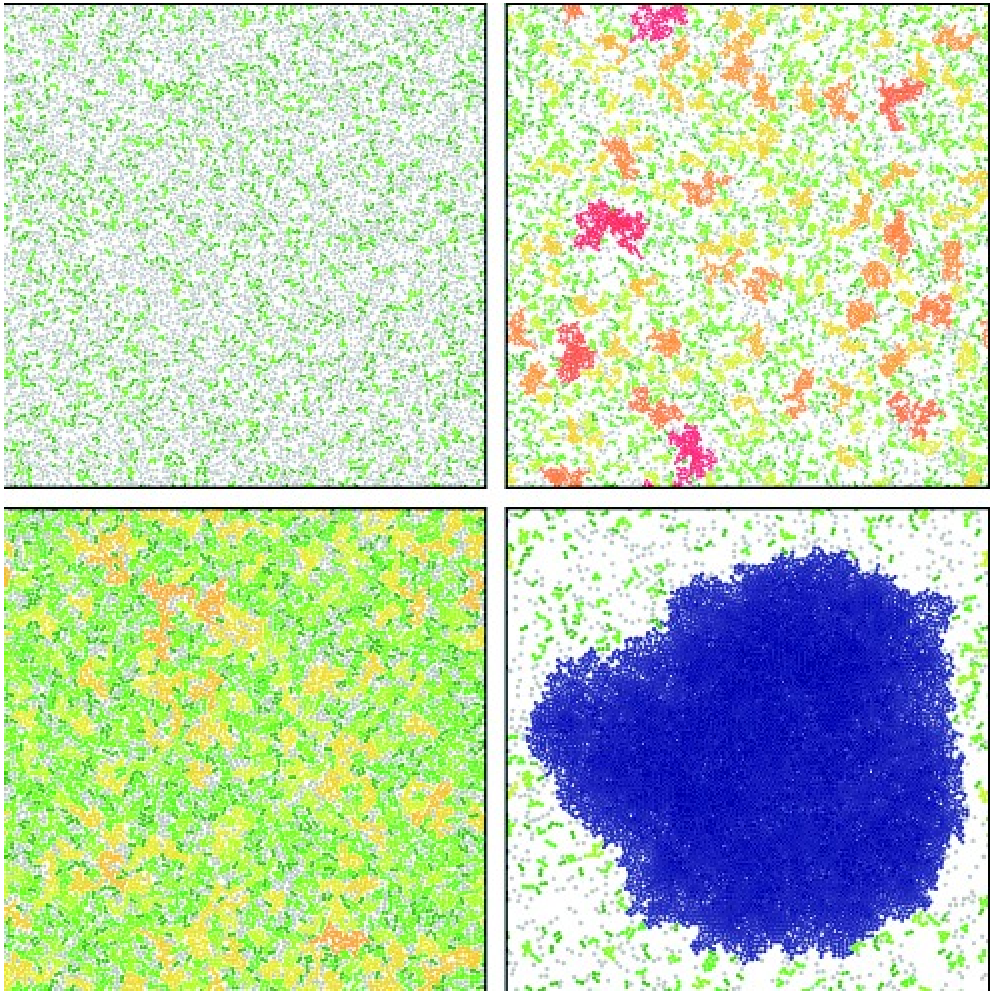
Trapping efficiency $\eta \equiv N_0 a/A_t$

N_0 = # at zero velocity

a = projected area of particle

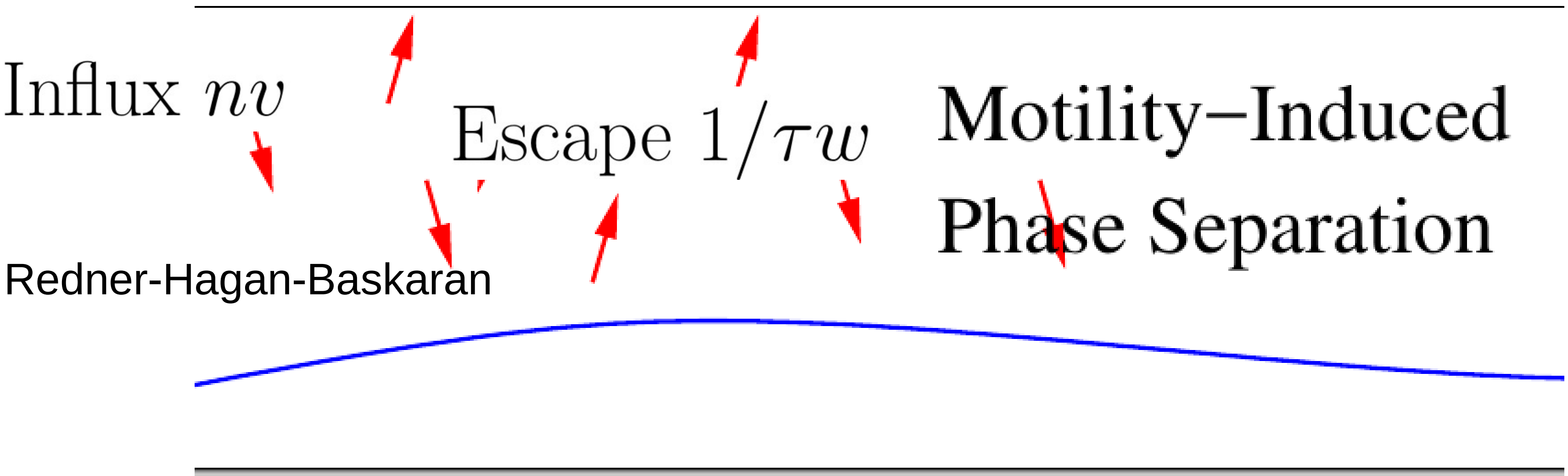
A_t = area of trap

Persistent motion → condensation without attraction



Motility-induced phase separation
Non-aligning SPPs: Fily & Marchetti; Redner, Hagan, Baskaran; Tailleur & Cates;
SP rods: S Weitz, A Deutsch, F Peruani

Theory of trapping



self-propelling speed v

persistence time $\sim 1/D_{rot} = \tau$

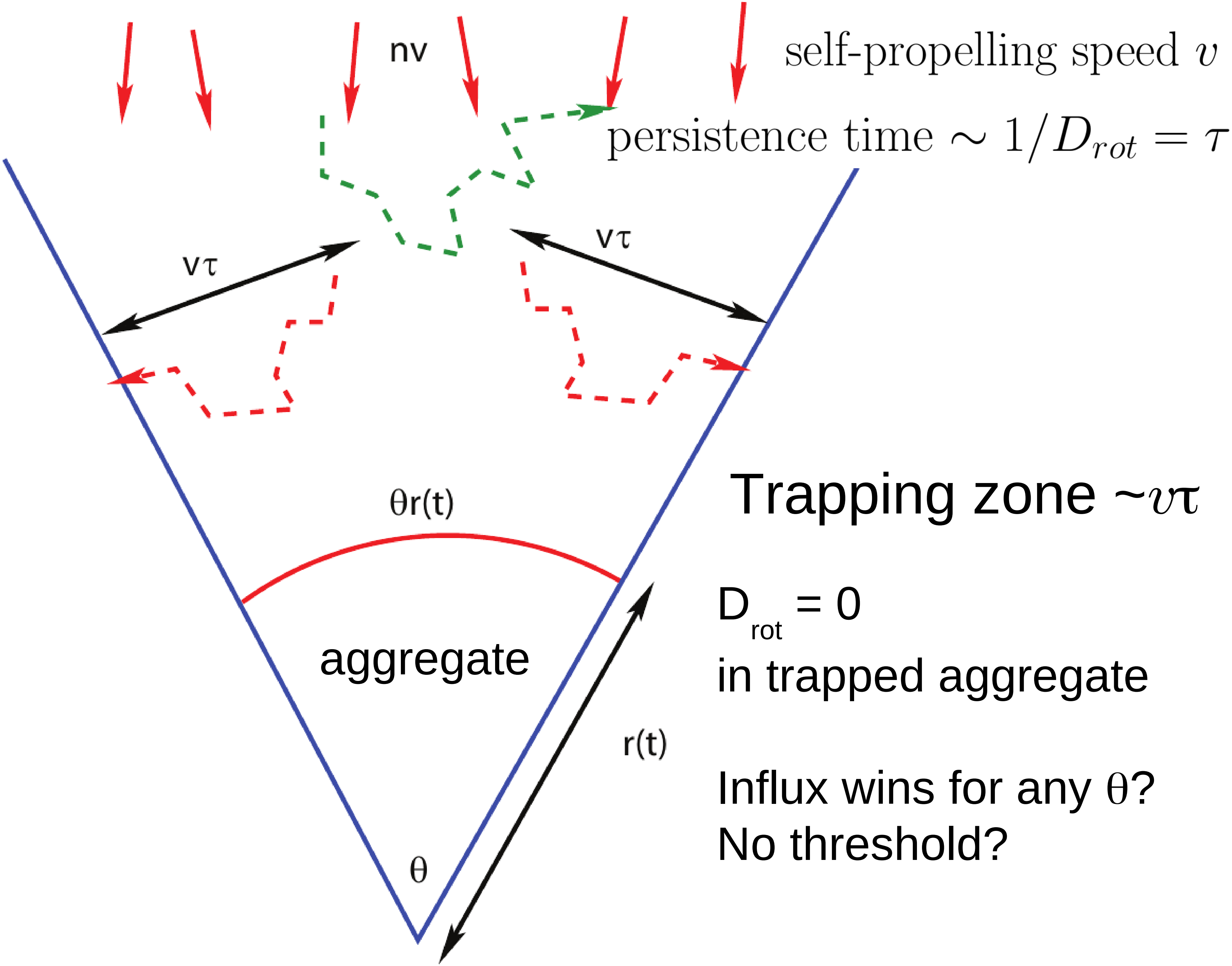
concentration n

particle dimensions $\ell \times w$

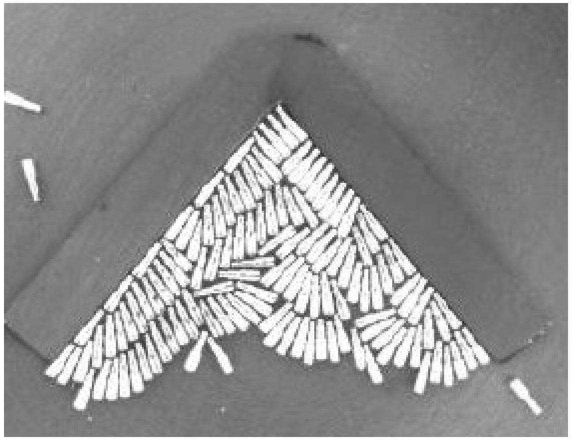
particle area fraction $\phi = n\ell w$

Bulk, no MIPS: $\phi v\tau/\ell \ll 1$

No condensation without traps
Clearly no bulk MIPS
What do traps do?

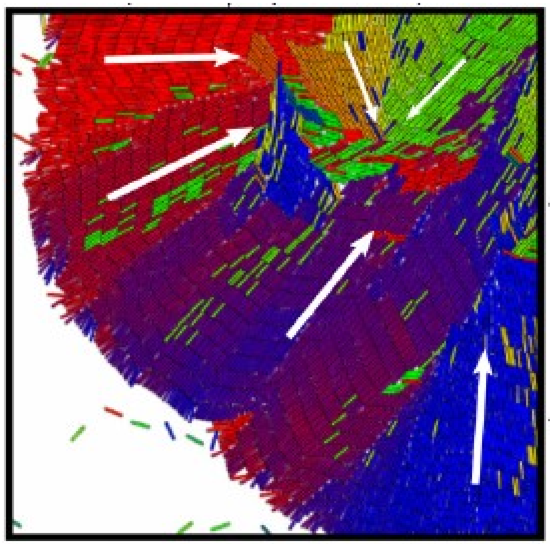

nv
self-propelling speed v
persistence time $\sim 1/D_{rot} = \tau$
vτ
vτ
θr(t)
aggregate
θ
r(t)
Trapping zone ~$v\tau$
D_{rot} = 0
in trapped aggregate
Influx wins for any θ?
No threshold?

Resistance to growth: defects?

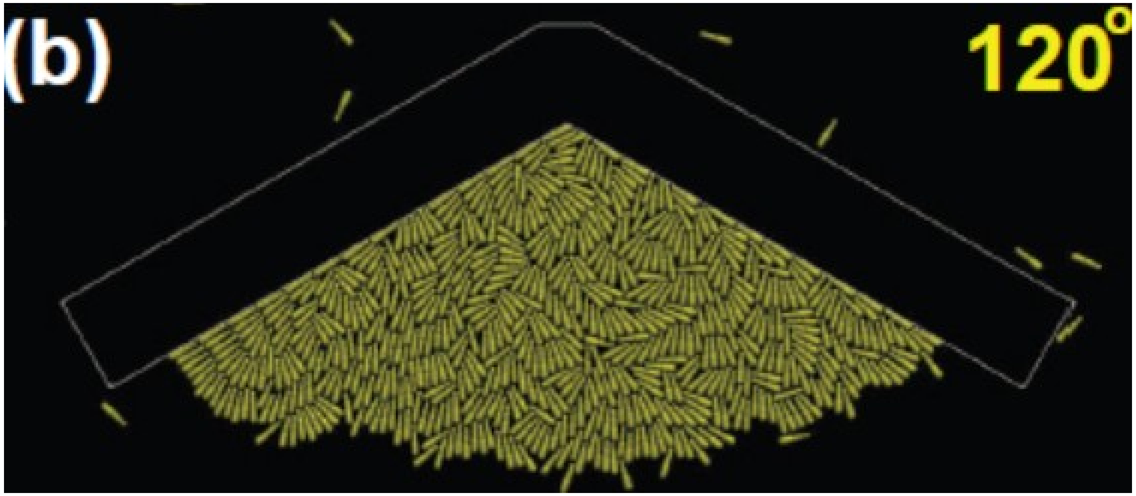


Single disclination fragment? "energy" ~ θ log r

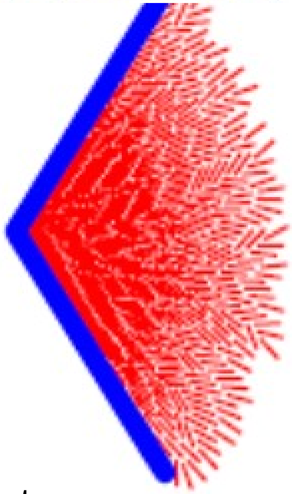
Tilt wall ~ θ r



S Weitz et al 2015
SP-rods

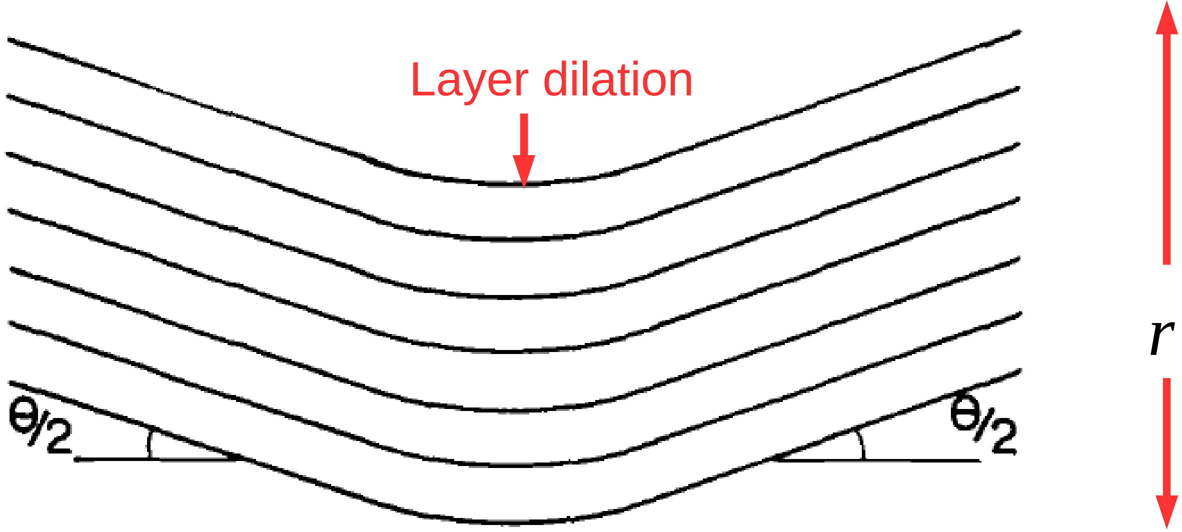


transient trapping



Kaiser et al

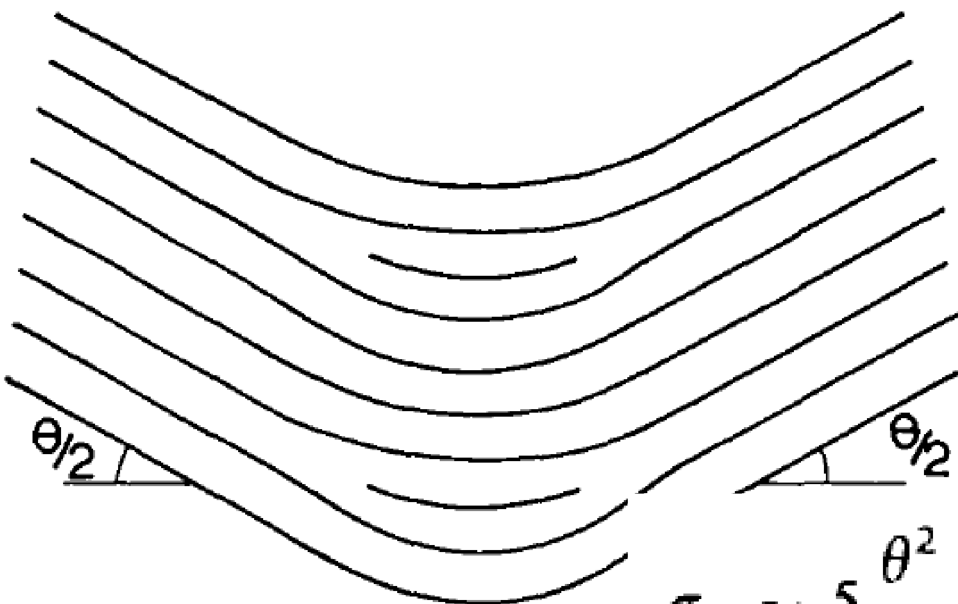
Gowrishankar & Rao asters



(a)

Energy per unit length

$$\sigma_W = \frac{16}{3} B\lambda\theta^3$$



(b)

$$\sigma_d \sim 5\frac{\theta^2 K_1}{\lambda} + \frac{4K_1}{\pi}\frac{\theta^2}{nd}\ln\frac{n}{2} + \frac{\theta^2}{2nd}\tau'_c$$

C. Williams, M. Kléman. DISLOCATIONS, GRAIN BOUNDARIES AND FOCAL CONICS IN SMECTICS A. Journal de Physique Colloques, 1975, 36 (C1), pp.C1-315-C1-320.

Dynamics of collective coordinate r

Effective flux: $nv - 1/\ell\tau \to nv$

Capture zone width: $W_\tau = v\tau$

Wedge "energy" $\sim \theta^\alpha r$

Free edge length $r\theta \to$ mobility $M \sim 1/r\theta$

$\alpha = 2$ or 3

Influx

defect-induced expulsion

$$\frac{dr}{dt} = \phi v \frac{v\tau}{r\theta} - D_{eff} \frac{\theta^\alpha}{r}$$

$$D_{eff} \sim M\,B$$

B = elastic constant for layered structure

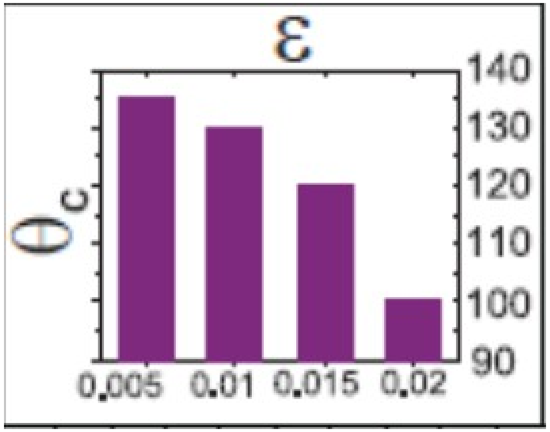
Predictions

Influx   defect-induced expulsion

$$\frac{dr}{dt} = \phi v \frac{W_\tau}{r\theta} - D\frac{\theta^{\alpha-1}}{r} \qquad D \sim MB$$

$$B = \text{effective smectic elastic constant}$$

Simulation confirms



Trapping: all or nothing ✔

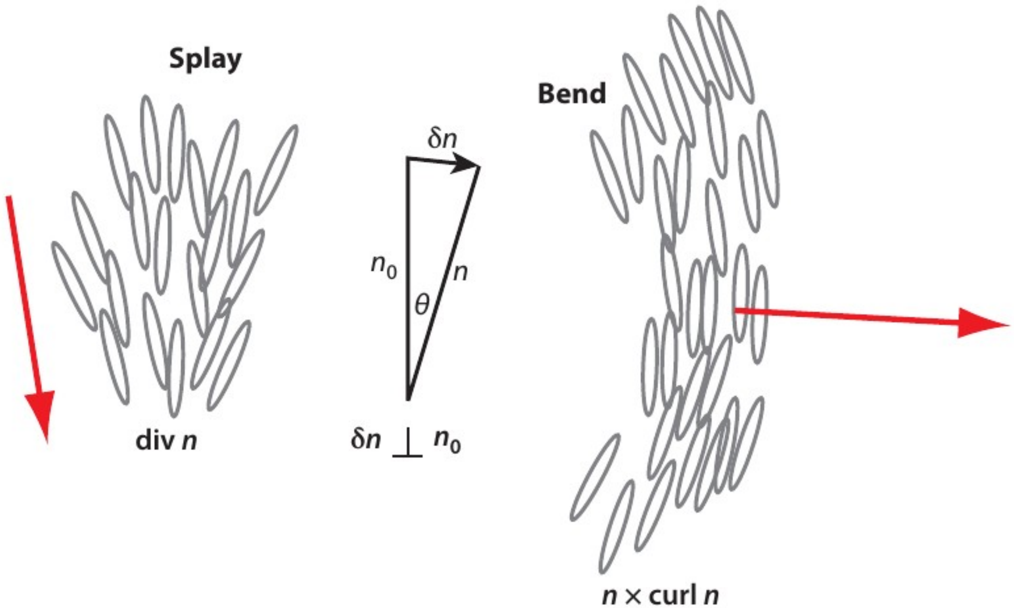
$t^{1/2}$ growth ?

Threshold θ ↓ as rotational noise ↑ ✔

ACTIVE NEMATICS II
topological defects

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

Shankar, Marchetti, SR, Bowick, arXiv 2018



Q = local alignment tensor

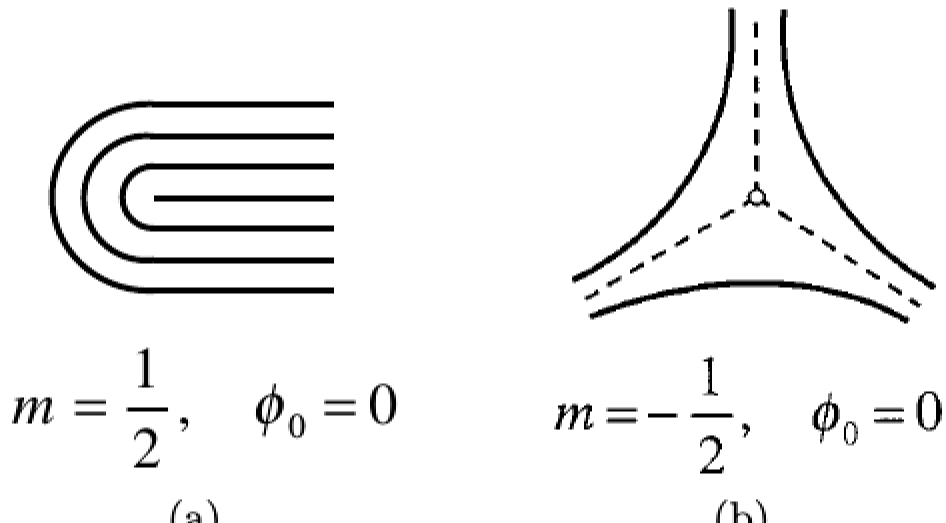
Gradients of **Q**; curvature

Div **Q**: vector

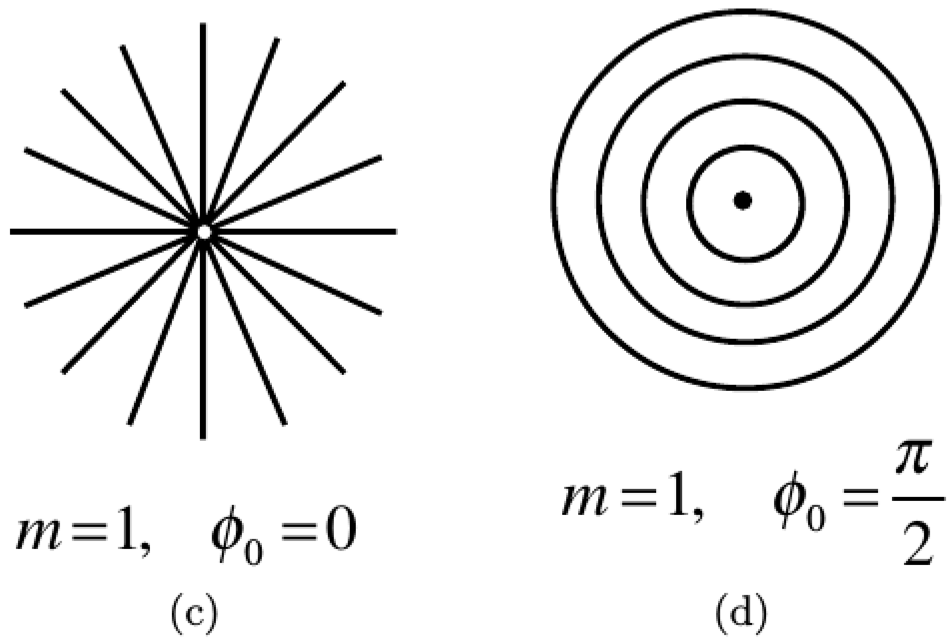
Active: local current ~ div **Q**

SR, Simha, Toner 2003

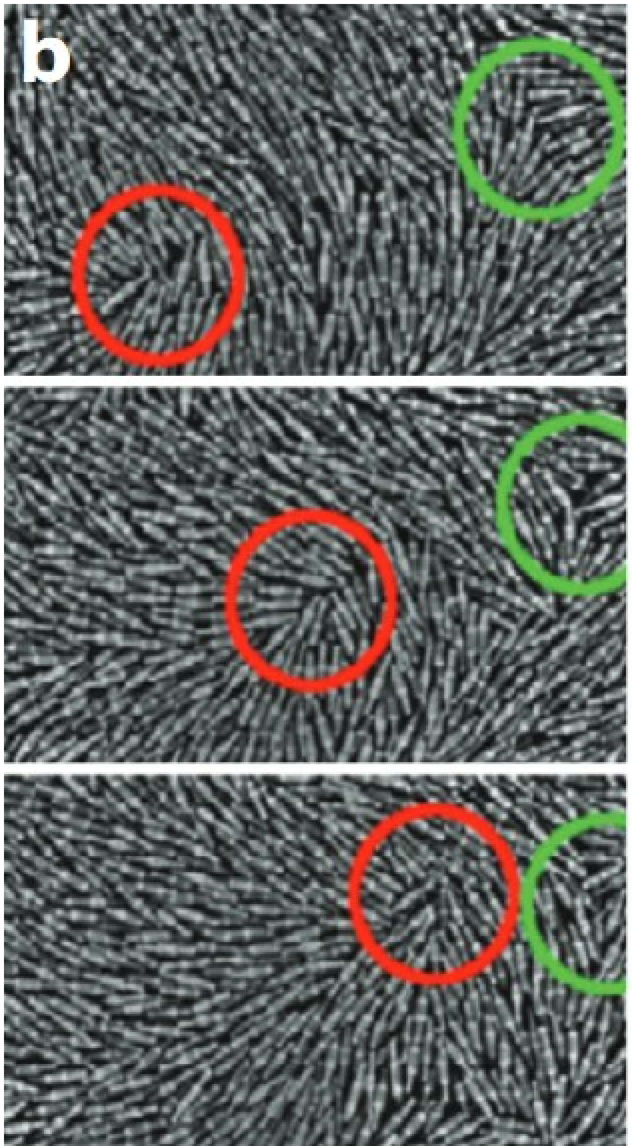
Topological defects in a nematic



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



Defect unbinding in active nematics



Suraj Shankar, M C Marchetti, SR, MJ Bowick

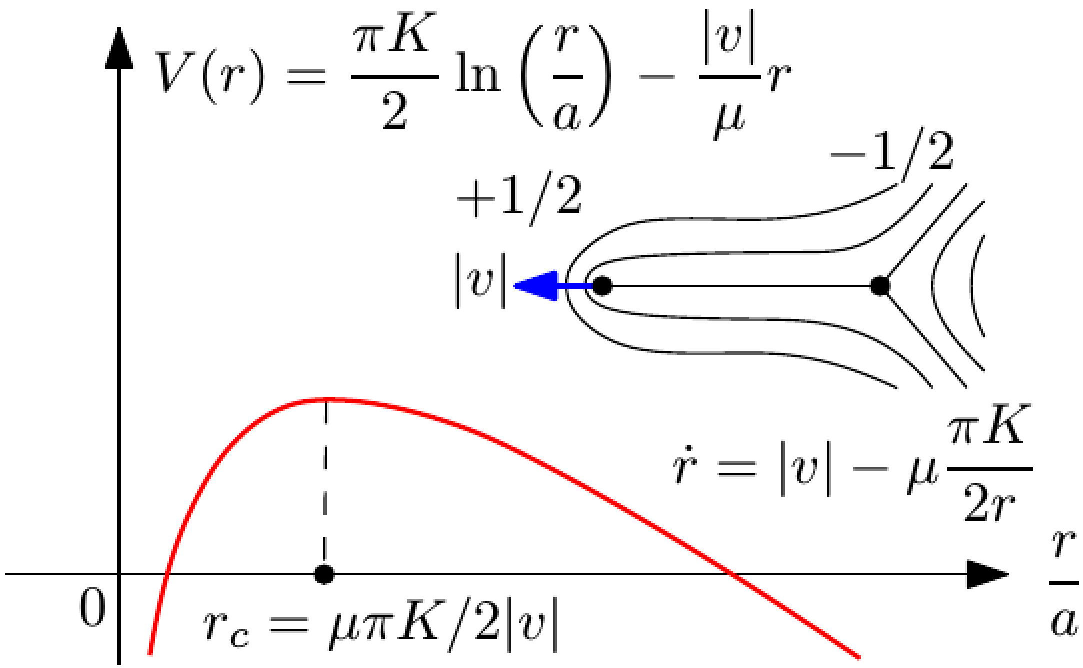
The symmetry of the field around the strength -1/2 defect will result in no net motion, while the curvature around the +1/2 defect has a well-defined polarity and hence should move in the direction of its “nose” as shown in the figure.
V Narayan et al., Science **317** (2007) 105

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

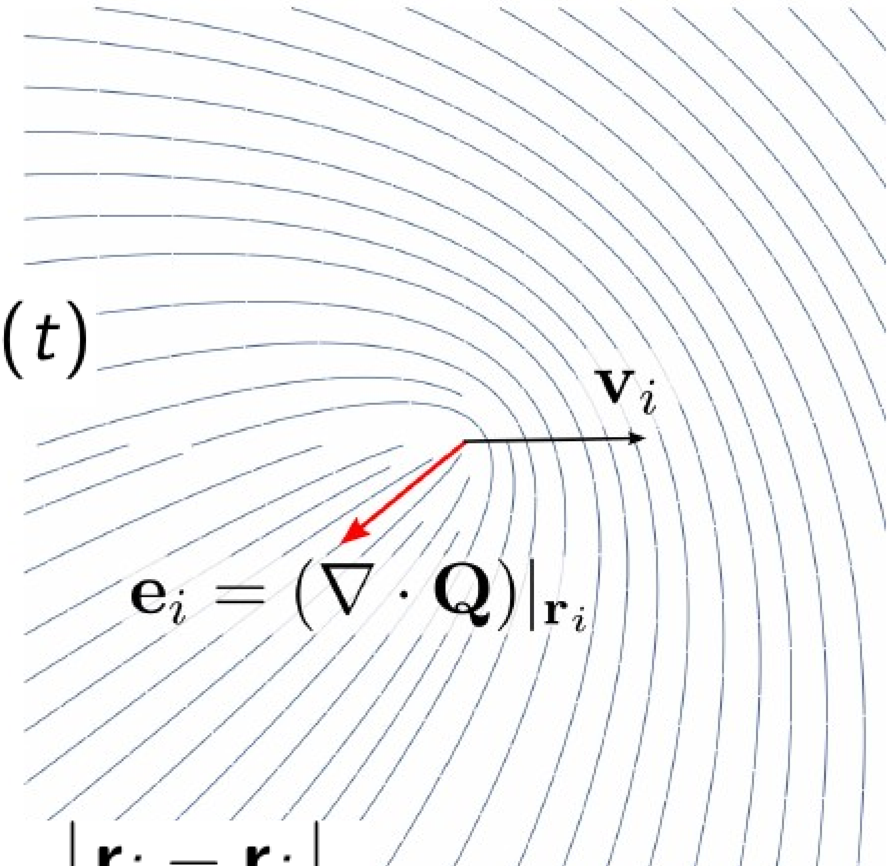
Shankar et al. arXiv 2018:

From active nematic dynamics

+1/2 self-velocity ∝ polarization

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

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



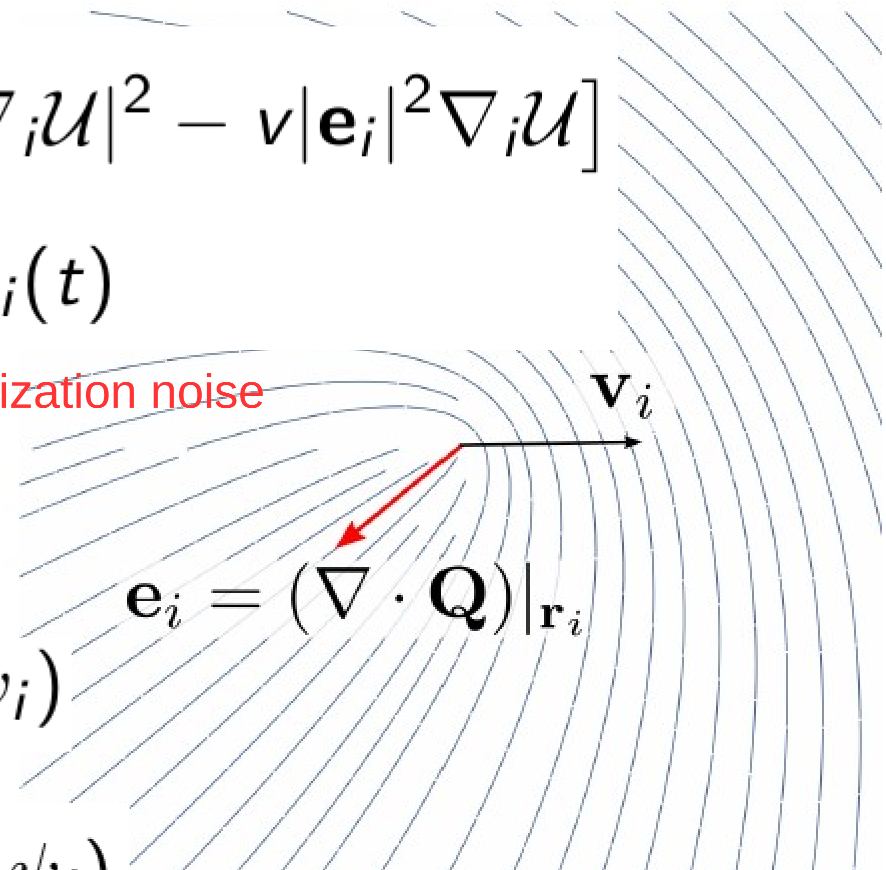
$$\mathcal{U} = -2\pi K \sum_{i\neq j} q_i q_j \ln\left|\frac{\mathbf{r}_i - \mathbf{r}_j}{a}\right|$$

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

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

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

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

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

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

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:

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

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

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

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

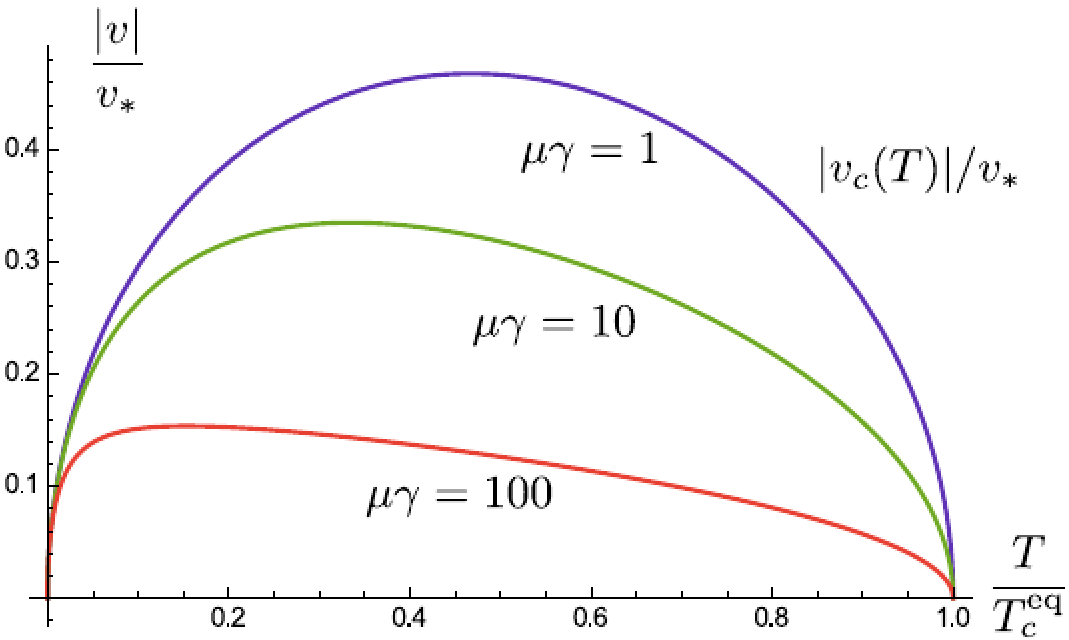
Threshold activity

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

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)

Summary

- Unified picture of fluctuating active dynamics
  - natural language to describe living materials
- Confined active fluids
  - new force density: stable nematics
  - polar: super−stable / −unstable

Maitra et al
arXiv:1711.02407

- Artificial motile systems — a great test−bed
  - a few motile particles can mobilize a big group
  - trapping: motility−induced condensation vs defect energy

Kumar, Soni, Sood, SR
NComm 2014 & in prep

Kumar et al
arXiv:1803.02278

- Pair sedimentation of discs
  - analogies with self−propelled systems

Chajwa, Menon, SR arXiv:1803.10269