BUGS, MOTORS, COPPER RODS AND BROWNIAN INCHWORMS

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Based on

- [K Vijay Kumar, SR, Madan Rao](#), in preparation
- [S Mishra](#) and SR, cond-mat/0603051
- [R A Simha Ph D thesis](#), IISc 2003
- [R A Simha](#) and SR, Phys Rev Lett **89** (2002) 058101
Support

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DIRECTED MOTION

Herds, bird flocks

Fish schools, bacteria

Crawling cells/fragments, treadmilling actin

Cell extracts: motors + filaments

Rods on a vibrating surface
Collective behaviour of *many* moving things

Approach: nonequilibrium statistical mechanics

Drawn to questions of how *one* thing moves: noise $\rightarrow$ directed motion

For this workshop: common features of treadmilling actin, translocating motors, granular arrowheads
TALK PLAN

- Background, systems of interest
  - What are active particles?

- Self-propelled suspensions, force dipoles
  - Rheological consequences of activity

- Active granular matter
  - Apolar vs polar; giant number fluctuations

- Force dipoles, tension and propulsion from noise
  - Brownian inchworms

- Conclusion and prospect
SYSTEMS OF INTEREST

Fish liquid crystals

http://fins.actwin.com/fish/marine-pics/anchovie.MOV
Active topological defects

kinesin + microtubules
Nedelec et al. 1997

http://www.cytosim.org/others/princeton/
Order and instabilities in bacterial suspensions

Ott, Kessler, Goldstein
U. of Arizona
B. subtilis

http://math.arizona.edu/ lega/UG/Colonies/Colonies.htm
Membranes + pumps
SR/Toner/Prost 2000
Bassereau et al. 2001

Active fission-fusion
Sarasij/Rao 2001

Active filaments

Actin-myosin (Spudich), treadmilling actin (Theriot), helicase (Schulten, Ha)

http://www.dictybase.org/tutorial/myosinassays.htm
http://cmgm.stanford.edu/theriot/movies.htm
Polar and apolar particles

Polar
- Fish, Bacteria
- Motor–filament
  - fore-aft asymmetric

Apolar
- Melanocytes,
  - Symmetric rods,
  - Bundles
  - symmetric
Polar and apolar order

POLAR ORDER
fore-aft asym particles

apolar order

APOLAR ORDER
can order symmetrically
Melanocyte aggregates
Kemkemer et al. 2000

APOLAR active systems

Fig. 8. A set of -1/2 disclination is shown for melanocytes. The bar is 100 μm. Different possibilities are shown: (a) the core of the disclination is an empty hexagon. (b) The core of the disclination is an annulus with concentrically distributed cell. (c) The core of the disclination is occupied by a star shaped cell. The cells which form the annular fluid are in an elongated bipolar state.

V Narayan, N Menon, SR
Absorb and dissipate energy: nonequilibrium steady state
Motion self-directed
Common features of our systems

Self-driven, interacting, correlated, noisy

Orientable particles: ordering?

Fixed energy *throughput*, not budget

All particles forced independently, not from boundary

not like shear flow or 3d granular
SELF-PROPELLED SUSPENSIONS

Why do they form? HARD
Mechanism of motion? HARD

ASSUME in or near ordered state EASIER
Response to disturbance? Hydrodynamic approach
Fluctuation statistics?

Construct equations of motion for slow variables

Related: Lau, Lubensky PRL 2003, Kruse et al. PRL 2004
Our interest

Symmetry, conservation laws $\rightarrow$ coarse-grained eqns of motion

Nonequilibrium steady state; infer statistics from eqns of motion: no Gibbs distribution, no Onsager symmetry.

Focus: qualitative difference from dead Brownian particles
Earlier work

Reynolds 1987: computer graphics for movies

Vicsek et al 1995: simulations

Toner and Tu 1998: field theory – moving XY model

Only polar order: can’t describe nematics

No fluid flow: misses physics of suspensions

Fluid dynamics literature (Lighthill, Pedley-Kessler): doesn’t consider ordering
Generic hydrodynamic eqns for active-particle systems

Ordered phases

- Travelling waves
- Giant number fluctuations, tails
- Ordered low-Re swimmers always break up into finite domains (expts)

Isotropic phase: novel rheology; nonequilibrium noise

- Increase correlations $\rightarrow$ stiffen or soften
- activity $\rightarrow$ giant noise-temperature, tails

HOW?
Active-particle concentration $c(x, t)$

Momentum density of particles + fluid $g(x, t) = \rho u$

$u = \text{hydrodynamic velocity field}$

Incompressible: $\rho = \text{constant}; \nabla \cdot u = 0$

Polar order parameter: active-particle velocity relative to solvent: $v(x, t)$

Simha and SR PRL 2002

See also Kruse et al. “active gels” PRL 2004
Building equations of motion

Number conservation: \( \partial_t c = -\nabla \cdot J \)

Newton II:  \( \partial_t g = -\nabla \cdot \sigma + F_{ext} \)

Order-parameter:  \( \partial_t v = \text{Forces and Torques} \)

Express \( \sigma, \ J, \) forces and torques in terms of slow variables.
Easiest: concentration equation

\[ \partial_t c = -\nabla \cdot J \]

\[ J = c(v + u) \]

\( \mathbf{v} \) is velocity \textit{relative} to medium

Galilean invariance of particles + fluid
Momentum equation

Activity: internal forces: Total momentum (particles + solvent) conserved

\[ \partial_t \mathbf{g} \equiv \partial_t (\rho \mathbf{u}) = -\nabla \cdot \mathbf{\sigma} \]

\[ \mathbf{\sigma} = -\eta \nabla \mathbf{u} + \rho \mathbf{l} + \mathbf{\sigma}^a \]

viscosity  pressure  activity
Modelling active stresses

Guess (symmetry permits)

\[ \sigma_{ij}^a(x, t) \propto c u_i u_j \]

because of noneq activity

**CONTRAST:** for thermal equilibrium uniaxial phase
structure anisotropic, mean stress isotropic

More microscopically:
One active particle

\[ F_{\text{ptcl-med}} = -F_{\text{med-ptcl}} \]

Force-density has zero monopole moment

Active particle = permanent force dipole

Brennen and Winet 1977
Point forces, equal magnitude, opposite direction

\[ a \neq b: \text{mover (polar, vectorial); velocity } \mathbf{v}_\alpha = v_0 N_\alpha \]

\[ a = b: \text{shaker (apolar, nematic); velocity } = 0 \]

Coarse-grain: \( \mathbf{v}_\alpha \rightarrow \mathbf{v}(\mathbf{x}, t) ; \mathbf{v}_\alpha \mathbf{v}_\alpha - \frac{1}{3} v_\alpha^2 \rightarrow \mathbf{Q}(\mathbf{x}, t) \)
Examples

steady-state activity $\leftrightarrow$ permanent force dipoles

$$\sigma^a = K Q; \text{sgn}(K)?$$
Force density

\[ \text{Force density} = \nabla \cdot (a + b) f \mathbf{Q} + (a - b) f \mathbf{Q} \mathbf{Q} \]

in continuum limit

\[ c = \text{local concentration} \]

\[ \mathbf{Q} \sim \mathbf{v} \mathbf{v} = \text{local alignment tensor} \]

Simha and SR PRL 2002

Motor-filament calculation: Liverpool and Marchetti 2006
Driven state: curvature (asymmetry) $\rightarrow$ flow (Curie)
Polar order-parameter dynamics

\[ \dot{v} \sim + (\nabla u \cdot v) + \alpha v - \beta |v|^2 v - \nabla (cQ) + O(\nabla \nabla v) + \therefore \]

- advection
- speed limit
- stress
- elasticity

Toner-Tu + fluid flow

Flow rotates orientation
Bacteria: stokesian limit

Include viscosity, ignore inertia

Viscous forces balance active forces

\[-\eta \nabla^2 u_\perp \sim \partial_z \delta n_\perp - \nabla c + \ldots\]

\[\partial_t c \sim -\partial_z c - \nabla \cdot \delta n_\perp + \ldots\]

\[\partial_t \delta n_\perp \sim \partial_z u_\perp + \nabla_\perp c + \ldots\]

\[\Rightarrow\] Effective eqn of motion

\[(\partial_t + v_0 \partial_z) \delta n_\perp \sim \tau^{-1} c^{\cos 2\theta} \delta n_\perp\]

Instability near 45°!
\[ \tau \sim \frac{\eta}{ac_0} f \sim 0.1 \text{ sec} \]

\( a = \text{particle size}, \ c_0 = \text{mean conc.}, \ f = \text{active force} \)

Convective instability for \( \text{Re} \ll qa \ll 1 \)

\( q = \text{wavenumber} \)

Relevant regime for bacteria

Only \textit{finite-scale} ordered domains!

Simha and SR PRL 2002

Experiments? Dombrowski \textit{et al.} PRL 2004

Effect of shear (S Muhuri, Raman Instt)

Instabilities in film flow: SR in preparation
Isotropic phase: active rheology


\[
\frac{\text{stress}}{\text{strain}} = \frac{\sigma(\omega)}{\epsilon(\omega)} = G^*(\epsilon, \omega) = G_{\text{struct}}^* + G_{\text{activ}}^*
\]

Liverpool et al 2001 (polymers) Liverpool-Marchetti, Fabry et al., Lau, Lubensky
Shape and activity

Assume flow-aligning

SHEAR -- ORIENTED ACTIVITY
ACTIVITY -- REDUCES FLOW

stable

unstable?

SHEAR -- ORIENTED ACTIVITY
ACTIVITY ENHANCES FLOW
Active viscoelasticity

In general
$$\partial_t \mathbf{Q} + \tau^{-1} \mathbf{Q} \sim \nabla \mathbf{u}$$
relaxation, coupling to flow

Active:
$$\partial_t \sigma^a + \tau^{-1} \sigma^a \sim K \dot{\varepsilon} \quad \text{(shear-rate)}$$

$$G''_{\text{activ}} \sim K \frac{(\omega \tau)^2}{1 + (\omega \tau)^2}$$

Strong viscoelasticity if $K > 0$; strong softening if $K < 0$.
This plus instability: fragile jammed matter à la Cates (SR + M Rao 2006)?
Not like equilibrium

Contrast: equilibrium systems near orientational ordering transitions:

\[ \sigma \sim \frac{\delta F}{\delta Q} \quad \text{(field conjugate to } Q; \rightarrow 0 \text{ at transition)} \sim T - T_* \]

\[ G_{\text{passive}}' \sim \frac{\omega^2 \tau}{1 + (\omega \tau)^2} \]

All effects discussed on previous slide \( \rightarrow 0 \) as system approaches ordering transition
Isotropic phase

Wu-Libchaber, Soni et al. – bacterial swimming

- Active stresses: noise source for dynamics of fluid velocity
- Estimate $T_{eff}$ from variance of $\sigma^a$
- Find $10^5 – 10^6$ Kelvin, similar to Wu-Libchaber bacterial water-polo

Basmati: smectic?
flat tip: tetratic?
tapered: nematic
Other apolar active systems

Melanocyte aggregates
Kemkemer et al. 2000

rod monolayer
V Narayan, N Menon, SR
Shaken monolayers of rods


V Narayan, N Menon, SR 2006

rod swirls

polar rods move
Driven steady state

Not thermal equilibrium

Don’t have Boltzmann-Gibbs

Must construct equations of motion by “pure thought”

Infer statistics from dynamics
Active nematics: different

True nematic order: fore-aft symmetric, mean velocity zero
Just like equilibrium nematic? Effective temperature?

Variables:
Concentration $c$, 1 order parameter fluctuation $\delta n_\perp$
Ignore velocities
Substrate: momentum sink
Splay or bend $\rightarrow$ current

ASYMMETRY LEADS TO CURRENT

\[ J_x \propto \partial_z \theta \quad J_z \propto \partial_x \theta \]
Curvature $\rightarrow$ current

\[ J^{(a)} \propto \nabla \cdot Q \]

Curvature $\Rightarrow$ left-right asymmetry $\Rightarrow$ current
Giant number fluctuations

Recall

$$\langle (\delta \theta)^2 \rangle \sim \frac{T}{K} \ln \frac{L}{a}$$

and

Flux $\propto \delta \theta$

Thus concentration fluctuation (almost) indep of $L$.

Hence $\delta N_{rms} \propto N$.

Cf. particles sliding down fluctuating surface
Das-Barma-Majumdar, Drossel-Kardar
Not an effective temperature

Note:
\[ \langle |c(\mathbf{q})|^2 \rangle \sim q^{-2} \]

system size \( L \Rightarrow \langle (\delta N)^2 \rangle / N \propto L^2 \propto N^{2/d} \)

\( d = 2 \): standard deviation \( \propto \) mean!

\[ \langle \delta c(x,0)\delta c(x,t) \rangle \sim \ln(1/t) \]

None of this can be described by effective temperature
Phase separation?

Simulation: Mishra and SR cond-mat/0603051 — particles actively advected by nematic fluctuations.

Uniform distribution → coarsening:

fluctuation dominated phase separation
Das, Barma, Majumdar 2000

Chaté et al. PRL 2006: independent confirmation in computer experiment

Experiments on biological systems?
Shradha’s results

\[ L(t) = 1280.4t^{0.49} \]

steady state \( L(t) \)
A BROWNIAN INCHWORM

Turn noise into directed motion?

No substrate sawtooth potential?

Build a moving dimer: K Vijay Kumar and M Rao
Equations of motion

\[ m_i \ddot{x}_i + \zeta_i \dot{x}_i = -\partial_i U(x) + f_i \]

\( x, \; X \) = relative and C of M coordinates

\[ \langle f_i(0) f_j(t) \rangle = A_i \delta_{ij} \delta(t) \]

Only \( \zeta_1 \) depends on \( x, \zeta_2, A_1, A_2 \) don’t.

\( U \) symmetric, \( \zeta_1 \) asymmetric, or vice versa \( \rightarrow \) drift of \( X \).
The Brownian inchworm

one moving dimer
Features

Clear analogy to Ha-Schulten 2006

Relate their parameters to these?

Restoring equilibrium: $A_1 \propto \sqrt{\zeta_1}$ kills drift

In noneq steady state, $\langle \partial_1 U \rangle \neq 0$
Velocity and force time-series

Asymmetric damping, harmonic $U(x)$, no FDT
Asymmetric damping, harmonic $U(x)$, no FDT
Symmetric damping, noncentrosym $U(x)$, no FDT
Probability distributions

Symmetric damping, noncentrosym $U(x)$, no FDT
Velocity and force time-series

Asymmetric damping, harmonic $U(x)$, with FDT
Asymmetric damping, harmonic $U(x)$, with FDT
Dynamics of the distribution

distributions from an ensemble: equil vs noneq
Thus: steady state tension, spontaneous motion, force dipole

Can interpret $x$ as length of actin treadmill, tilt of polar granular rod

Many obvious generalisations: collections of inchworms, longitudinal or transverse chain, immerse in fluid etc.
CONCLUSION AND THE FUTURE

- Framework for mechanics of living soft matter
- Ordered phases
  - Orientational order $\rightarrow$ shear rigidity, waves
  - Giant number fluctuations, long-time tails
  - Long-ranged order unstable for low Reynolds no.
- Isotropic phase
  - Active shear-thickening of contractile filaments
  - Giant noise-temperature as in bacteria experiments
- Rod monolayers: promising analogue
- Simple Brownian inchworm model for individual active particles