

Synchronization and LC order in soft active matter



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Plan

- 1. Introduction ...
- 2. Focus on active elements ...
- 3. Cycles, synchronization ...
- 4. Dynamic active particle suspensions (time)
- 5. Outlook



active matter ?

Collection of interacting self- driven units with emergent behavior at large scales

Energy input that maintains the system out of equilibrium is on each unit, not at boundaries

Robust behavior in the presence of noise (generally nonthermal)

Orientable units \rightarrow states with orientational order





(soft) active matter?

swimming bacteria, janus particles, cell cytoskeleton



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Legionella



Active suspension



Tubulin - green, Actin -red, Nucleus- blue

Active elements – complex fluid constituents

- polymers, colloids, membranes, ...

Weak interactions ~ k_BT , slow dynamics, fluctuations, ...

+

Life - an internal source of energy KITP, April 2014



Cycles in the Cytoskeleton

- Filaments/motors
- Cytoskeletal filaments



- F-actin and Myosin use ATP to turn chemical energy into mechanical work (duty cycle)
- Kinesin 'walks' along Microtubules using ATP as fuel
- Collective behaviour of fiaments/motors





Schaller et al, (2010, 2013)













Strokes of micron sized swimmers





Butler & Camilli, (2005)



Weibel et al, PNAS (2005)











Lighthill, SIAM review (1976)

Collective behaviour of bacillus subtilis

Zhang et al, (2010)





Phenomenology of active units







Liquid crystals

Anisotropic objects (mesogens) -> "between" liquid & crystal

Increase density, decrease T ۲ Mesophase isotropic smectic A smectic C nematic **Broken** rotational translational + trans. + none **Symmetry** rotational rot. Other phases : columnar, cholesteric KITP, April 2014

Order parameters



 $Q_{ij} = Q_0 \left(\hat{n}_i \hat{n}_j - \frac{1}{3} \delta_{ij} \right) \qquad \text{director:} \\ \hat{\mathbf{n}} \leftrightarrow -\hat{\mathbf{n}}$

Isotropic $Q_0 = 0$

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Nematic

 $Q_0 \neq 0$



Order parameters

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BRISTOL Broken continuous symmetries

d=3





modelling collective behaviour

Identify large scale degrees of freedom

Generic models of possible behaviours



Bottom-up modelling

Properties of ingredients

Macroscopic properties



simplifications required to make process tractable



Programme ?

Simple models for micron sized self propelled objects (SPO) – obtain design principles

Simplified physical theory that links microscopic properties of SPO to macroscopic behaviour

Understand macroscopic mechanical properties (initially qualitative -> eventually quantitative)



Micro-hydrodynamics

 ${\rm Re}=\rho VL/\eta\ll 1$

Micron sized objects in fluid

$$\rho (\partial_t \mathbf{v} + \mathbf{v} \cdot \nabla \mathbf{v}) = \eta \nabla^2 \mathbf{v}(\mathbf{r}, t) - \nabla p \quad \nabla \cdot \mathbf{v} = 0 \qquad \begin{array}{c} \rho = 1000 \text{ kg m}^{-3}, \text{ V} = 10^{-6} \text{ m s}^{-1} \\ \text{L} = 10^{-6} \text{ m }, \eta = 10^{-3} \text{ Pa s} \\ \text{Re} = 10^{-6} \end{array}$$



Total force on colloid from fluid balances external force Neutrally buoyant swimming = no external forces - zero total force from fluid !!



Phenomenology of active units

Contractile/Extensile Sign of force dipole

• $\alpha < 0 / \alpha > 0$

Pushers/Pullers

E-Coli/Chlamydomonas



We can classify/understand some aspects of the collective behaviour in terms of these force dipoles.

Pushers : regions of orientational order, disordered on large lengthscales

Pullers : disordered on all lengthscales



Phenomenology of behaviour

Contractile/Extensile

Sign of force dipole





What about the duty cycle ?

Q: Does this internal phase variable have consequences on the behaviour of active matter?

Phase differences -> possibility of synchronization

Place where this happens is collective behaviour of cilia



Collective behaviour of cilia

Ciliated organisms – paramecium (100 μm , 10 lengths/s)



Collective transport by cilia – mucociliary tract





Can the cilia transport material on scales >> size ?



Structure of axonemic cilia

Microtubules (M), Dynein (D), Nexin spring (N)



Generic simplified model – single object subject to time varying force

$$\dot{f}_{\tau} = \frac{f}{\gamma} \qquad \gamma = 6\pi\eta a \quad \text{sphere radius, a}$$

$$\dot{f} = -\frac{k}{\tau}x + \mu \frac{f}{\gamma}(1 - \sigma x^2) + \alpha x^3$$

Viscosity dominated dynamics



Oscillator

Viscosity dominated dynamics -> spontaneous oscillations





Filaments/motors -> oscillator

Force balance



 $F_m = -\kappa y$ $F_s = -Kx - \Lambda x^3$ Binding, Unbinding rate $\omega_b < \gamma/K, \gamma/\kappa < \omega_u$ Fm (b) **Parameters** Step length = d $\frac{k}{\tau} \sim \omega_u^0 \frac{d^2 \kappa K}{k_B T} \quad , \quad \mu \sim (\kappa - K)$ $\sigma \sim \frac{3\Lambda}{\kappa - K} \quad , \quad \alpha \sim -\frac{d\kappa}{k_B T} \Lambda$ Hin K (c)



Hydrodynamic interactions

• On lengthscales large compared to object, micron sized object as collection of point forces on fluid

$$\eta \nabla^2 \mathbf{v} - \nabla p = \mathbf{g}(\mathbf{r}) \quad ; \quad \nabla \cdot \mathbf{v} \qquad \mathbf{g}(\mathbf{r}) = \mathbf{f} \delta(\mathbf{r})$$

• Green's function $\mathbf{v}(\mathbf{r}) = \mathbf{H}(\mathbf{r}) \cdot \mathbf{f}$ $\mathbf{H}(\mathbf{r}) = \frac{1}{8\pi\eta r} (\mathbf{I} + \hat{\mathbf{r}} \cdot \hat{\mathbf{r}})$ Oseen tensor

1.5



Two interacting oscillators

 $\alpha \neq 0$ means amplitude-dependent frequency of oscillations



Hydrodynamic interactions -

 $r = d + x_2 - x_1$

 $\dot{x}_1=rac{1}{\gamma}\left(f_1+H(r)f_2
ight);$

$$\dot{x}_2=rac{1}{\gamma}\left(f_2+H(r)f_1
ight),$$

$$\dot{f}_i = -rac{k}{\tau} x_i + \mu rac{f_i}{\gamma} (1 - \sigma x_i^2) + lpha x_i^3$$

 $H(r) \sim rac{1}{r}$ bulk
 $H(r) \sim rac{h^2}{r^3}$ near wall

Fast variable : amplitude

Slow variable : phase

Average over fast modes -> effective equation for slow modes



Hydrodynamic Synchronization

Weakly interacting limit

$$\begin{split} d \gg x_2 - x_1 & a/d \ll \mu/k, \alpha \tau/k\sigma \\ x_k = \frac{1}{2} \left(A_k e^{i\omega t} + A_k^* e^{-i\omega t} \right) & k = 1,2 \\ \text{Average over fast oscillations} \implies & \bar{A}_k = R_k e^{i\phi_k} \\ \text{Phase difference } \psi = \phi_2 - \phi_1 & \dot{\psi} = f(\cos \psi) \sin \psi \\ \text{Enhanced when } & \alpha \neq 0 \\ \text{In phase - } & \alpha > 0 \\ \text{Antiphase - } & \alpha < 0 \\ \text{Much slower if } & \alpha = 0 \end{split}$$



Tutorial example: Brownian motion

Langevin equation in over-damped limit (no inertia)



Probability density of finding particle in vol. $d^d x$ around \mathbf{x} $P(\mathbf{x},t) = \langle \delta (\mathbf{x} - \mathbf{r}(t)) \rangle$ $\langle .. \rangle \equiv$ average over noise



From stochastic trajectory to probability

Dynamical equation for prob. density



Stochastic trajectory to probability II

N interacting particles + fluctuations

$$\frac{\partial \vec{x_i}}{\partial t} = \vec{V_i} \left(\{ \vec{x_1}, \dots, \vec{x_N} \} \right) + \vec{\xi_i}(t) \\ \langle \xi_{i\alpha}(t) \xi_{j\beta}(t') \rangle = 2D_{i\alpha} \delta_{ij} \delta_{\alpha\beta} \delta(t - t')$$

Up to pairwise interactions

$$ec{V}_i\left(\{ec{x}_1,\ldots,ec{x}_N\}
ight) = ec{v}^{(1)}(ec{x}_i) + \sum_{j
eq i} ec{v}^{(2)}(ec{x}_i,ec{x}_j)$$

One particle density $c_1(ec{r},t) = \sum_{i=1}^N \langle \delta\left(ec{r} - ec{x}_i(t)
ight)
angle$
Conservation law : $\partial_t c_1 + ec{
abla} \cdot ec{J}_1 = 0$



Stochastic trajectory to probability III

Current :

$$\vec{J_1}(\vec{r_1},t) = \vec{v}^{(1)}(\vec{r_1})c_1(\vec{r_1},t) + \int d\vec{r_2} \ \vec{v}^{(2)}(\vec{r_1},\vec{r_2})c_2(\vec{r_1},\vec{r_2},t)$$

 $-D\vec{\nabla}c_1$ 2-particle density
 $\partial_t c_2 = F[c_2,c_3] \dots$

Closure problem (usual non-equil. Stat. mech. prob.)

Mean field approximation $c_2(\vec{r_1}, \vec{r_2}, t) = c_1(\vec{r_1}, t)c_1(\vec{r_2}, t)$

(ignore correlations)



Statistic Stochastic trajectory to probability IV One particle density $c_1(\vec{r},t) = \sum_{i=1}^N \langle \delta(\vec{r} - \vec{x}_i(t)) \rangle$ $\partial_t c_1 + \vec{\nabla} \cdot \vec{J_1} = 0$ Conservation law : $\vec{J_1}(\vec{r_1},t) = -D \vec{\nabla} c_1 + \vec{v}^{(1)}(\vec{r_1}) c_1(\vec{r_1},t)$

Nonlinear current :

 $-D \nabla c_{1} + v^{(1)}(r_{1})c_{1}(r_{1},t) + \int d\vec{r}_{2} \ \vec{v}^{(2)}(\vec{r}_{1},\vec{r}_{2})c_{1}(\vec{r}_{1},t) \ c_{1}(\vec{r}_{2},t)$

Interacting oscillators :

$$\vec{r_i} = \{\phi_i, y_i\}$$

Velocities $\vec{v}^{(2)} = \{ \dot{\phi}_1 - \dot{\phi}_2, 0 \}$

Gradient operator $\vec{\nabla} = \{\partial_{\phi}, \partial_y\}$



Coarse-graining the dynamics ...

Project on to moments (hydrodynamic modes) :

$$egin{aligned} &
ho(y,t) := \int_0^{2\pi} d\phi c(\phi,y,t); \ &\Phi(y,t) := \int_0^{2\pi} d\phi e^{i\phi} c(\phi,y,t); \end{aligned}$$

Density

Phase coherence

Coarse-grain in space/time

 $a \ll d \ll h \ll r$

Global behaviour

$$\partial_t \Phi^0 = -\left(D - \frac{\chi}{\beta} \frac{3ak}{4\omega\tau\gamma}\rho^0\right) \Phi^0 + \text{h.o.t}$$

$$\partial_t \rho^0 = 0$$
 $\chi = \frac{3}{8} \frac{\alpha}{\gamma \omega}$ $\beta = \frac{\mu \sigma}{\gamma}$

Synchronized state for $\alpha > 0$

Leoni, TBL (2012)



Coarse-graining the dynamics ...

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Coarse-grain in space/time

Density

Phase coherence

 $a \ll d \ll h \ll r$

 $\alpha > 0 \Rightarrow$ Globally inphase

 $\alpha < 0 \Rightarrow$ Locally antiphase + long wavelength phase modulations





Cyclic swimmers

• (Re=0) Stokes equation is linear

$$\eta \nabla^2 \mathbf{v} - \nabla p = 0 \quad ; \quad \nabla \cdot \mathbf{v}$$

• Swimming is a periodic sequence of shape changes



If e.g. forward stroke = backward stroke → no net motion







Purcell (1977)



Swimming stroke = oscillation

Identical swimmers = all oscillations in phase



Another possible broken symmetry

Dissipative oscillator – single object subject to time varying force

$$\dot{x} = \frac{f}{\gamma} \qquad \gamma = 6\pi\eta a \quad \text{sphere radius, } a$$

$$\dot{f} = -\frac{k}{\tau}x + \mu \frac{f}{\gamma}(1 - \sigma x^2) + \alpha x^3$$

Viscosity dominated dynamics -> spontaneous oscillations $\mu > 0$

An 'Ising model' of swimmers



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An 'Ising model' of swimmers



 $d_1 \simeq d\cos(\omega t + \varphi)$ $d_2 \simeq d\sin(\omega t + \varphi)$

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- - $\alpha > 0$

- Average over fast period ->
- Swimmer characterised by

$$\mathbf{X} = (\hat{\mathbf{u}}, \mathbf{r}, \varphi)$$





Stochastic trajectory to probability II

Nonlinear current :

$$\begin{split} \vec{J}_{1}(\vec{r}_{1},t) &= -D\,\vec{\nabla}c_{1} + \vec{v}^{(1)}(\vec{r}_{1})c_{1}(\vec{r}_{1},t) \\ &+ \int d\vec{r}_{2}\,\vec{v}^{(2)}(\vec{r}_{1},\vec{r}_{2})c_{1}(\vec{r}_{1},t)\,c_{1}(\vec{r}_{2},t) \\ \partial_{t}c_{1} + \vec{\nabla}\cdot\vec{J}_{1} &= 0 \qquad D = D(\vec{r}_{1}) \end{split}$$

Interacting objs : $\vec{r}_{i} = \{\mathbf{r}_{i},\hat{\mathbf{u}}_{i},\varphi_{i}\}$

Velocities : $v^{(i)} = \{ \mathbf{v}^{(i)}, \boldsymbol{\omega}^{(i)}, \varphi_i \}$ Gradient operator $\vec{\nabla} = \{ \nabla, \mathcal{R}, \partial_{\omega} \}$ $\mathbf{\nabla} = \frac{\partial}{\partial \mathbf{r}}$ $oldsymbol{\mathcal{R}} = \hat{\mathbf{u}} imes rac{\partial}{\partial \hat{\mathbf{u}}}$



Interactions

Interactions between swimmers (no fluctuations)



• Take account of phase

Leoni, TBL, (2010, 2014)

• Interactions mediated by fluid (averaging over a cycle)



Length/timescales

- Internal motions ~ 10 nm
- in ms timescales
- Stall force of $\sim 10 \text{ pN}$
- Objects of length ~ 1 micron

Separation of scales

- Looking for phenomena
- on lengthscales > 100 microns
- Timescales of seconds-minutes



Projecting on to hydrodynamic variables Polarized state

Moment expansion of concentration + truncation :

$$\rho(\mathbf{r},t) = \int d\hat{\mathbf{u}} \, d\varphi \, c(\mathbf{r},\hat{\mathbf{u}},\varphi,t) \quad \text{density - conserved quantity}$$

$$\rho\mathbf{P}(\mathbf{r},t) = \int d\hat{\mathbf{u}} \, d\varphi \, \hat{\mathbf{u}} \, c(\mathbf{r},\hat{\mathbf{u}},\varphi,t) \quad \text{possible broken symmetries}$$

$$\rho\Phi(\mathbf{r},t) = \int d\hat{\mathbf{u}} \, d\varphi \, e^{i\varphi} \, c(\mathbf{r},\hat{\mathbf{u}},\varphi,t) \quad \text{possible broken symmetries}$$

Dynamics on length-scales much bigger than *L*

 \Rightarrow Gradient expansion

3 bead model



One arm spontaneous osciilator

Additional phase variable

 $\phi = 0, 2\pi$

Leoni, Liverpool, PRL, in press (2014)

Order parameters



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<u>.</u>

Polarization

Phase coherence

$$\mathbf{P}(t) = \frac{1}{N} \sum_{n=1}^{N} \hat{\boldsymbol{u}}_n(t)$$
$$\mathbf{\Phi}(t) = \frac{1}{N} \sum_{n=1}^{N} e^{i\phi_n(t)}$$



Synchronization & polar order $\mathbf{P} = P \,\hat{\mathbf{p}} \quad \mathbf{\Phi} = M \, e^{iQ}$ $\partial_t P = (b + vM^2)P$ $\partial_t M = (\zeta + \xi P^2) M$ $v = \frac{\Gamma_b \Gamma_v (\kappa - 1)}{\rho \Gamma_v - D_r}$ $b = -D_r + \rho(1-\kappa)\Gamma_b$ $\zeta = \kappa (2\kappa + 1) \Gamma_{\mathcal{C}}$ $\xi = \frac{v}{\Gamma_{x}}$

Leoni, Liverpool, PRL, in press (2014)

$$\kappa < 1$$
 pushers

 $\kappa > 1$ pullers



Phase-force dipole duality





Summary

Q: Does an internal phase variable have consequences on the behaviour of active matter?



Summary

• A: Yes !!

Studied collective behaviour of simple model swimmer with a dynamic phase variable and simple force multipole to show this

These consequences are not dependent on specific model (can be obtained by phenomenology – writing down most general terms allowed by symmetry)

Leoni, Liverpool, PRE, (2012)

Furthauer, Ramaswamy, PRL, (2013)

Leoni, Liverpool, PRL, in press (2014)



Summary

We focused on oscillators which synchronise in phase $\alpha > 0$ 'Ferromagnets'

Very interesting to explore oscillators which synchronize out of phase (metachronal waves,)

'antiferromagnets'