Self-propelled colloids: from single to collective behaviour

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I) Introduction
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III) Transport powered by bacterial turbulence
IV) Crystallization for active particles
V) Phase separation for active particles
VI) Summary
penguins!

I) Introduction

“active“ (self-propelled) “particles“ occur in many different situations

- dissipation of energy
- intrinsically in nonequilibrium
- different from “passive“ particles driven by external fields

goal of the talk: discuss simple models for (single and) collective properties of active particles
From "passive" to "active" "particles"
From “passive“ to „active“ particles in the microworld (soft matter)

inert colloidal particle
in an external field

self-propelled „particles“ with an internal motor

- bacteria (E. coli)

- sperm

- bacillus subtilis

SFB TR6
Colloidal Dispersions in External Fields
(2002-2013)

http://www.youtube.com/watch?v=IEdb3wTMSBo

COLLOIDAL MICROSWIMMERS

catalytically driven colloidal Janus particles

W. F. Paxton et al, JACS 128, 14881 (2006)
G. Mino et al, PRL 106, 048102 (2011)

Thermally/diffusionally driven colloidal Janus particles

Model: Brownian dynamics of self-propelled rods

Yukawa segment interaction

\[ U_{\alpha\beta} = \frac{U_0}{n^2} \sum_{i=1}^{n} \sum_{j=1}^{n} \exp\left[-\frac{(r_{ij}^{\alpha\beta})^2}{\lambda r_{ij}^{\alpha\beta}}\right] \]

\[ r_{ij}^{\alpha\beta} = |\Delta r_{\alpha\beta} + (l_i \hat{u}_{\alpha} - l_j \hat{u}_{\beta})| \]

\[ a = \frac{\ell}{\lambda} \]

\( n \): number of segments

\( \lambda \): screening length

aspect ratio
Completely overdamped equations of motion

\[
\begin{align*}
  f_T \cdot \partial_t r_\alpha &= -\nabla_{r_\alpha} U + F\hat{u}_\alpha \\
  f_R \cdot \partial_t \hat{u}_\alpha &= -\nabla_{\hat{u}_\alpha} U.
\end{align*}
\]

\[
U = \frac{1}{2} \sum_{\beta, \alpha: \beta \neq \alpha} U_{\alpha\beta}
\]

internal drive

total potential energy

\[
\begin{align*}
  f_T &= f_0 \left[ f_{\parallel} \hat{u}_\alpha \hat{u}_\alpha + f_{\perp} (I - \hat{u}_\alpha \hat{u}_\alpha) \right] \\
  f_R &= f_0 f_R I,
\end{align*}
\]

friction tensors for translation and rotation

\[
\begin{align*}
  \frac{2\pi}{f_{\parallel}} &= \ln a - 0.207 + 0.980a^{-1} - 0.133a^{-2} \\
  \frac{4\pi}{f_{\perp}} &= \ln a + 0.839 + 0.185a^{-1} + 0.233a^{-2} \\
  \frac{\pi a^2}{3f_R} &= \ln a - 0.662 + 0.917a^{-1} - 0.050a^{-2}
\end{align*}
\]

Stokesian friction coefficient \( f_0 \)

explicit expressions for hard cylinders

(Tirado et al, JCP 81, 2047 (1984))

- no hydrodynamic interactions
- no noise (zero temperature \( T=0 \)), but noise can be included
- two spatial dimensions
length unit

\( \lambda \)

time unit

\( \tau_0 = \lambda f_0 / F \)

energy unit

\( F\lambda \)

remaining parameters of the model

\[ \tilde{U}_0 = \frac{U_0}{F\lambda} \approx 250 \]

\( a = l/\lambda \) (aspect ratio)

\[ \phi = \frac{N}{A} \left[ \lambda(\ell - \lambda) + \frac{\pi \lambda^2}{4} \right] \] effective volume fraction
Single particle limit

trivial linear trajectory along orientation \( \hat{u} \)

\( \hat{u} \) fixed

\[ \vec{R}(t) = \vec{R}(0) + \frac{F}{f_0 f_{11}} \hat{u} t \]

Brownian noise for translation and rotation

→ stochastic equations with known moments, see e.g.


also valid for circle swimmers (constant interval torque)

← PARENTHESIS ←

interactions: → nontrivial collisions and many-body phenomena
parenthesis: Brownian circle swimmers (1)
circling of human walkers

- Trajectory of “Sample 5”.

Obata et al., J. Korean Phys. Soc. 2005
parenthesis: Brownian circle swimmers (2)

thermally driven colloidal Janus particles


spira mirabilis for the noise-averaged trajectory

Helical-like swimming in three dimensions: The Brownian spinning top

molecular dynamics

self-propelled biaxial particle (in 3d)

internal (constant in the body-fixed frame)

external (constant in the lab-frame)

- complicated equations of motion (see de la Torre et al, Doi for passive particles)

- translation-rotation coupling for a chiral particle (Brenner et al)

R. Wittkowski, HL, PRE 85, 021406 (2012)
Single particle limit

trivial linear trajectory along orientation $\hat{u}$

$\hat{u}$ fixed

$$\vec{R}(t) = \vec{R}(0) + \frac{F}{f_0 f_{11}} \hat{u} t$$

Brownian noise for translation and rotation

stochastic equations with known moments, see e.g.


also valid for circle swimmers (constant interval torque)

interactions: nontrivial collisions and many-body phenomena
binary collisions

non-central forces

non-elastic collisions

tendency of mutual alignment

\( \hat{u}_1 \longrightarrow \hat{u}_2 \)

swarming

(Viczek et al, I. Aranson)
II) Meso-scale turbulence in living fluids

- no temperature,
- repulsive Yukawa segment interactions, swarming behaviour

Fig. 1. (A) Schematic non-equilibrium phase diagram of the 2D SPR model and snapshots of six distinct phases from simulations: D-dilute state, J-jamming, S-swarming, B-bionematic phase, T-turbulence, L-laning. Our analysis focusses on the bionematic and turbulent regimes B/T

H. H. Wensink and HL

H. H. Wensink et al,
PNAS 109, 14308 (2012)
experiments on 2d-confined solutions (Drescher, Goldstein et al) of bacillus subtilis
turbulent phase in a quasi-2D homogeneous B. subtilis suspension (channel thickness approximately 5 μm).
Continuum model (generalization of Toner-Tu theory)

\[ \nabla \cdot v = \partial_t v_i = 0, \quad i = 1, \ldots, d, \]

\[ (\partial_t + v \cdot \nabla)v = -\nabla p - (\alpha + \beta |v|^2)v + \nabla \cdot E, \]

\[ E_{ij} = \Gamma_0(\partial_i v_j + \partial_j v_i) - \Gamma_2 \Delta (\partial_i v_j + \partial_j v_i) + S q_{ij}, \]

\[ q_{ij} = v_i v_j - \delta_{ij} \frac{d}{d} |v|^2 \]

incompressibility

Navier-Stokes equation

rate-of strain-tensor \( E \)

see also: J. Dunkel, S. Heidenreich et al, PRL 110, 228102 (2013)
Fig. 2. Experimental snapshot (A) of a highly concentrated, homogeneous quasi-2D bacterial suspension (see also Movie S07 and Fig. S8). Flow streamlines $\mathbf{v}(t, r)$ and vorticity fields $\omega(t, r)$ in the turbulent regime, as obtained from (B) quasi-2D bacteria experiments, (C) simulations of the deterministic SPR model ($a = 5, \phi = 0.84$), and (D) continuum theory. The range of the simulation data in (D) was adapted to the experimental field of view (217 $\mu$m x 217 $\mu$m) by matching the typical vortex size (scale bars 50$\mu$m). Simulation parameters are summarized in the SI Text.
Figure 5. (a) Enstrophy $\Omega$ (in units $\tau_0^{-2}$) versus filling fraction for a number of aspect ratios $a$ in the turbulent regime. The maxima correspond to the densities where mixing due to vortical motion is the most efficient. (b) Spatial velocity autocorrelation function for a number of bulk volume fractions in the turbulent flow regime for two different aspect ratios $a$. 
energy spectrum:

\[ E(k) \sim k \int dr \exp[-ik \cdot r] \langle \mathbf{v}(t, 0) \cdot \mathbf{v}(t, r) \rangle_t \]

**Fourier transform of the VACF**

Kolmogorov-Kraichnan scaling for 2d classical turbulence:

\[ E(k) \propto k^{-5/3} \]

(inertial regime)
Fig. 4. Equal-time velocity correlation functions (VCFs), normalized to unity at $R = \ell$, and flow spectra for the 2D SPR model ($\alpha = 5$, $\phi = 0.84$), B. subtilis experiments, and 2D continuum theory based on the same data as in Fig. 3. (A) The minima of the VCFs reflect the characteristic vortex size $R_v$ [47]. Data points present averages over all directions and time steps to maximize sample size. (B) For bulk turbulence (red squares) the 3D spectrum $E_3(k)$ is plotted ($k_\ell = 2\pi/\ell$), the other curves show 2D spectra $E_2(k)$. Spectra for the 2D continuum theory and quasi-2D experimental data are in good agreement; those of the 2D SPR model and the 3D bacterial data show similar asymptotic scaling but exhibit an intermediate plateau region (spectra multiplied by constants for better visibility and comparison).


- not consistent with Kolmogorov-Kraichnan scaling
- self-sustained turbulence!
- maximal swirl size
Summary

- At high density there is mesoscale turbulence in living or active fluids „bacterial turbulence“
- The energy spectrum does not follow Kolmogorov-Kraichnan scaling
III) Transport powered by bacterial turbulence

What to do with bacterial turbulence?

length units in µm

mesoscopic carrier, „bulldozer“

with I. Aranson, A. Peshkov (Argonne), A. Sokolov (Paris)

Andreas Kaiser (Düsseldorf)

Borge ten Hagen (Düsseldorf)
simulation

experiment
turbulence maximizes transport efficiency

idea: extract useful mechanical energy out of turbulence
transport mechanism
swirl depletion

- wedge creates a shielded area
- swirls cannot reach cusp
How to clean the corners?
- low concentration: direction (almost) random
- intermediate concentration: directed along x-axis
- high concentration: occurrence of a double peak
  -> zig-zag motion
underlying reason for tilted carrier motion
IV) Crystallization for active particles

spherical particles (one segment)

2d

plus noise

(≡ finite temperature in equilibrium)

rotational noise decoupled (minimal model)

interaction coupling parameter

\[ \Gamma = \frac{v_0\sqrt{\rho}}{k_B T} \]

propulsion strength

\[ f = \frac{F}{k_B T \sqrt{\rho}} \]

with drive: structural and dynamical diagnostics of freezing differ!
snapshot across the freezing transition

„bubbles“

without propulsion | with self propulsion
microscopic field-theoretical model for crystallization

 travellng and resting crystals

resting crystal

no migration

direction of migration

travelling crystal

\[ \psi_1(\vec{r}, t) \quad \text{density field} \quad \vec{P}(\vec{r}, t) \quad \text{polarization field} \quad \text{as coupled order parameters} \]

PFC model  

reduced Toner-Tu model  
Toner, Tu, PRL 75, 4326 (1995)

self-propagation speed

total functional
\[ \mathcal{F} = \mathcal{F}_{pf} + \mathcal{F}_P \]

with
\[ \mathcal{F}_{pf} = \int d^2 r \left\{ \frac{1}{2} \psi [\varepsilon + (1 + \nabla^2)^2] \psi + \frac{1}{4} \psi^4 \right\} \]

and
\[ \mathcal{F}_P = \int d^2 r \left\{ \frac{1}{2} C_1 P^2 + \frac{1}{4} C_4 (P^2)^2 \right\} \]

either \( c_1 > 0 \) or \( c_1 < 0 \) and \( c_4 > 0 \)
FIG. 2. Different phases observed when increasing the active drive $v_0$ at $(\tilde{\psi}, \varepsilon, C_1, C_4) = (-0.4, -0.98, 0.2, 0)$: (a) resting hexagonal, $v_0 = 0.1$, (b) traveling hexagonal, $v_0 = 0.5$, (c) traveling quadratic, $v_0 = 1$, (d) traveling lamellar, $v_0 = 1.9$. The phases are depicted by plotting the density field $\psi_1$. Thin bright needles illustrate the polarization field $\mathbf{P}$ that points from the thick to the thin ends. In panels (b)-(d) the predominant direction of motion is indicated by the bright arrows. Only a fraction of the numerical calculation box is shown.

FIG. 3. Sample-averaged magnitude $v_m$ of the crystal peak velocities (left scale) and polar order parameter $p_v$ of the crystal peak velocity vectors (right scale) as a function of $v_0$ for $(\tilde{\psi}, \varepsilon, C_1, C_4) = (-0.4, -0.98, 0.2, 0)$. The threshold corresponds to the onset of collective crystalline motion. Thick arrows mark the positions where the snapshots of Fig. 2 were taken: the black star just below threshold and the black triangle indicate the intersection points with the phase diagrams in Figs. 1(b) and 1(c), respectively. The region above threshold where regular swinging motion could be observed is marked in gray. Inset: peak trajectories illustrating a state of regular swinging motion in a hexagonal crystal; different colors correspond to different peaks; only trajectories of a horizontal row of density peaks are shown that started at the bottom and were traveling to the top of the picture while tracking was performed.

A. M. Menzel, HL, PRL 110, 055702 (2013)
• There are stable active crystals

  – The crystallization transitions is different from bulk freezing

  – Active crystals can be collectively migrating (traveling crystals)
motility-induced phase separation
(Tailleur and Cates)

spherical particles (one segment)

rotational noise decoupled (minimal model)

interaction coupling parameter
\[ \Gamma = v_0 \sqrt{\rho} / k_B T \]

propulsion strength
\[ p_e = \frac{F}{k_B T \sqrt{\rho}} \]

the mechanism of clustering

FIG. 5: (a) Consecutive close-ups of a cluster, where we resolve the orientations (arrows) of the caps. Particles along the rim mostly point inwards. The snapshots show how the indicated particle towards the bottom (left) leaves the cluster (center) and is replaced by another particle (right). (b) Sketch of the self-trapping mechanism: for colliding particles to become free, they have to wait for their orientations to change due to rotational diffusion and to point outwards.
FIG. 4: Phase separation: (a) Mean strength $P$ of the largest cluster as a function of swimming speed $v$. Shown are experimental results (open symbols) and simulation results (closed symbols). (b) Simulation snapshot of the separated system at $\phi = 0.5$ and speed $\text{Pe} = 100$. (c) Experimental snapshot at $\phi \approx 0.25$ and $v \approx 1.45 \text{μm/s}$. 

instability theory

Fig. 3. Simulation results neglecting translational diffusion for: (H) soft spheres with harmonic repulsion, (GCM) the Gaussian core model, and (Y) the Yukawa potential. (a) Structure factors $S(q)$ for different speeds $v_0$ increasing from bottom to top. (b) Force coefficient $\zeta$ as a function of the propulsion speed $v_0$ (note that the unit of time compared to Fig. 2 is $1/100$). Open symbols correspond to homogeneous systems, closed symbols to phase separated systems. (c) Snapshot at speed $v_0 = 0.2$ and (d) at speed $v_0 = 0.5$ for (H). Every particle is colored according to Eq. [27] with $\Delta t = 25$ quantifying the persistence of particle motion with respect to the initial particle orientation.

scaling of cluster growth for coagulating particles

\[ N_C \propto t^\gamma \]

explosive growth possible \( N_C \to \infty \) for \( t \to t_0 < \infty \)

Simple „sweeping argument“ to derive scaling (in the ballistic regime)

number density $\rho$ of particles

in time interval $\Delta t$ the cluster sweeps out a volume of $v \Delta t R^{d-1}$

Therefore

$$\Delta N_C = \rho R^{d-1} v \Delta t$$

$$\Rightarrow \dot{N}_C \propto N_C^{\beta+(d-2)/2}$$

$$N(t) = \begin{cases} 
\left[N_0^{2/d-\beta} + C(2/d - \beta)t\right]^{\frac{1}{2/d-\beta}} & \beta < 2/d, \\
N_0 \exp(C t) & \beta = 2/d, \\
C(\beta - 2/d) (t_c - t)^{-\frac{1}{\beta-2/d}} & \beta > 2/d,
\end{cases}$$
Confirmation of the scaling predictions by particle resolved simulations

Fig. 3: Cluster size evolution obtained from simulations in \( d = 2, 3 \) dimensions with various values of the persistence parameter \( \kappa \) and the total propulsion force scaling exponent \( \beta \). Algebraic growth in the diffusive regime (a), (b) as well as in the ballistic regime (c), (d) occurs with the predicted exponents as indicated in the plots. Exponential growth (e) in the ballistic regime occurs faster than in the diffusive regime as indicated by the much higher slope. For high persistence and high force scaling, explosive cluster growth occurs (f). The dashed lines are fits using eqs. (3) and (4) respectively.
Summary

- Active particles exhibit phase separation purely induced by the drive
- New scaling behaviour
- Nucleation?
VI) Conclusions

active colloidal particles reveal fascinating collective features!

Thanks to:
