LECTURE I

INTRODUCTION

- What is active matter?

  collection of interacting active particles, each ~~generating~~ self-driven and capable of converting stored energy in motion / forces, and collectively generating coordinated motion

- How does it differ from other noneq. system?

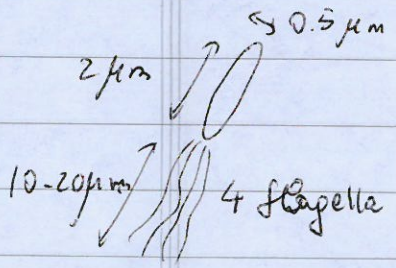
  drive is local on each unit, not global (field) or at boundary → reverse energy cascade

- SP motion is "force free" (≠ sedimentation under gravity)

⇒ emergent behavior
(not mechanisms of motility)

EXAMPLE OF ACTIVE PARTICLE

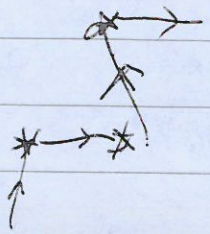
E. coli rod-shaped 1% gut flora



converts chemical energy into motion via an internal cyclic transformation

run-and-tumble
not a conventional RW

$v_0 \sim 10-40\ \mu m/s$
$\alpha \sim 1\ s^{-1}$



MANY E. coli : swarming, turbulent flow, pattern formation, biofilms

- not motility mechanisms, but collective behavior
- time >> cycle (but some recent work on activity and synchronization)

EXAMPLES ON MANY SCALES → {movies}

- inside a cell : cytoskeleton → cell motility, division, mechanics (Joanny)
- many cells → tissues : mechanics, collective migration, wound healing (Manning)
- fish, birds, people (Toner)
- synthetic microswimmer

What do they have in common?

- drive on each unit / symmetry broken locally, breaks TRS
- emergent behavior, order/disorder transition
- [liquid xstalline order] → living LC

{GOALS} Use methods from noneq. stat mech + SoftCM

- Which new states of active matter are possible?
- Can we classify behaviors and identify generic properties?
- What do we tune to change from one state to another?

MCM et al, RMP 85, 1143 (2013)

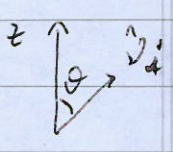
CLASSIFICATION

Types of orientational order

POLAR : bacteria, fish, ...

ferromagnetic order $\langle \vec{v} \rangle \neq 0$
moving state

O.P. vector
velocity / polarization

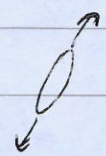


$$\vec{P} = \sum_i \hat{\nu}_i \delta(\vec{r} - \vec{r}_i)$$

$$P_z \sim \langle \cos\theta_i \rangle$$

→ TONER

APOLAR : melanocytes, rods, ...



O.P. tensor

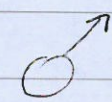
$$Q_{\alpha\beta} = \left\langle \sum_i \left(\hat{\nu}_{\alpha i}\hat{\nu}_{\beta i} - \frac{1}{2}\delta_{\alpha\beta}\right) \times \delta(r - r_i) \right\rangle$$

$$Q_{zz} \sim \langle \cos^2\theta_i \rangle$$

no state with mean motion

→ Dogic

SPHERICAL : active colloids



No orientational order, but surprising collective behavior

→ MCM

Role of medium : "dry" vs "wet"

Forces on environment : contractile vs extensile

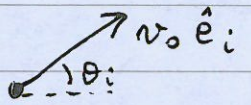
puller pusher

→ ← ← →

VICSEK MODEL OF FLOCKING 1995 Craig Reynolds 1987

inspired by analogy with ferromagnetism

→ flying XY spins



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

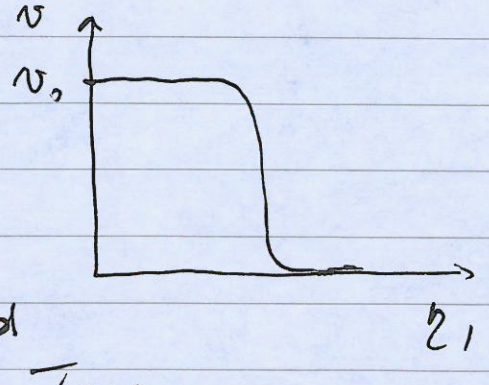
- N point particles
- fixed speed v_0
- align w/ neighbors with noisy rules
- overdamped dynamics

~~$\vec{r}_i(t+\Delta t) = \vec{r}_i(t) + v_0 \hat{e}_i \Delta t$~~ R_i

$$\begin{cases} \vec{r}_i(t+\Delta t) = \vec{r}_i(t) + v_0 \hat{e}_i \Delta t \\ \theta_i(t+\Delta t) = \langle \theta_i(t) \rangle_R + \xi_i(t) \end{cases}$$

ξ_i random ≠ uniform in $[-\eta/2, \eta/2]$

OP $\quad v = \left| \frac{1}{N} \sum_i \vec{v}_i(t) \right|$



- first order
- spontaneous breaking of continuous symmetry in 2d (* ≠ Mermin-Wagner) → Toner

Agent or rule-based model → demo

→ continuum : Toner-Tu model

separation of time scales :

- most fluctuations decay on microscopic time scales
- some are 'slow' : $\underbrace{\omega(k)}_{\text{decay rate}} \to 0 \quad k \to \infty$

TUTORIAL : from Langevin dynamics to Smoluchowski

Brownian particle

$$m \frac{d\vec{v}}{dt} = \underbrace{-\zeta \vec{v}}_{\text{mean drag}} + \underbrace{\vec{\eta}(t)}_{\text{random component of effect of collisions with fluid atoms}}$$

$\zeta = 6\pi\eta a$ (3d)

$\langle \vec{\eta}(t) \rangle = 0$

time scale $\tau = m/\zeta$

$\langle \eta_\alpha(t) \eta_\beta(t') \rangle = 2\Delta \delta_{\alpha\beta} \delta(t-t')$

Gaussian, white

$$\langle |\vec{v}(t)|^2 \rangle \xrightarrow[t \gg m/\zeta]{} \frac{\Delta}{\zeta m} d = \langle v^2 \rangle_{th} = d \frac{k_B T}{m}$$

↑ equilibrium

$\Delta = k_B T \zeta$ FD theorem

$$\langle [\Delta \vec{r}(t)]^2 \rangle = 2d \frac{k_B T}{\zeta} \left\{ t - \tau \left[1 - e^{-t/\tau} \right] \right\}$$

balance of dissipation and noise

$t \ll \tau$ $\quad \langle [\Delta \vec{r}(t)]^2 \rangle = d \frac{k_B T}{m} t^2$ ballistic

$t \gg \tau$ $\quad \langle [\Delta \vec{r}(t)]^2 \rangle = 2Ddt$ diffusive

$$D = \frac{k_B T}{\zeta}$$ Einstein

Many particle, interactions : Langevin dynamics hard, not well suited to analytics

→ eq. for probability distribution

Overdamped dynamics $t \gg m/\zeta$

$\zeta \vec{v} = \vec{\eta}(t)$ $\quad \langle [\Delta \vec{r}(t)]^2 \rangle = 2Ddt$ all times

Derive Eq. for noise-averaged probability distribution

- overdamped dynamics
- 1d

$$v = \frac{dx}{dt} = -\frac{1}{\zeta} U'(x) + \eta(t) \qquad \langle \eta(t) \rangle = 0$$

$$\langle \eta(t)\eta(t') \rangle = 2\Delta\, \delta(t-t')$$

$\hat{\psi}(x,t)$ probability density — Gaussian, white but no FD

all t $\int_V dx\, \hat{\psi}(x,t) = 1$ — conservation law $\Rightarrow \partial_t \hat{\psi}$ is the divergence of a flux $J = \hat{\psi} v$ (cf fluid dynamics)

$$\partial_t \hat{\psi} = -\partial_x v \hat{\psi}$$

$$\partial_t \hat{\psi} = \overbrace{-\partial_x \left[-\frac{1}{\zeta} U' \hat{\psi} \right]}^{L\hat{\psi}} - \partial_x (\eta \hat{\psi})$$

We want an eq. for $\psi = \langle \hat{\psi} \rangle$

$$\hat{\psi}(t) = e^{-\hat{L}t} \hat{\psi}(0) - \int_0^t ds\, e^{-\hat{L}(t-s)} \partial_x (\eta(s) \hat{\psi}(s))$$

$\hat{\psi}(t)$ only depends on noise at time $s < t$

$$\partial_t \hat{\psi} = -L\hat{\psi} - \partial_x \eta(t) e^{-Lt} \hat{\psi}(0)$$

$$+ \partial_x \int_0^t ds\, \eta(t) e^{-L(t-s)} \partial_x (\eta(s) \hat{\psi}(s))$$

noise average

- assume $\hat{\psi}(0)$ does not depend on noise $\langle \eta(t) \hat{\psi}(0) \rangle = 0$
- $\langle \eta(t) \eta(s) \hat{\psi}(s) \rangle$ Gaussian: only terms with $\eta \neq 0$ — Wick's theorem

$\langle \xi(t)\eta(s)\psi(s)\rangle$ —

$\langle \xi(t)\eta(s)\rangle\langle\psi(s)\rangle \sim \delta(t-s)$

\

$\langle \xi(t)\eta(s')\rangle \sim \delta(t-s')$

↑

from $\psi(s) \Rightarrow s' < s$

but $t > s > s'$ $t = s'$ vanishes

Smoluchowski equation

$$\partial_t \psi = -\partial_x\left[\underbrace{-\frac{1}{\zeta}U'\psi}_{\text{force}} - \Delta\partial_x\psi\right]$$

← when FD holds $\Delta = D$

Note: noise was <u>not</u> assumed to be small

<u>Many interacting particles</u>: hierarchy of Smoluchowski eqns. for $\psi_s(\vec{r}_1,\dots,\vec{r}_s,t)$

$\mu = 1/\zeta$

$$\partial_t \psi_1 = \vec{\nabla}_1 \cdot \Delta \vec{\nabla}_1 \psi_1 - \vec{\nabla}_1 \cdot \Big[\mu \underbrace{\int d\vec{r}_2 \left(-\vec{\nabla}_1 U(\vec{r}_{12})\right)\psi_2(\vec{r}_1,\vec{r}_2,t)}_{\text{interaction force density}}\Big]$$

ψ_2 couples to ψ_3

etc.

molecular chaos $\psi_2 = \psi_1\psi_1$

$$\partial_t \psi_1 = \Delta\nabla_1^2\psi_1 - \mu\vec{\nabla}_1\cdot\int d\vec{r}_2\left(-\vec{\nabla}_1 U(\vec{r}_{12})\right)\psi_1(r_2)\psi_1(r_1)$$

Non-Gaussian noise ⇒ higher order gradient terms

MICROSCOPIC → HYDRODYNAMICS

Describe large scale dynamics in terms of a small number of continuum fields that are 'slow' → field theory
$\omega(k) \to 0 \quad k \to \infty$

- conserved densities
- broken symmetry fields

3 ways of constructing dynamical eqs:

- phenomenological (symmetry) → TONER
- entropy production (near eq.) → JOANNY
- derive by coarse graining microscopic dynamics

EXAMPLE : Vicsek model (continuous time) *
→ Toner-Tu eqs.

$$\frac{d\vec{r}_i}{dt} = v_0 \hat{e}_i$$

neglect translational thermal noise

$$\frac{d\theta_i}{dt} = \gamma \sum_j \underbrace{F(\theta_j - \theta_i,\ \vec{r}_j - \vec{r}_i)} + \sqrt{2D_r}\,\eta_i(t)$$

$$= \sin(\theta_j - \theta_i)/\pi R^2 \qquad r_{ij} < R$$

$$= 0 \qquad \text{otherwise}$$

$\eta_i \in [-1/2, 1/2]$

Now $\psi = \psi(\vec{r}, \theta, t)$

$$\partial_t \psi = -\vec{\nabla}\cdot(v_0 \hat{e}\psi) - D_r \partial_\theta^2 \psi$$

$$-\gamma \partial_\theta \int d\theta' \int d\vec{r}' \underbrace{F(\theta' - \theta, \vec{r}' - \vec{r})}\ \psi(\vec{r}', \theta')\,\psi(\vec{r}, \theta)$$

$$\sin(\theta' - \theta)\,\delta(\vec{r} - \vec{r}')$$

* E. Bertin, M. Droz, G. Gregoire, J Phys A: Math Th. 42, 445001 (2009)
S. Mishra, A. Baskaran, MCM, PRE 81, 061916 (2010) (banding)

Continuum fields such as density etc. as moments of ψ

$$\rho(\vec{r},t) = \int \frac{d\hat{e}}{2\pi}\, \psi \qquad \psi_k(\vec{r},t) = \int \frac{d\theta}{2\pi}\, e^{ik\theta}\, \psi$$

$$\rho \vec{P} = \int \frac{d\hat{e}}{2\pi}\, \hat{e}\, \psi \qquad \psi_0 = \rho$$

$$\psi_1 = \rho(P_x + iP_y)$$

$$\rho Q_{\alpha\beta} = \int \frac{d\hat{e}}{2\pi} (\hat{e}_\alpha \hat{e}_\beta - \tfrac{1}{2}\delta_{\alpha\beta})\psi \qquad \psi_2 = \rho(Q_{xx} + iQ_{xy})$$

... ...

Eqn for $\psi(\vec{r},t) \longrightarrow$ infinite set of Eqs. $\{\psi_k\}$

$$\partial_t \psi_k + \frac{v_0}{2}\partial_x(\psi_{k+1} - \psi_{k-1}) + \frac{v_0}{2i}\partial_y(\psi_{k+1} - \psi_{k-1})$$

decay $= -K^2 D_r \psi_k + \frac{i\chi K}{2\pi} \sum_s \psi_s F_{-s} \psi_{k-s}$

need closure!

$F_1 = -i/2 \quad F_{-1} = F_1^* \quad$ others $\emptyset$

$$\partial_t \psi_0 + \frac{v_0}{2}(\partial_x - i\partial_y)\psi_1 = 0 \longrightarrow \partial_t \rho = -\vec{\nabla}\cdot(v_0 \rho \vec{P})$$

$\psi_0 \sim \rho$ conserved field ✓

$\psi_1 \sim \vec{P}$ order parameter ✓

$-\frac{i}{2}(\psi_1^* \psi_{k+1} - \psi_1 \psi_{k-1})$

Assume $\psi_k = 0 \quad k > 3$

$\dot{\psi}_2 = 0$

Can be made systematic as an expansion in a small parameter ε near ME transition where

$\rho - \rho_0 \sim \varepsilon \qquad \psi_1 \sim P \sim \varepsilon \qquad \partial_t \sim \nabla \sim \varepsilon \qquad f_2 \sim \varepsilon^2$

[see Peshkov et al., EPJ Special Topics 223 1315 (2014)]

Toner-Tu Eqs of flocking :

$\vec{\nabla}$(pressure)

$$\partial_t \rho = -\vec{\nabla}\cdot(v_0 \rho \vec{p})$$

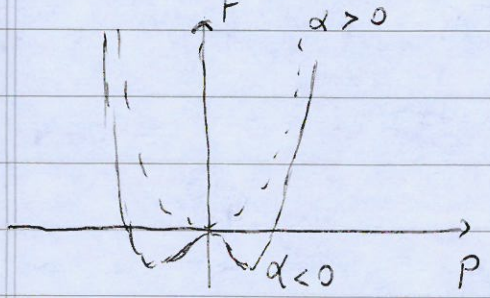
$$\partial_t \vec{p} + \lambda_1 (\vec{p}\cdot\vec{\nabla})\vec{p} = -[\alpha(\rho) + \beta p^2]\vec{p} - \frac{v_0}{2}\vec{\nabla}\rho + \frac{\lambda_3}{2}\vec{\nabla}p^2 + \lambda_2 \vec{p}(\vec{\nabla}\cdot\vec{p}) + K_3 \nabla^2 \vec{p} + (K_1 - K_3)\vec{\nabla}(\vec{\nabla}\cdot\vec{p})$$

all parameters given in terms of D_r, γ, v_0, ρ_0

$$\alpha(\rho) = D_r - \frac{1}{2\pi}\gamma\rho$$

$$\beta = \gamma^2\rho^2 / 3\pi^2 D_r$$

Dual role of $\vec{p}$



nonlinear friction

$$-\frac{1}{\gamma}\frac{\delta F}{\delta \vec{p}}$$

$$F = \frac{1}{2}\int_{\vec{r}} \left\{ \frac{\alpha}{2} p^2 + \beta/4\, p^4 \right\}$$

$\lambda_1 = v_0$ if Galilean invariance

substrate → non universal parameter

Disordered $|\vec{p}| = 0$ → ordered $p_0^2 = -\alpha/\beta$

↑

$\alpha = 0$

$\rho_c = 2D_r\pi/\gamma$

Banding instability

ordered phase linearly unstable for $\alpha \to 0^-$ $\rho_0 \to 0^+$

$|\delta \vec{p}|$ decay at rate $|\alpha_0| \to 0$

$\delta\rho$, $|\delta \vec{p}|$ fluctuations unstable along $\vec{p}$

at a wavelength $\lambda_c \sim (\rho_c - \rho_0)^{-3/2}$ (see Refs. on p.5)

$\Rightarrow$ bands, observed ubiquitously

Fluctuations about ordered state

$\rho = \rho_0 + \delta\rho$

$\vec{P} = P_0 \hat{x} + \delta\vec{p}$ $\qquad$ $\vec{P} = P\hat{P}$

$\delta\vec{p} = \delta p\,\hat{x} + P_0\,\delta\hat{P}_y$

spatial variations along x

$\delta\rho$, δp decouple $\sim e^{iqx}$

$$\partial_t \delta\rho = -iq v_0 \rho_0 \delta p - iq v_0 P_0 \delta\rho$$

$$\partial_t \delta p = a\,\delta\rho - 2|\alpha_0|\,\delta p - \frac{v_0}{2} iq\,\delta\rho$$

generic instability

propagating wave $\qquad \delta\rho, \delta p \sim e^{st}$

$$\mathrm{Re}\, s = -s_2 q^2 - s_4 q^4 \qquad a \sim -\frac{\partial\alpha}{\partial\rho}$$

$$s_2 = \frac{v_0^2}{2|\alpha_0|}\left[1 - \frac{v_0 a^2 \rho_0^2}{4 v_0 |\alpha_0| \beta}\right]$$ ← unstable even for small v_0 near MFT

no noise : propagating solitary waves as bands

→ seen in simulation and experiments.

Two comments:

1) Method can be used to derive eqs for model with other symmetry, and to include flow
   - SP rods w/ steric repulsion Baskaran + MCM PRL 2008
   - dry "Vicsek nematic" Bertin et al, NJP 2013
   - polar and nematic w/ flow, Liverpool + MCM 2008 in "Cell motility", P. Lenz ed.
   - active polymers: Ahmadi, MCM, Liverpool, PRE 2006

3) Eq. for one-particle distribution with noise:
   David Dean, J. Phys. A: Math Gen 29, L613 (1996)
   White, Gaussian noise in microscopic dynamics
   → multiplicative noise in coarse-grained dynamics.

LECTURE II

DENSE ACTIVE SYSTEMS : activity and crowding

- Recall Lisa's confluent cell layers
- Show penguin movie

Today's lecture : activity and exclude volume / steric effects

FIRST → SP dynamics vs Brownian dynamics

■ Overdamped Brownian particle ($d=2$)

$$\frac{d\vec{r}}{dt} = \vec{v} = \vec{\eta}(t) \qquad \langle \vec{\eta}(t) \rangle = 0$$

$$\langle [\Delta \vec{r}(t)] \rangle = 4Dt \qquad \langle \eta_\alpha(t)\eta_\beta(t') \rangle = 2D\delta_{\alpha\beta}\delta(t-t')$$

$$D = k_B T/\zeta$$

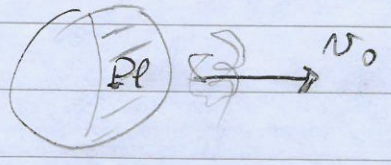
■ SPP

- active colloids
- cells on substrate

- Fily & MCM PRL 108 235702 (2012)
- Fily, Henkes, MCM Soft Matter 10, 2132 (2014)

→ Palacci's low density movie + high density

Ayusman Sen 2005

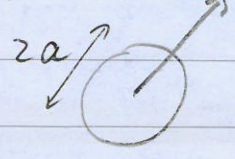


$v_0 \sim 1-15\,\mu m/s$

from different rates of H_2O_2 consumption on two sides

$$\frac{d\vec{r}}{dt} = v_0 \hat{e} + \vec{\eta}(t) \qquad \hat{e} = (\cos\theta, \sin\theta)$$

$$\frac{d\theta}{dt} = \eta_R(t)$$



$$\langle \eta_R(t) \rangle = 0$$

$$\langle \eta_R(t)\eta_R(t') \rangle = 2D_r\delta(t-t')$$

$[D] = [\ell^2 t^{-1}]$

$[D_r] = [t^{-1}]$

equilibrium : noise $\sim kT$

$D \sim a^2 D_r$

HW : calculate MSD

$$\langle [\Delta \vec{r}(t)]^2 \rangle = 4Dt + \frac{2v_0}{D_r}\left[t - \frac{1 - e^{-D_r t}}{D_r} \right]$$

$t \ll D_r^{-1}$ $\quad \sim v_0^2 t^2$

$t \gg D_r^{-1}$ $\quad \frac{2v_0^2}{D_r} t$

$$t \gg D_r^{-1}$$

$$\langle [\Delta \vec{r}(t)]^2 \rangle \simeq 4\left[D + \frac{v_0^2}{2D_r} \right] t$$

persistence length

$$\ell_p = v_0 / D_r$$

$$\frac{v_0^2}{2D_r} \sim \ell_p^2 D_r$$

How does this compare to run-and-tumble ? (E.coli)

continuous diffusion at rate D_r VS discrete tumble events

mean-time between tumbles exponentially distributed

tumble rate α

$$D_{sp} \sim \frac{v_0^2}{d(d-1)D_r}$$

$(d-1)D_r \to \alpha$

$$D_{sp} \sim v_0^2 / d\alpha$$

$$D_{sp} = \frac{v_0^2}{d[\alpha + (d-1)D_r]}$$

(some E.coli mutants do not tumble)

Differences disappear upon coarse graining.

Apparent only when there is a small-scale structure in the problem, e.g., traps of size large compared to run length: ABP trapped at walls.

For more : Solon, Cates, Tailleur EPJ 224, 1231 (2015)

Some numbers

$D = \frac{k_B T}{6\pi \eta a}$

$k_B T \sim 1.38 \times 10^{-23} \frac{J}{K} \, 300K \sim 5 \times 10^{-21} J$

$\eta_{H_2O} \sim 10^{-3} Pa\,s$

$a \sim \mu m \sim 10^{-6} m$

$D \sim 0.2 \times 10^{-12} m^2/s$

$\sim 0.2 \, \mu m^2/s$

$D_{sp} \sim v_0^2 / D_r$

$v_0 \sim 10 \, \mu m/s$

$D_r \sim 10^{-3} - 10^{0} \, s^{-1}$

$\alpha \sim 1 \, s^{-1}$

$D_{sp} \sim 10^2 \, \mu m^2/s$

$D_{sp} >> D$

We can neglect translational noise

Both systems:

- particles do not exert torques on each other nor on a surrounding solvent.
  The angular dynamics of each particle is unaffected by that of the others or by interactions

Key simplification

Peclet number $Pe = v_0 / a D_r = l_p / a$

Effective temperature

tempting, but ...

$$\left.\begin{aligned}\frac{d\vec{r}}{dt} &= \hat{e}(\vartheta)v_0 \\ \frac{d\vartheta}{dt} &= \eta_R(t)\end{aligned}\right\} \quad \frac{d\vec{r}}{dt} = \vec{\xi}_{eff}(t)$$

$$\langle \xi_\alpha(t)\xi_\beta(t')\rangle = v_0^2 e^{-D_r|t-t'|} \to \frac{v_0^2}{D_r}\delta(t-t') \quad D_r \to \infty$$

Non-Markovian noise

$$k_B T_{eff} = \frac{v_0^2}{2\mu D_r}$$

$$P_{ideal} = \rho k_B T_{eff}$$

$[D_r] = t^{-1}$

$[\mu] = [m^{-1}t^{+1}]$

skip

- Equilibrium: linear response $R = \left(\frac{\partial\langle v\rangle}{\partial f}\right)_{f=0} = \mu = 1/\zeta$

  FD: $C/R = k_B T$ correlation function $C = D = \frac{1}{a}\int_0^\infty dt\,\langle \vec{v}(t)\cdot\vec{v}(0)\rangle$

- Glassy systems: $C/R = k_B T_{eff}$ a useful concept sometimes $T_{eff}(\omega)$

Here:

- Single active particle in an external force, e.g., confining potential V_{ex}; equilibrium notion effective only if

$$\nabla V_{ext} \ll F_{sp} = v_0/\zeta$$

or characteristic length set by balance of external and SP force $\sim V_{ex}\zeta/v_0 \gg l_p$

- Most striking phenomenon → MIPS = motility-induced phase separation

many particles $1/D_r \ll \tau_{coll} \sim 1/2a v_0 \rho$

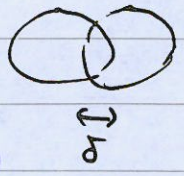
Interacting SPP : only repulsion

$$\frac{d\vec{r}_i}{dt} = v_0 \hat{e}_{\theta_i} + \mu \sum_j \vec{f}_{ij}$$

$$\frac{d\theta_i}{dt} = \eta_{R_i}(t)$$

Repulsive forces :

- soft $\quad \vec{f}_{ij} = -\delta k \hat{r}_{ij}$



- hard spheres

- WCA, LJ, ...

2d + 3d

Time scales

$1/D_r$

a/v_0

$1/\mu k$

$\tau_c = 1/2a v_0 \rho$

$v_0/a \gg \mu k$ pass through

$v_0/a\mu k \to 0$ athermal packing

$D_r \to \infty$ thermal

Phase separation with no attraction → MIPS motility-induced

→ movies : • our simulations
• Palacci clusters

phase separation if $\tau_r > \tau_c$

$Pe\rho \gg 1$

MIPS :

- mean speed of particles along propulsion direction decreases with increasing density ($\neq$ equipartition)
- particles accummulate when they move slowly (not possible in equilibrium systems because speed distribution does not depend on position)

$v_0 \to v(\rho) \simeq v_0(1 - \lambda\rho)$ numerics fits to MSD

Schnitzer, PRE 48, 2553 (1993)

1 d run-and-tumble w/ spatially varying speed

$V(x)$ speed of run

α tumble rate

$R(x)/L(x)$ = density of right/left moving particles

$$\begin{cases} \dot{R} = -\partial_x(vR) - \frac{\alpha}{2}R + \frac{\alpha}{2}L \\ \dot{L} = \partial_x(vR) + \frac{\alpha}{2}R - \frac{\alpha}{2}L \end{cases}$$

factor of $\frac{1}{2}$ because $\frac{1}{2}$ of tumbles are $R \to R$ or $L \to L$ direction switches at rate $\alpha/2$

$\rho = R + L$ = density

$\sigma = R - L$ = polarization

$J = v\sigma$ = current

$$\begin{cases} \partial_t \rho = -\partial_x J & \text{conserved} \\ \partial_t \sigma = -\partial_x(v\rho) - \alpha\sigma & \text{relaxational} \end{cases}$$

time $\gg 1/\alpha$ $\quad \sigma \simeq -\frac{1}{\alpha}\partial_x(v\rho)$ "adiabatic" approximation

$$\partial_t \rho = -\partial_x\left[-\frac{v}{\alpha}\partial_x v\rho\right]$$

$$\partial_t \rho = -\partial_x\left[-\frac{v^2}{\alpha}\partial_x\rho + \frac{vv'}{\alpha}\rho\right]$$

cf convection-diffusion

current $J = V\rho - D\partial_x\rho$

~~$\partial_t \rho = \partial_x[D(x)\partial_x\rho] + \partial_x[V(x)\rho]$~~

$D(x) = v^2(x)/\alpha$

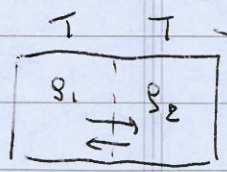
$V(x) = -\frac{v(x)v'(x)}{\alpha}$ drift towards regions of smaller v (- sign)

- $v(x) = \text{constant}$

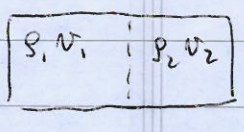
  $\partial_t \rho = D \partial_x^2 \rho$ only stationary solution is $\rho = \rho_0$

- $v(x) \neq \text{constant}$

  steady state $J(x) \equiv \text{const} = 0$ no flux



$\rho_1 v_{th} = \rho_2 v_{th}$



$\rho_1 v_1 = \rho_2 v_2$

$\frac{1}{\rho}\partial_x \rho = -\frac{1}{v}\partial_x v$

$$\rho(x) = \rho_0 \frac{v(0)}{v(x)}$$

This result depends critically on having an upper bound for speed, as opposed to a speed distribution (e.g. M-B) that allows (even if with small probability) arbitrarily large speeds.

Many interacting particles $v \to v(\rho)$

$\rho \sim \frac{1}{v(\rho)}$ feedback yields phase separation

Continuum Model

ρ conserved

$\vec{p}$ no phase transition

Non interacting particles:

$$\frac{d\vec{r}_i}{dt} = v_0 \hat{e}_i + \vec{\eta}_i(t)$$

$$\frac{d\theta_i}{dt} = \eta_{R_i}(t)$$

$$\partial_t \psi(\vec{r},\theta,t) = -\vec{\nabla}\left[v_0 \hat{e}\psi - D\vec{\nabla}\psi\right] + D_r \partial_\theta^2 \psi$$

$$\partial_t \rho = -\vec{\nabla}\cdot\left[v_0 \rho \vec{p} - D\vec{\nabla}\rho\right]$$

$$\partial_t \vec{p} = -D_r \vec{p} - \frac{v_0}{2}\vec{\nabla}\rho + \cancel{k}(\nabla^2 \cancel{\vec{p}}$$

interactions here are repulsive steric effect.
do not yield alignment, but reduce motility

$$v_0 \to v(\rho) \simeq v_0(1-\lambda\rho)$$

λ depends on pair correlation function

higher probability of finding particles ahead of you than behind

Clustering of inelastic systems arise from combining the dynamics of a conserved field (density) with non-conserving noise. This gives $S(k) \sim 1/k^2$, like GNF in ordered state

$$\partial_t \rho = -\vec{\nabla}\cdot[v(\rho)\rho\vec{p}] + D\nabla^2\rho$$

$$\partial_t \vec{p} = -D_r\vec{p} - \frac{1}{2}\vec{\nabla}[\rho v(\rho)] + O(\nabla^2)$$

$t \gg 1/D_r$ $\quad \vec{p} \propto -\frac{1}{2D_r}\vec{\nabla}[\rho v(\rho)]$ quasi-thermal limit

$$\partial_t \rho = \vec{\nabla}\cdot D(\rho)\vec{\nabla}\rho$$

$$D(\rho) = D + \frac{v^2(\rho)}{2D_r} + \frac{v\rho v'}{2D_r}$$

$$v(\rho) = v_0(1-\lambda\rho)$$

minimum Pe required for phase separation

$$D_{eff} = D + \frac{v_0^2}{2D_r}(1-\lambda\rho)(1-2\lambda\rho)$$

$D_{eff} < 0$ spinodal phase separation

Kinetic estimate of λ

$\tau_c \sim (2a v_0 \rho)^{-1}$ mean free time

$v(\rho) \sim v_0(1-\tau/\tau_c)$ τ ~ mean delay caused by collisions

- $\tau_1 \sim a/v_0$ escape by traveling a while maintaining orientation
- $\tau_2 \sim 1/D_r$ must rotate to escape

$\frac{1}{\tau} = \frac{1}{\tau_1} + \frac{1}{\tau_2}$ faster mechanism wins (back)

finite D_r: retain dynamics of $\vec{p}$ and examine stability of homogeneous state $\rho = \rho_0$, $\vec{p} = 0$ by letting up $\rho = \rho_0 + \delta\rho$

$$\vec{p} = \delta\vec{p}$$

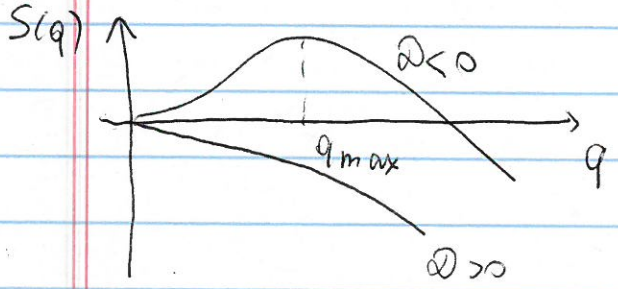
$$\delta\rho(\vec{r},t), \delta\vec{p}(\vec{r},t) \sim e^{st + i\vec{q}\cdot\vec{r}}$$

$$(\partial_t + Dq^2)\,\delta\rho_q + i v(\rho_0)\,\vec{q}\cdot\vec{p} = 0$$

$$(\partial_t + D_r \overset{+kq^2}{\Gamma})\,\delta\vec{p} + \tfrac{1}{2}(v + \rho_0 v')\, i\vec{q}\,\delta\rho = 0$$

small q : mode

$$s(q) = -q^2 D(\rho_0) + q^4 B$$



$$q_{max} \sim \sqrt{-\frac{D}{2kD}}$$

This result can also be interpreted in the context of a Landau-type MFT (ignoring gradient terms, i.e., $v(\rho(r))$ is local.

In fact one can map repulsive SPP with $v(\rho)$ onto a Landau-like MFT of a system of attractive particles undergoing liquid gas phase separation.

Pressure

- force/area on walls of container
- thermodynamics : $P = -\left(\frac{\partial F}{\partial V}\right)_N \Rightarrow$ eqn. of state
- hydrodynamics : $P = \rho k T + \frac{1}{6V}\left\langle \sum_{i \neq j} \vec{r}_{ij} \cdot \vec{F}_{ij} \right\rangle$ or virial

trace of stress tensor

or $\frac{1}{3V}\left\langle \sum_i \vec{r}_i \cdot \vec{f}_i \right\rangle$ virial

Ideal gas of SP particles :

$\zeta \dot{\vec{r}}_i = \zeta v_0 \hat{e}_i$

$\dot{\theta}_i = \eta_i(t)$ → SP force $\vec{f}_i^{SP}$

$$P_{act/swim} = \frac{1}{2A}\left\langle \sum_i \vec{r}_i \cdot \vec{f}_i^{SP} \right\rangle$$

$$= \frac{1}{2A}\int_{-\infty}^{t} dt' \left\langle v_0 \hat{e}_i(t') \cdot \zeta v_0 \hat{e}_i(t) \right\rangle$$

$$P_{act/swim} = \frac{\rho v_0^2}{2\mu D_r}\left(1 - e^{-D_r t}\right) \xrightarrow[t \to \infty]{} \frac{\rho v_0^2}{2\mu D_r} = \rho k T_{eff}$$

in a container $t \sim L/v_0$

$$P_{swim}(t \sim L/v_0) \sim \begin{cases} \rho k T_{eff} & \text{if } L \gg \ell_p \\ \frac{\rho v_0 L}{2\mu} & L \ll \ell_p \end{cases}$$

Detailed calculations have shown

$$P_{swirl} = \frac{\rho v_0 v(\rho)}{2\mu D_r}$$