DENSE ACTIVE SYSTEMS : activity and crowding

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

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

$\boxed{\text{First}}$ → SP dynamics vs Brownian dynamics

■ Overdamped Brownian particle $(d=2)$

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

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

$$D = K_BT/\zeta$$

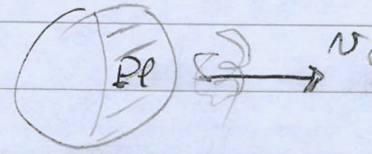
■ SPP

- active colloids
- cells on substrate

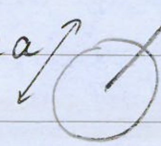
- Fily & MCM PRL 108 235702 (2012)
- Fily, Henkes, MCM Soft Matter 10, 2132 (2014)

→ Palacci's low density movie + high density

Ayusman Sen 2005



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



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

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

from different rates of H_2O_2 consumption on two sides

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

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

$[D] = [l^2 t^{-1}]$ equilibrium : noise $\sim KT$

$[D_r] = [t^{-1}]$ $D \sim a^2 D_r$

HW : calculate MSD

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

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

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

$$\boxed{\begin{array}{l} t \gg D_r^{-1} \\ \langle[\Delta\vec{r}(t)]^2\rangle \simeq 4\left[D + \frac{v_0^2}{2D_r}\right]t \end{array}}$$

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

$D_{sp} \sim \frac{v_0^2}{d(d-1)D_r}$ $\quad \boxed{(d-1)D_r \to \alpha}$ $\quad D_{sp} \sim v_0^2/d\alpha$

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

(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 ~~comparable~~ to run length : ABP trapped at walls.

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

Some numbers

$D = \frac{K_B T}{6\pi\eta a}$ $\qquad$ $K_B T \sim 1.38\times10^{-23}\,J/K \; 300K \sim 5\times10^{-21}\,J$

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

$D \sim 0.2\times10^{-12}\,m^2/s$ $\qquad$ $a \sim \mu m \sim 10^{-6}\,m$

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

$D_{sp} \sim v_0^2/D_r$ $\qquad$ $v_0 \sim 10\,\mu m/s$

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

$D_{sp} \sim 10^{2}\,\mu m^2/s$ $\qquad$ $\alpha \sim 1\,s^{-1}$

$\boxed{D_{sp} \gg D}$ $\qquad$ <u>We can neglect translational noise</u>

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 $\qquad Pe = v_0/aD_r = l_p/a$

Effective temperature

tempting, but...

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

$$\langle \xi_\alpha(t)\xi_\beta(t')\rangle = v_0^2\, e^{-D_r|t-t'|}$$

Non-Markovian noise

$$\rightarrow \frac{v_0^2}{D_r}\,\delta(t-t') \qquad D_r\to\infty$$

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

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

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

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

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 $C = D = \frac{1}{d}\int_0^\infty dt\,\langle\vec{v}(t)\cdot\vec{v}(0)\rangle$

- 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., ~~[illegible]~~ 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 $\sim V_{ex}\,\zeta/v_0 \gg \ell_p$

- Most striking phenomenon $\longrightarrow$ MIPS = motility-induced phase separation

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

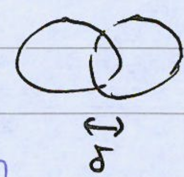
Interacting SPP : only repulsion

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

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

Repulsive forces :

- Soft $\quad \vec{f}_{ij} = -\delta K\, \hat{r}_{ij}$



- hard spheres $\quad \boxed{2d + 3d}$
- WCA , LJ , ...

Time scales

$1/D_r$

a/v_0

$1/\mu K$

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

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

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

$D_r \to \infty$ thermal

Phase separation with no attraction $\to$ MIPS motility-induced phase separation if $\tau_r > \tau_c$

$\Rightarrow$ movies : • our simulations
• Palacci clusters

$\boxed{Pe\, \rho \gg 1}$

MIPS :

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

$v_0 \to v(\rho) \simeq v_0 (1 - \lambda \rho)$ $\quad$ 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 ½ because ½ 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

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

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

cf convection-diffusion

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

$\cancel{\partial_t \rho = \partial_x(V(x)\rho) + \partial_x D(x)\partial_x \rho}$

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

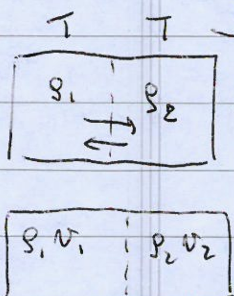
$V(x) = - \dfrac{v(x)\, v'(x)}{\alpha}$ drift towards regions of smaller v ($-$ sign)

- $v(x) =$ constant

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

- $v(x) \neq$ constant

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



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

$\rho_1 v_1 = \rho_2 v_2$

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

minimum Pe required for phase separation

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

$\mathcal{D}_{eff} < 0$ spinodal phase separation

$\boxed{\text{Kinetic estimate of } \lambda}$

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

$v(\rho) \sim v_0(1-\tau/\tau_c)$ $\quad \tau \sim$ 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 mechanisms wins (back)

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

$$\rho = \rho_0 + \delta\rho$$
$$\vec{p} = \delta\vec{p}$$

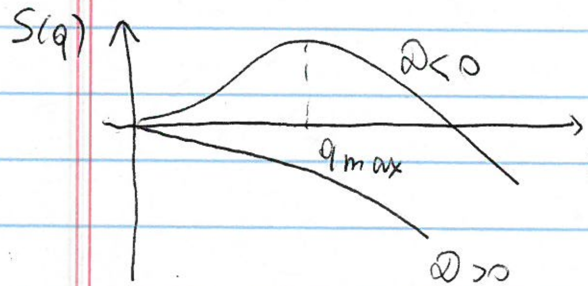
$$\delta\rho(\vec{r},t),\ \delta\vec{p}(\vec{r},t) \sim e^{st + i\vec{q}\cdot\vec{r}}$$

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

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

small q : mode

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



$$q_{max} \sim \sqrt{-\mathcal{D}/2K\mathcal{D}}$$

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.

$\boxed{\text{Pressure}}$

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

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

Ideal gas of SP particles :

$$\zeta \dot{\vec{r}}_i = \underbrace{\zeta v_0 \hat{e}_i}_{\text{SP force } \vec{f}_i^{\,SP}}$$

$$\dot{\theta}_i = \eta_i(t)$$

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

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

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

in a container $t \sim L/v_0$

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

Detailed calculations have shown

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