2019 Boulder condensed matter summer school

Active living matter

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- Many biological systems involve interactions between large numbers of objects at relatively high densities that are "active" – energy is injected at the smallest scales

- Condensed matter physicists have developed a sophisticated set of tools to predict the emergent, collective behavior of dense, interacting systems.

- How can we extend these tools to active living matter?
  challenges:
  - far from equilibrium
  - what is the right level of model? (objects are not simple atoms/molecules)
  - different types of interactions/transitions
    - alignment/flocking
    - steric/glass or jamming or MIPS
      Motility Induced Phase Separation

Focus today on "active matter":

- local force on each agent; not driven by boundary conditions (e.g. shear) or by a global field (e.g. gravity)

Examples of active matter in biology (lots)

- inside a nucleus: active chromatin remodeling?
- inside a cell: cytoskeleton: cell division, cell motility

  liquid-liquid phase separation: intrinsically disordered proteins + active motors
- many cells: tissues + colonies
  - development,
  - collective migration
  - wound healing
  - bacteria colonies
  - cancer tumors
- organisms: human crowds, birds, insects, fish, sheep
- synthetic: extensible microtubule systems (e.g. Dogic lab)
  active colloids

Outline for lectures

① classification of active matter systems
② Statistical physics of single particles: brownian + self-propelled
(remainder Lecture I)

③ Interactions + emergent behavior

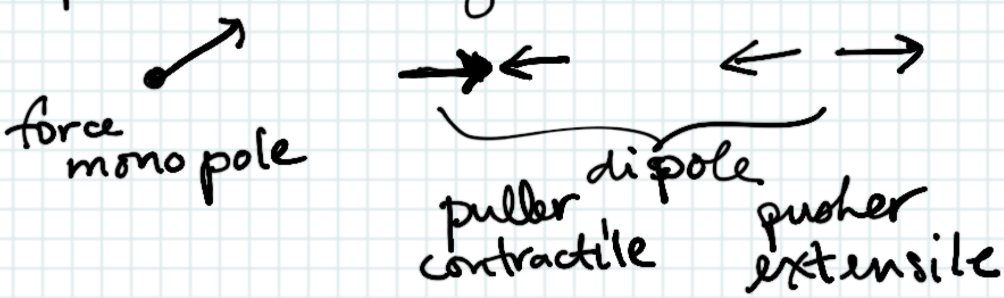
A. Alignment + flocking (Lecture II)
- vicsek model
- Toner-Tu hydrodynamics

B. Steric interactions (metric-based) (Lecture III)
- particle-based models
- motility induced phase separation
- jamming/glass physics

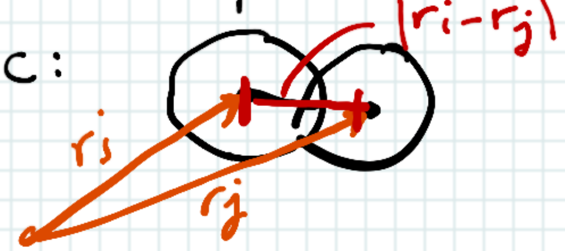
C. Shape-based interactions (topology-based)
- vertex models
- calculations of shear modulus
(Lecture IV)

Classification of Active matter systems:

- types of force generation

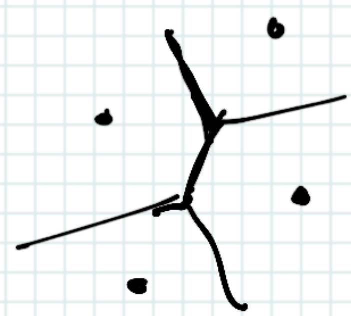


- types of particle-particle interactions
  - steric:



metric $|r_i - r_j|$

- OR -



topological: voronoi or Wigner-Seitz; depends on neighbor relationship, not distance

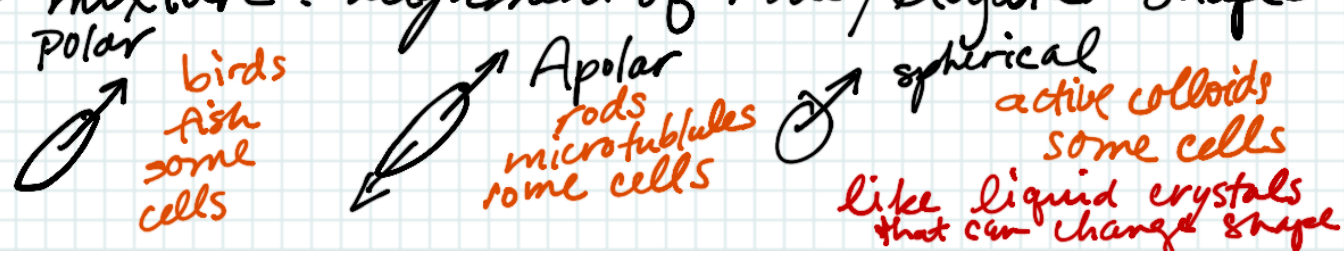
  - alignment: $\hat{n}_i$ $\hat{n}_j$

metric

- OR -

topological

  - mixture: alignment of rods/elogated shapes



Interactions with environment:

- hydrodynamic interactions with walls or other particles
- drag/friction forces with substrate or other particles
- global fields such as gravity or morphogen gradients

2.1 Passive particle (Review from stat mech)

Jean Perrin: colloids in solvent

$$ma = \sum F$$

effect of collisions from solvent molecules

$$m\dot{v} = \underbrace{F_{pot}}_{-\nabla U} + \underbrace{F_{drag}}_{-\zeta v} + \underbrace{F_{random}}_{\eta(t)}$$

for a spherical particle in 3d $\zeta = 6\pi \nu a$

viscosity (ν), particle radius (a)

noise is Gaussian or white

$$\begin{cases} \langle \eta(t) \rangle = 0 \\ \langle \eta_\alpha(t)\, \eta_\beta(t') \rangle = 2\Delta\, \delta_{\alpha\beta}\, \delta(t-t') \end{cases}$$

time average: $\int \eta(t')dt'$

magnitude of noise (Δ)

$$\boxed{m\dot{v} = -\zeta v + \eta(t)}$$

standard grad. stat mech references: McQuarrie, Kardar

underdamped Brownian motion in absence of a potential

$\exists$ characteristic timescale $\tau_m = m/\zeta$

$$\langle |v(t)|^2 \rangle = \frac{d\Delta}{m\zeta}\left(1 - e^{-2|t|/\tau_m}\right)$$

equipartition

for $t \gg \tau_m$ $\langle |v(t)|^2 \rangle = \frac{d\Delta}{m\zeta} = \frac{dT}{m}$

$$\Rightarrow \Delta = \zeta T$$

can show:

$$\langle \Delta r^2(t)\rangle = \langle [r(t)-r(0)]^2\rangle$$

$$= 2d\,\frac{T}{\xi}\left[|t| - \tau_m\left(1-e^{-|t|/\tau_m}\right)\right] = \begin{cases} \dfrac{dT t^2}{\xi\,\tau_m} & t \ll \tau_m \\ \dfrac{2dT}{\xi}|t| & t \gg \tau_m \end{cases}$$

$$D_t \equiv \lim_{t\to\infty}\frac{\langle \Delta r^2(t)\rangle}{2dt} = \frac{T}{\xi}$$

ref. Fily + Marchetti PRL 108 (2012)

2.2 Self-propelled particles (non-interacting)

$\Sigma F = m\cancel{a} \overset{0}{}$ → overdamped limit, neglect inertial forces

$F_{drag} + F_{spp} + \cancel{F_{interaction}} \overset{0}{} = 0$ neglect for now

$$-\xi v + F_0\hat{n} = 0$$

$$\Rightarrow \boxed{\begin{aligned}\frac{\partial \vec{r}}{\partial t} &= v_0\hat{n} \\ \frac{\partial\theta}{\partial t} &= \eta^R(t)\end{aligned}}\ ;\quad \underset{\text{self-propelled velocity}}{v_0} \equiv \frac{F_0}{\xi}$$

SPP

$$\langle \eta^R(t)\,\eta^R(t')\rangle = 2D\,\delta(t-t')$$

$$\langle \eta^R(t)\rangle = 0$$

$$\frac{\partial x}{\partial t} = v_0\cos\theta$$

$$\frac{\partial y}{\partial t} = v_0\sin\theta$$

What is $\chi = \langle v_0\cos\theta(t')\,v_0\cos\theta(t)\rangle$?

$$\theta(t) = \int_0^t \eta^R(t')\,dt'$$

$$\cos\theta(t) = \tfrac{1}{2}\left(e^{i\theta(t)} + e^{-i\theta(t)}\right)$$

$$\langle v_0\cos\theta(t')\,v_0\cos\theta(t)\rangle = \frac{v_0^2}{4}\left\langle\left[e^{i\theta(t)} + e^{-i\theta(t)}\right]\left[e^{i\theta(t')} + e^{-i\theta(t')}\right]\right\rangle$$

Let $\phi = \theta(t) + \theta(t')$; $\omega = \theta(t) - \theta(t')$

$$\Rightarrow \chi = \frac{v_0^2}{2} \langle e^{i\phi} + e^{i\omega} \rangle$$

since θ is Gaussian, we use cumulant expansion

$$\langle e^{i\theta} \rangle = e^{-\frac{\langle \theta \rangle^2}{2}}$$

$$\chi = \frac{v_0^2}{2} \left[e^{-\frac{\langle \phi^2 \rangle}{2}} + e^{-\frac{\langle \omega^2 \rangle}{2}} \right]$$

$$\langle \phi^2 \rangle = \langle \underset{2Dt}{\theta^2(t)} + \underbrace{\theta(t')\theta(t)} + \underset{2Dt'}{\theta^2(t')} \rangle$$

$$\theta(t')\theta(t) = \int_0^t \int_0^{t'} \langle \eta(\tilde{t}) \eta(\tilde{t}') \rangle \, d\tilde{t} \, d\tilde{t}'$$

$$= 2D \int\int^{t\ t'} \delta(\tilde{t} - \tilde{t}') \, dt \, dt'$$

$$\begin{cases} \text{if } t' > t & 2D \int_0^t 1 \, dt = 2Dt \\ \text{if } t > t' & 2D \int_0^{t'} 1 \, dt' = 2Dt' \end{cases}$$

$$= 2D \min(t, t')$$

Similarly $\langle w^2 \rangle = 2Dt + 2Dt' - 4D \min(t, t')$

for $t > t'$

$$\chi = \frac{v_0^2}{2}\left(e^{-\frac{1}{2}(2Dt + 2Dt' + 4Dt')} + e^{-\frac{1}{2}(2Dt + 2Dt' - 4Dt')} \right)$$

small for $t, t' \gg \frac{1}{D}$ (steady state)

$$= \frac{v_0^2}{2}\left(\cancel{e^{-Dt - 3Dt'}} + e^{-D(t-t')} \right)$$

small for $t, t' \gg \frac{1}{D}$ (steady state)

for $t' > t$

$$\chi = \frac{v_0^2}{2}\left(\cancel{e^{-3Dt - Dt'}} + e^{-D(t'-t)} \right)$$

$$\boxed{\langle v_0 \cos\theta(t')\, v_0 \cos\theta(t) \rangle = \frac{v_0^2}{2} e^{D|t-t'|}}$$

translational noise on SPP particles non-Markovian with memory time $\sim 1/D$

Mean-squared displacement of SPP:

$$\frac{\partial x}{\partial t} = v_0 \cos\theta(t) \Rightarrow \langle (x(t))^2 \rangle = \int_0^t \int_0^{t'} \chi(\tilde{t}, \tilde{t}')\, d\tilde{t}\, d\tilde{t}'$$

$$\Rightarrow \langle (x(t))^2 \rangle = \frac{v_0^2}{2} \int_0^t \int_0^{t'} e^{D|\tilde{t} - \tilde{t}'|}\, d\tilde{t}\, d\tilde{t}'$$

$$= \frac{2 v_0^2}{2D} \int_0^t \left(e^{D\tilde{t}} + 1 \right) d\tilde{t}$$

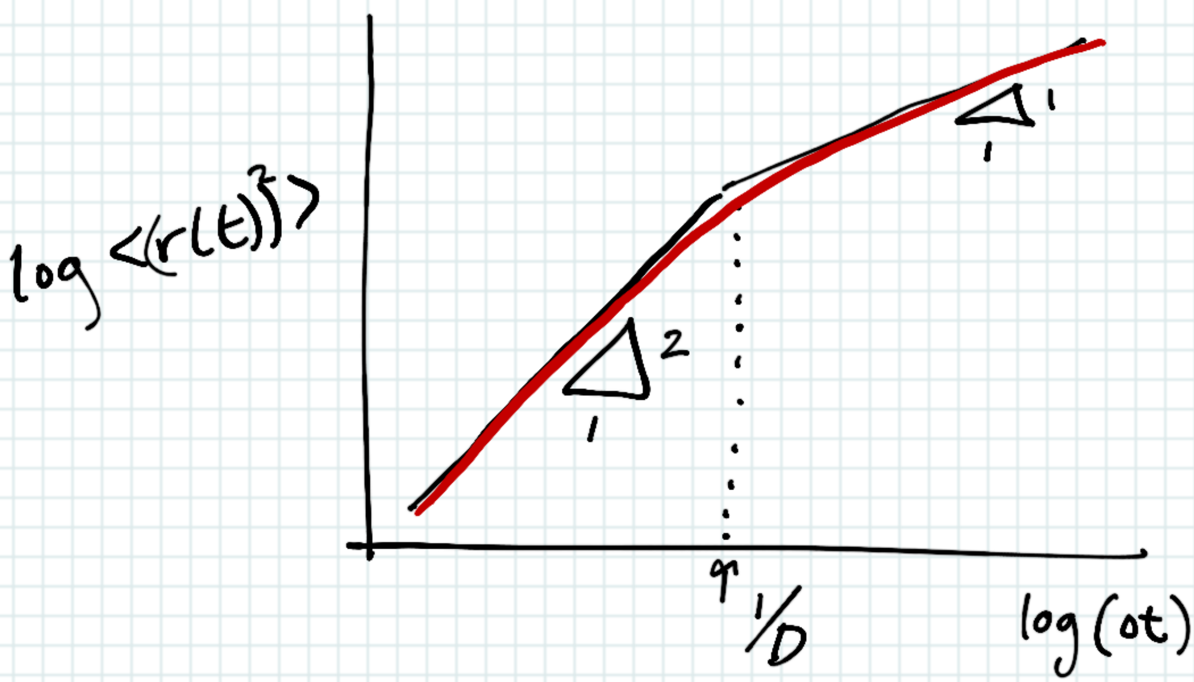
$$= \frac{v_0^2}{D}\left(t + \frac{1}{D}\left(e^{-Dt} - 1 \right) \right)$$

Similarly $\frac{\partial y}{\partial t} = v_0 \sin\theta(t) \Rightarrow$

$$\langle (y(t))^2 \rangle = \langle (x(t))^2 \rangle \Rightarrow$$

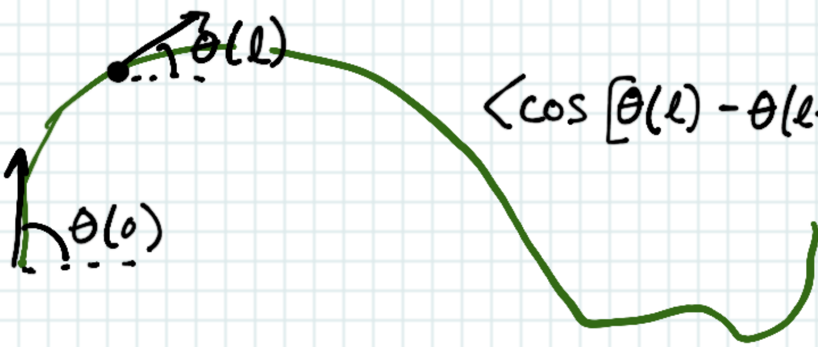
$$\langle (r(t))^2 \rangle = \frac{d v_0^2}{D}\left(t + \frac{1}{D}\left(e^{-Dt} - 1\right)\right)$$

$$\langle (r(t))^2 \rangle \sim \begin{cases} t \ll \frac{1}{D} & \sim \frac{d v_0^2}{D}\left[t + \frac{1}{D}\left(1 - Dt + \frac{(Dt)^2}{2} - 1\right)\right] \\ & \sim \frac{d}{2} v_0^2 t^2 \\ t \gg \frac{1}{D} & \frac{d v_0^2}{D} t \end{cases}$$



The dimensionless number used to describe the competition between self-propulsion and rotational noise is the Peclet number: $Pe \equiv \dfrac{v_0}{2RD_r}$

For non-interacting particles this can be extracted from the orientational autocorrelation function:



$$\langle \cos[\theta(l) - \theta(l+l')] \rangle \equiv e^{-(l/L)}$$

persistence length L

$$Pe = \frac{V_0}{2RD_r} = \frac{L}{2R} \Rightarrow L = \frac{V_0}{D_r}$$

R: characteristic lengthscale (say of cell, particle, etc)