Disorder in complex systems
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What are the origins of long-range velocity correllations in dense active matter systems?

1) for nearly arrested systems, explained by combined effect of persistent motion + elastic response

use notation from this → **Henkes et al, Nat Comm (2020)**

also c.f. Henkes, Fily, Marchetti PRE 2011
Bi, Yang, Marchetti Manning PRX 2016

2) for diffusive systems, explained by persistent motion + bulk modulus.

Flenner + Szamel EPL (2021)

Elastic response:

moves along a direction $\hat{n}$, and orientation angle experiences white noise

Let's investigate self-propelled particles with a simple two-body interaction potential:

$$m \frac{dv_i}{dt} = F_{int} + F_{propulsion} + F_{drag} + F_{positional\ noise}$$

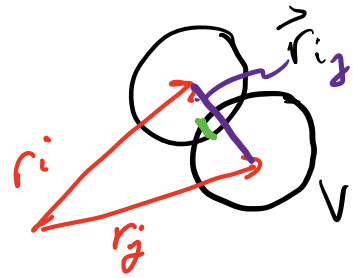
$$0 \qquad -\sum_j \frac{\partial V(r_{ij})}{\partial r_i} \qquad F_0 \hat{n}_i \qquad -\xi v_i \qquad 0$$

"overdamped limit"
inertial effects negligible compared to drag

$$\hookrightarrow \quad \frac{dr_i}{dt} = \frac{F_0}{\xi}\hat{n}_i - \frac{1}{\xi}\sum_j \nabla_i V(r_{ij})$$

Here we consider 2-body potentials

where $V(r_{ij})$ depends on distance between two particles



e.g.

$$V(r_{ij}) = \begin{cases} \epsilon\left[1-\frac{r_{ij}}{2\sigma}\right]^{\alpha}, & r_{ij}<2\sigma \\ 0 & \text{o.w.} \end{cases}$$

$$\circledast \Rightarrow \boxed{\dot{r}_i = v_0\hat{n} - \frac{1}{\xi}\sum_j \nabla_i V(r_{ij})}$$

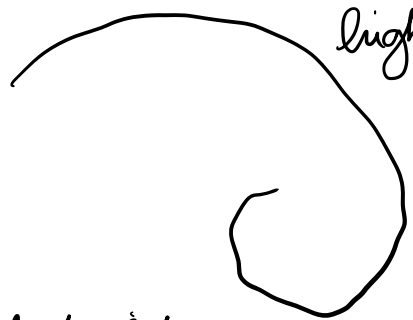
and $\hat{n}_i = \cos\phi_i\,\hat{x} + \sin\phi_i\,\hat{y}$

with $\dot{\phi}_i = \eta_i(t)$, $\langle \eta_i(t)\rangle = 0$

angle experiences white noise with persistence time

and $\langle \eta_i(t)\eta_j(t')\rangle = \frac{2}{\tau}\delta_{ij}\delta(t-t')$

low τ SPP trajectory

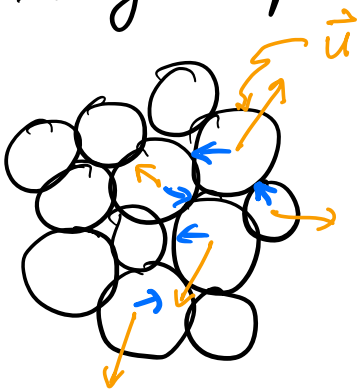


high τ SPP trajectory

Next: start from solid-like perspective:

At high densities, where system would be arrested in the absence of self-propulsion, we can define a <u>Dynamical Matrix</u> describing linear response around a mechanically stable state (local minimum of total potential energy $V_{tot} = \sum_{\substack{\text{all pairs} \\ \langle i,j \rangle}} V(r_{ij})$.

→ if you displace packing of particles by a field $\vec{u}$:



it will result in a set of restoring forces $\vec{f}$:

$$\vec{f} = \overleftrightarrow{M}\,\vec{u}$$

for N particles in 2d, $\vec{u} = \begin{bmatrix} u_{1x} \\ u_{1y} \\ u_{2x} \\ u_{2y} \\ \vdots \end{bmatrix}$, in general is an $Nd \times 1$ vector

$\vec{f} = \begin{bmatrix} f_{1x} \\ f_{1y} \\ \vdots \end{bmatrix}$ is also an $Nd \times 1$ vector.

One can show

$$M_{\substack{i\alpha j\beta \\ j \neq i}} = \frac{\partial^2 V(|r_i - r_j|)}{\partial r_{i\alpha}\, \partial r_{j\beta}}$$

and

$$M_{i\alpha i\beta} = -\sum_j \frac{\partial^2 V(r_{ij})}{\partial r_{i\alpha}\, \partial r_{j\beta}}$$

and $\vec{f}_i = \overleftrightarrow{M}_{ij}\, \partial \vec{r}_j$, where $\vec{f}_i = \sum_j \nabla_i V(r_{ij})$

$\vec{f}_i$: 2-comp. vector in 2D; $\overleftrightarrow{M}_{ij}$: 2x2 matrix; $\partial \vec{r}_j$: 2-comp vector

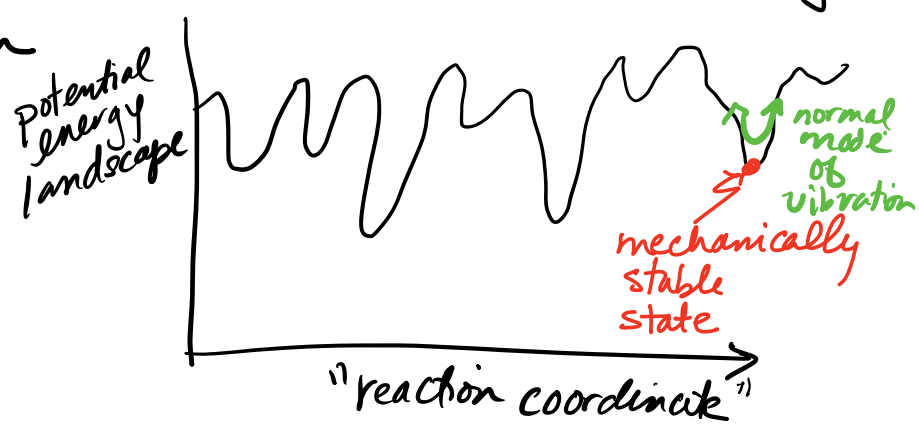
The eigenvalues of this matrix are related to the frequencies of the normal modes of vibration:

$$\omega_\nu^2 = \lambda_\nu$$ ← labels mode index

and the histogram of is the density of vibrational states.

the eigenvectors ξ_ν are the normal modes of vibration. (complete basis set)

They describe the curvatures around a local energy minimum



We can look at dynamics of dense SPP system around such a state:

Let $\vec{r}_{oi}$ be a mechanically stable "inherent state"

Let $\delta\vec{r}_i$ be the displacement from that state:

$$\delta\vec{r}_i = \vec{r}_i - \vec{r}_{oi}$$

Expand $\delta\vec{r}_i$ into the basis of normal modes:

$$\delta\vec{r}_i = \sum_{\nu=1}^{2N} a_\nu \xi_i^\nu \quad \text{or} \quad \delta|r\rangle = \sum_\nu a_\nu |\xi\rangle$$

$\hat{n}_i$ can also be represented in normal mode basis:

$$|n\rangle = \sum_\nu \eta_\nu |\xi\rangle \quad \text{or} \quad \hat{n}_i = \sum_{\nu=1}^{2N} \eta_\nu \xi_i^\nu$$

Note that ⊛ can be linearized around $\vec{r}_{oi}$ and written as:

2 by 2 block of dynamical matrix

$$\delta \dot{\vec{r}}_i = v_0 \hat{n}_i - \frac{1}{\zeta}\sum_j M_{ij} \cdot \delta \vec{r}_j \qquad (\star\star)$$

so projecting $(\star\star)$ on the normal modes we have

$k_\nu = \frac{\lambda_\nu}{\zeta}$

$$\boxed{\frac{d}{dt} a_\nu = -\frac{\lambda_\nu a_\nu}{\zeta} + v_0 \eta_\nu} \qquad (\star\star\star)$$

both unit vectors

note $\eta_\nu = \langle n | \xi \rangle = \sum_{i=1}^{2N} \hat{n}_i \cdot \hat{e}^\nu_i$;

very important in rest of this: projection of SPP onto normal modes

$= \cos(\theta_\nu - \phi)$ polarization angle

θ_ν: eigenvector angle

with $\dot{\phi}$ = white noise

$\langle \cos(\phi) \rangle = 0$

So $\langle \eta_\nu(t) \rangle = 0$

Note $(\star\star\star)$ looks like a single SPP tethered to a spring

Solving it explicitly:

$$(4) \quad a_\nu(t) = a_\nu(t=0)\, e^{-k_\nu t} + v_0 \int_0^t dt' \, \frac{\eta_\nu}{\zeta} e^{-k(t-t')}$$

where $k = \frac{\lambda_\nu}{\zeta}$

Now let's average over the noise:

As shown in the appendix,

$$\underbrace{\langle \eta_\nu(t)\eta_{\nu'}(t')\rangle}_{\text{correlation of noise in eigenvalue basis}} = \langle \cos[\phi(t)-\phi(t')]\rangle \delta_{\nu\nu'}$$

$$= \underline{e^{-|t|/\tau}\delta_{\nu\nu'}}$$

So from (4) One can show that as $t \to \infty$

$$\langle a_\nu^2\rangle = \frac{\zeta}{\lambda_\nu}\int_0^\infty d\nu \, \frac{v_0^2}{2} e^{-|\nu|/\tau} e^{-\zeta\nu}$$

$$= \frac{\zeta v_0^2}{2\lambda_\nu}\int_0^\infty d\nu \, e^{-\left(\frac{1}{\tau}+\frac{\lambda_\nu}{\zeta}\right)\nu}$$

$$= \frac{\zeta v_0^2 \tau}{2\lambda_\nu\left(1+\frac{\lambda_\nu}{\zeta}\tau\right)}$$

average energy per mode:

$$\Rightarrow E_\nu = \left\langle \frac{1}{2}\lambda_\nu a_\nu^2\right\rangle = \frac{\zeta v_0^2 \tau}{4\left(1+\frac{\lambda_\nu}{\zeta}\tau\right)}$$

$$E_\nu \approx \begin{cases} \zeta \dfrac{v_0^2\tau}{4} & \tau \ll \zeta\lambda_\nu^{-1} \text{ (equipartition) } \sim \text{thermal} \\ \dfrac{\zeta^2 v_0^2}{4\lambda_\nu} & \tau \gg \zeta\lambda_\nu^{-1} \text{ dominated by soft modes!} \end{cases}$$

Velocity correlation in fourier space:

$$\hat{G}(\vec{q}) = \langle v(q) \cdot v^*(q) \rangle ; \quad v(\vec{q}) = \frac{1}{N} \sum_{j=1}^{N} e^{i\vec{q}\cdot r_j^0} \delta \dot{r}_j$$

$$= \sum_{\nu,\nu'} \langle \dot{a}_\nu \dot{a}_{\nu'} \rangle \xi_\nu(\vec{q}) \xi_{\nu'}^*(\vec{q}) ; \quad \xi_\nu(\vec{q}) = \frac{1}{N} \sum_{j=1}^{N} e^{i\vec{q}\cdot r_j^0} \xi_j^\nu$$

from above (~~***~~)

$$\langle \dot{a}_\nu \dot{a}_{\nu'} \rangle = \frac{1}{\zeta^2} \left[\lambda_\nu^2 \langle a_\nu^2 \rangle - 2\lambda_\nu \underbrace{\langle a_\nu \eta_\nu \rangle} + \langle \eta_\nu^2 \rangle \right] \delta_{\nu,\nu'}$$

$$\frac{1}{\zeta} \int_0^\infty dt' \langle \eta_\nu(t') \eta_\nu(t) \rangle e^{-k(t-t')}$$

$$= \frac{\zeta v_0^2}{2} \frac{\tau}{1 + \frac{\lambda_\nu}{\zeta}\tau} \quad \text{(similar to above)}$$

$\downarrow$

math

$\downarrow$

$$\langle \dot{a}_\nu^2 \rangle = \frac{v_0^2}{2(1 + \frac{\lambda_\nu}{\zeta}\tau)} \Rightarrow \hat{G}(q) = \sum_\nu \frac{v_0^2}{2(1 + \frac{\lambda_\nu \tau}{\zeta})} \| \xi_\nu(q) \|^2$$

and by Parsevals theorem

$$\langle |v|^2 \rangle = \frac{1}{N} \sum_{j=1}^{N} \langle |\delta \dot{r}_j|^2 \rangle = \sum_q \hat{G}(q)$$

$$\langle |v|^2 \rangle = \frac{L^2}{(2\pi)^2} \int d^2q \sum_\nu \frac{v_0^2}{2\left(1+\frac{\lambda_\nu \tau}{\rho}\right)} \|\xi_\nu(q)\|^2$$

velocity correlations are dominated by lowest frequency modes for $\tau \gg \rho \lambda_\nu^{-1}$

There is a continuum elastic formulation, too. But, it has very similar logic:

$$\langle \hat{n}(\vec{r},t), \hat{n}(\vec{r}\,',t') \rangle = a^2 \delta(\vec{r}-\vec{r}\,') e^{-|t-t'|/\tau}$$

$$\Downarrow$$

$$\langle F^{act}(q,\omega), F^{act}(-q,\omega') \rangle = 2\pi N \rho v_0^2 \frac{2\tau}{1+(\tau\omega)^2} \delta(\omega+\omega')$$

$$\Downarrow$$

$$\langle \tilde{v}(q,t), \tilde{v}(q',t) \rangle = 2\pi a^2 v_0^2 \delta(\vec{q}+\vec{q}\,') \left[\frac{1}{1+\underbrace{\left[\frac{(B+\mu)\tau}{\rho}\right]}_{\xi_L^2} q^2} + \frac{1}{1+\underbrace{\frac{\mu\tau^2}{\rho}}_{\xi_T^2} q^2} \right]$$

$$\xi_L = \left(\frac{(B+\mu)\tau}{\rho}\right)^{1/2} \Leftarrow$$

longitudinal length scale squared

transverse length scale squared

B and μ come from isotropic continuum linear elasticity

bulk modulus

shear modulus

$$\nabla\sigma = f = \zeta\dot{u} = B\nabla(\nabla\cdot u) + \mu\Delta u$$

overdamped dynamics

So note that the correlation length in both transverse + longitudinal directions scales as $\xi_L \sim \xi_T \sim \tau^{1/2}$

Section 2: Fluid-like starting point:

Very briefly discuss work by Szamel + Flenner:

What about dense liquids where there is no elasticity or reference state?

same eqn:

$$\zeta\dot{\vec{r}}_i = -\nabla_i \sum_j V(r_{ij}) + \zeta v_0 \hat{n}_i$$

derive an expression relating velocity polarization + force fields:

(6) $$\rho\, \vec{v}(\vec{q},t) = \sum_j \sum_{k\neq j} \vec{F}_{jk}\, e^{-i\vec{q}\cdot\vec{r}} + \rho v_0 \hat{n}(q,t)$$

where $$\vec{v}(\vec{q},t) = \sum_j \dot{\vec{r}}_j\, e^{-i\vec{q}\cdot r_j(t)}$$

$$\hat{n}(q,t) = \sum_j \hat{n}_j\, e^{-i\vec{q}\cdot r_j(t)}$$

Trick; one can show the first term on RHS of (6) can be written so that it looks like the interaction part of the pressure tensor (fourier transform)

$$\underbrace{i\vec{q}\cdot \sum_j \sum_{k\neq j} \vec{r}_{jk} \frac{\vec{r}_{jk}}{\partial r_{jk}} V'(r_{jk}) \left[\frac{e^{i\vec{q}\cdot\vec{r}} - 1}{i\vec{q}\cdot\vec{r}}\right] e^{-i\vec{q}\cdot\vec{r}}}_{-i\vec{q}\cdot \Pi_v(\vec{q},t)}$$

Assume a virial expansion of Π in terms of ρ

$$\Pi_v(\vec{r},t) = \underset{\substack{\uparrow \\ \text{steady state} \\ \text{pressure} \\ \Downarrow \\ \text{math}}}{P_v} + \frac{\partial P_v}{\partial \rho}\left(\rho(r,t) - \underset{\substack{\nearrow \\ \text{steady state avg density}}}{\rho}\right)$$

$$\langle |\hat{q}\cdot v(q)|^2 \rangle = \frac{N v_0^2}{2} \frac{1}{1 + \frac{q^2 \tau B_v}{\rho}} \Rightarrow \xi_L = \sqrt{\frac{\tau B_v}{\rho}}$$

Appendix note that the two point correlation fn for weights η is:

$$\langle \eta_\nu(t)\, \eta_{\nu'}(t') \rangle = \frac{1}{2} \langle \cos[\phi(t) - \phi(t')] \rangle$$

dot product is just cos difference b/w angles for unit vectors

recall $\dot{\phi} = \eta \qquad \langle \eta(t)\, \eta(t') \rangle = \frac{2}{\tau} \delta(t-t')$

$$\Rightarrow \phi(t) = \int_0^t \eta(t')\, dt'$$

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

(5) $$\langle \cos[\phi(t) - \phi(t')] \rangle = \left\langle \frac{1}{2}\left(e^{i(\phi(t) - \phi(t'))} + e^{-i(\phi(t) - \phi(t'))}\right) \right\rangle$$

If θ is Gaussian, use cumulant expansion:

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

$$= \frac{1}{2}\left(e^{-\frac{\langle [\phi(t) - \phi(t')]^2 \rangle}{2}} + e^{-\frac{\langle [\phi(t') - \phi(t)]^2 \rangle}{2}}\right)$$

$$\langle [\phi(t) - \phi(t')]^2 \rangle = \langle \underbrace{\phi(t)^2}_{1} - \underbrace{2\phi_t \phi_{t'}}_{2} + \underbrace{\phi(t')^2}_{3} \rangle$$

1 $$\int_0^t \int_0^{t'} \underbrace{\langle \eta(\tilde{t})\, \eta(\tilde{t}') \rangle}_{\frac{2}{\tau}\underbrace{\int_0^{t'} \delta(\tilde{t} - \tilde{t}')\, d\tilde{t}'}_{1}} d\tilde{t}\, d\tilde{t}' = \int_0^t \frac{2}{\tau}\, d\tilde{t} = \frac{2t}{\tau}$$

(2) $$\phi(t)\phi(t') = \int_0^t \int_0^{t'} \underbrace{\langle \eta(\tilde{t})\eta(\tilde{t}')\rangle}_{\delta(\tilde{t}-\tilde{t}')} d\tilde{t}\, d\tilde{t}' =$$

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

$$= \frac{2}{\tau}\min(t, t')$$

Assume time translation invariance, so WLOG $t' = 0$

then (5) $$= \frac{1}{2}\left(e^{-\frac{\langle \phi^2(t)\rangle}{2}} \left[e^{\frac{2\langle \phi(t)\phi(t')\rangle}{2}} + e^{\frac{2\langle \phi(t')\phi(t)\rangle}{2}} \right] \right)$$

$$= e^{-\frac{\langle \phi^2(t)\rangle}{2}} e^{\frac{2\langle \phi(t)\phi(t')\rangle}{2}}$$

$$= e^{t/\tau} e^{-\frac{2}{\tau}\min(t,t')}$$

$$= \begin{cases} e^{-t/\tau - 0} & t > 0 \\ e^{-t/\tau + \frac{2t}{\tau}} & t < 0 \end{cases}$$

$$= e^{-|t|/\tau}$$. Phew!