Interactions II

$\Rightarrow$ steric metric interactions

Focus first on particles with spherical symmetry $\rightarrow$ no alignment

Self-propelled particle models:

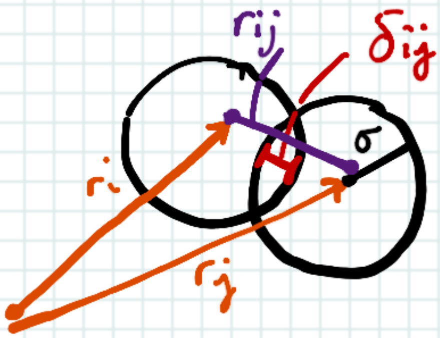
1. Interactions

$$V_{ij} = V(|\vec{r}_i - \vec{r}_j|) \equiv V(r_{ij})$$

Example: $V(r_{ij}) = 4\varepsilon\left[\left(\frac{\sigma}{r_{ij}}\right)^{12} - \left(\frac{\sigma}{r_{ij}}\right)^{6}\right]$ why?

-OR-

$V(r_{ij}) \sim \tilde{\epsilon}\,(\delta_{ij})^{\alpha}$ for $\delta_{ij} > 0$ $\quad \begin{cases} \alpha = 2 & \text{harmonic} \\ \alpha = 5/2 & \text{hertzian} \end{cases}$



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

2. Activity: Recall

$$\underbrace{\cancel{m\frac{dv_i}{dt}}}_{0} = \underbrace{\cancel{F_{int}}}_{\sum_j -\frac{\partial V(r_{ij})}{\partial r_i}} + \underbrace{\cancel{F_{propelled}}}_{F_0 \hat{n}_i} + \underbrace{\cancel{F_{drag}}}_{-\zeta v_i} + \underbrace{\cancel{F_{noise}}}_{0}$$

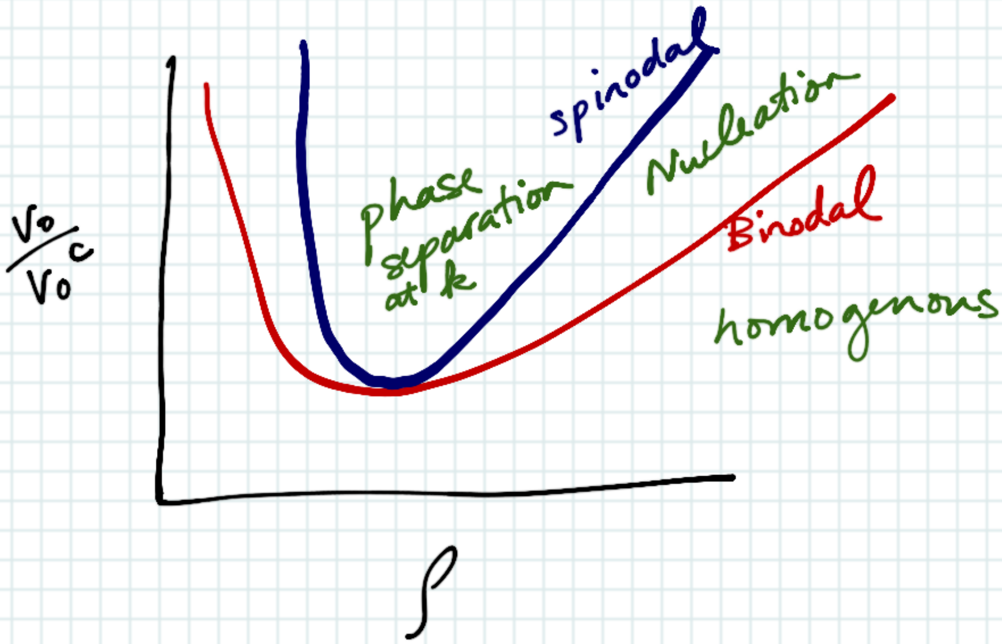
"over damped limit" inertial effects negligible compared to drag

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

$$\boxed{\dot{r}_i = v_0 \hat{n} - \mu \sum_j \nabla_i V(r_{ij})}$$

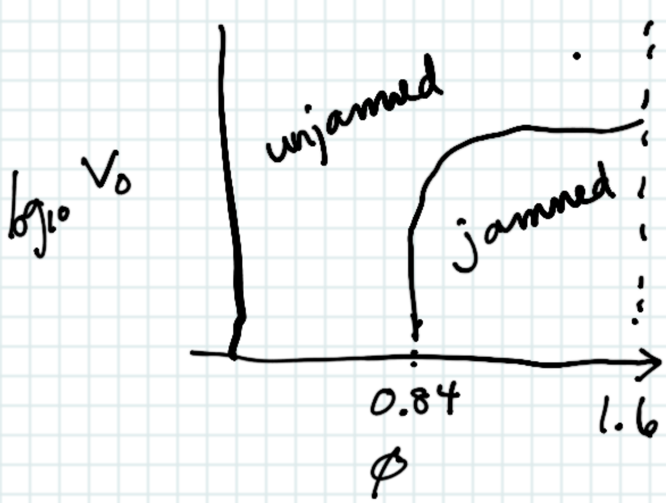
3. Lots of interesting stuff happens in these models.
Focus on two transitions:

⇒ Motility Induced Phase separation
Cates and Tailleur. ARCMP 6 219 (2015)



⇒ Glassy dynamics

2D { Henkes et al PRE 84 (2011)
Berthier PRL 112 (2014)



Control parameters:

V_0 (energy scale)

$$\phi = \sum_i \frac{\pi \sigma_i^2}{R^2}$$

packing fraction

box area

repulsive disk area

What about D_r (rotational diffusion)?

Motility - induced phase separation:

① intuitive mechanism

these particles
stick together for a time, ~ persistence time
of self-propulsion

at higher densities more collisions
are possible

but competing effect: lots of collisions reorient
particle velocities

Expect: higher Pe always enhances effect;
but there is a sweet spot in ρ where MIPS

② Hydrodynamic model for isotropic state at intermediate densities

→ no interactions b/w spins, just steric 

→ what is left from our old hydrodynamic theory?

no $\nabla\cdot\vec{P}$, $|\vec{P}|^2$, $(\vec{v}\cdot\vec{\nabla})\vec{P}$

still can have $\nabla\rho$, $\vec{P}$

→ new ingredient: each particle has a velocity
$v \neq v_0$ that depends on interactions with local
environment: $v(\rho)$

Then we have:

continuity

(1) $\partial_t \rho = -\nabla \cdot [v(\rho)\vec{p}]$

pressure-like term

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

Simplest assumption for $v(\rho)$ is an expansion in density, also matches simulation data

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

For timescales $t \gg \frac{1}{D_r}$ (2) $\Rightarrow$ $\vec{p} = -\frac{1}{2D_r}\nabla[v(\rho)\rho]$

$$\partial_t \rho = +\nabla \cdot \Big[\underbrace{\frac{(v(\rho))^2 + \rho\, v(\rho)\, v'(\rho)}{2D_r}}_{\mathcal{D}(\rho)} \nabla\rho \Big]$$

effective mean field dynamics:

homogenous for $\mathcal{D}(\rho) > 0$

Note: $v'(\rho) \equiv \frac{\partial v}{\partial \rho} < 0$

so $\mathcal{D}(\rho)$ changes sign

when $v(\rho) < -\rho\, v'(\rho)$

e.g at high densities

spinodal decomposition

$\mathcal{D}(\rho) < 0$

to go further, it would be nice to have an expression for

thermodynamic properties: pressure, chem potential with ρ

c.f. Takatori + Brady PRE 2015 → Caution Pe defined weirdly by Brady.
(also Yang, Manning, Marchetti (2014))
Yang . . . PNAS 2017

A. There are two contributions to the pressure in an active "swim" pressure that describes the flux of propulsive force $\frac{v_0}{\mu}\hat{n}_i$ across a boundary.

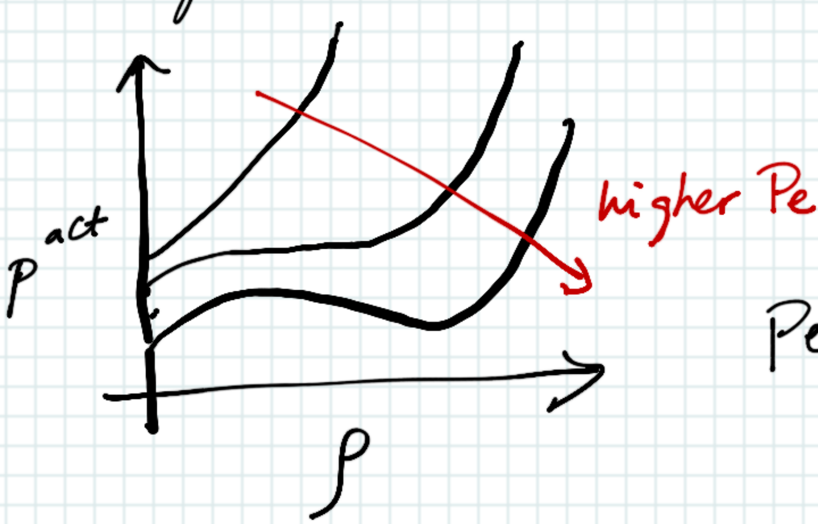
$$\sigma^{i\,(swim)}_{\alpha\beta} = \frac{-v_0}{\mu A_i} n^i_\alpha r^i_\beta$$

+ interaction pressure due to forces generated by interactions between particles (in 2D):

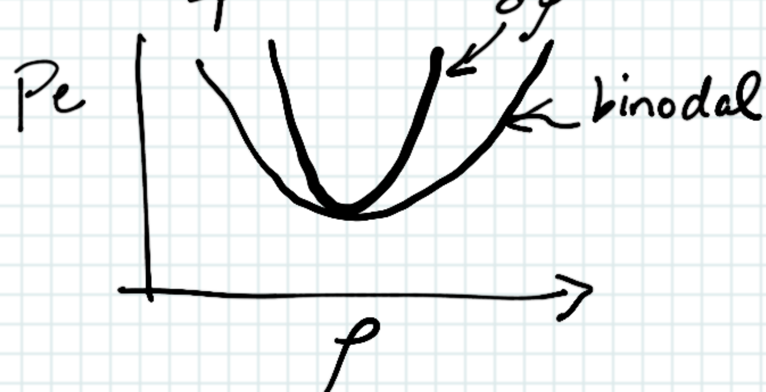
$$\sigma^{i\,(int)}_{\alpha\beta} = \frac{1}{2}\sum_{j\neq i} f_{ij}\, r_{ij}\, \frac{x_{ij}\, y_{ij}}{r_{ij}^{\,2}}$$

total pressure p^{act} is trace over sum of swim + interaction pressures

$$Pe = \frac{v_0}{2 R D_r}$$

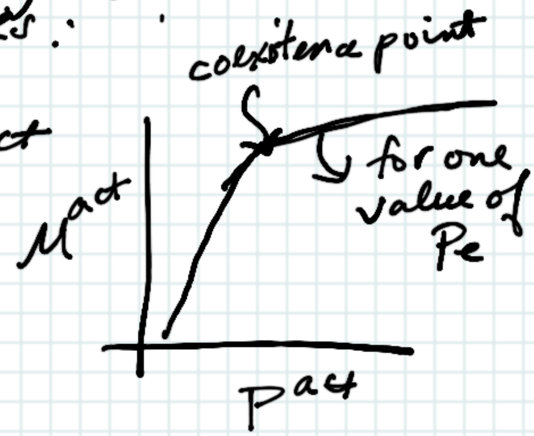


spinodal: $\frac{\partial p^{act}}{\partial \rho} = 0$



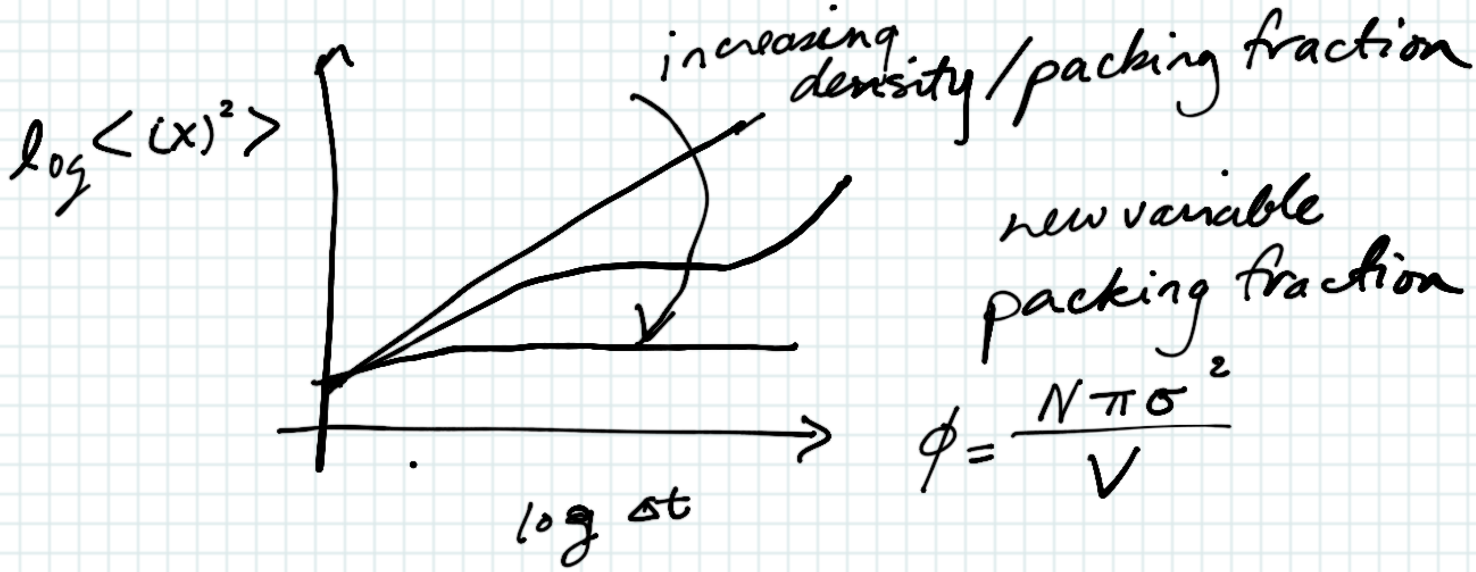
binodal: nucleating region, equality of chemical potential in dense + dilute phases:

$$n\left(\frac{\partial \mu^{act}}{\partial n}\right) = (1-\rho)\frac{\partial P^{act}}{\partial n} \Rightarrow \mu^{act}$$



That was for <u>intermediate</u> densities.

at high densities $v(\rho) \neq v_0(1-\lambda\rho)$ and instead, the dynamics becomes solid-like, in the sense that particles don't change their neighbors and get stuck in a "cage".

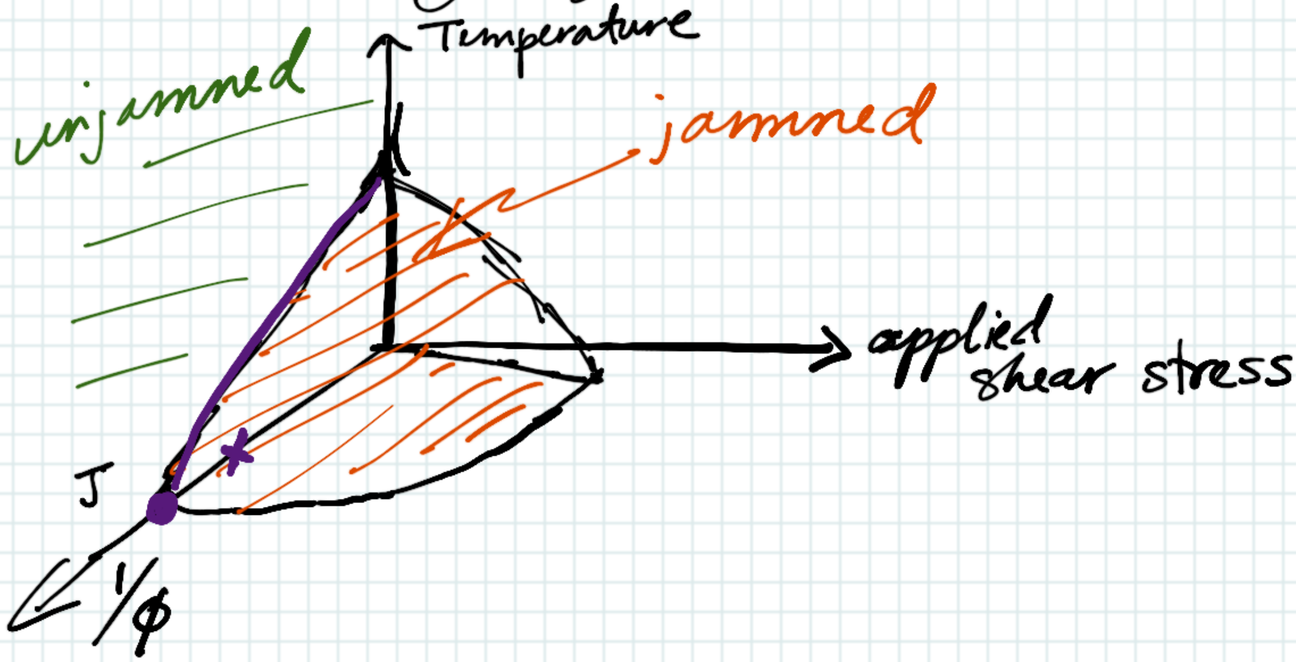


new variable packing fraction

$$\phi = \frac{N\pi\sigma^2}{V}$$

At high densities, then, much of the physics can be understood by using tools developed for non-active glassy or jammed systems

Completely uncomprehensive tutorial on physics of jamming & glasses:



Jamming transition:
- rigidity transition that occurs at zero temperature in disordered packings of soft, repulsive spheres
- occurs at critical packing fraction ϕ_J.

  $\phi < \phi_J$: no contacting particles

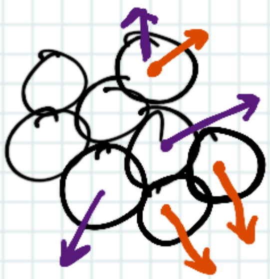
  $\phi = \phi_J$: system is <u>isostatic</u>

  # of DOF : DN

  # of constraints : $z/2 N$

  $\Rightarrow z_c = 2D$
- very unusual vibrational properties

In linear response



$$u = \begin{bmatrix} u_{1x} \\ u_{1y} \\ u_{2x} \\ u_{2y} \\ \vdots \end{bmatrix}$$

imposed displacements
$Nd \times 1$

$$f = \begin{bmatrix} f_{1x} \\ f_{1y} \\ f_{2x} \\ f_{2y} \\ \vdots \end{bmatrix}$$

restoring forces
$Nd \times 1$

Define Dynamical Matrix as :

$$f = \mathcal{M} u$$

for crystal, symmetries allow $\mathcal{M}$ to be small

for disordered solid
$\mathcal{M} = Nd \times Nd$

for systems with two-body interactions
can show

$$\mathcal{M}_{i\alpha j\beta} = \frac{\partial^2 V(|r_i - r_j|)}{\partial r_{i\alpha} \partial r_{j\beta}} \quad i \neq j$$

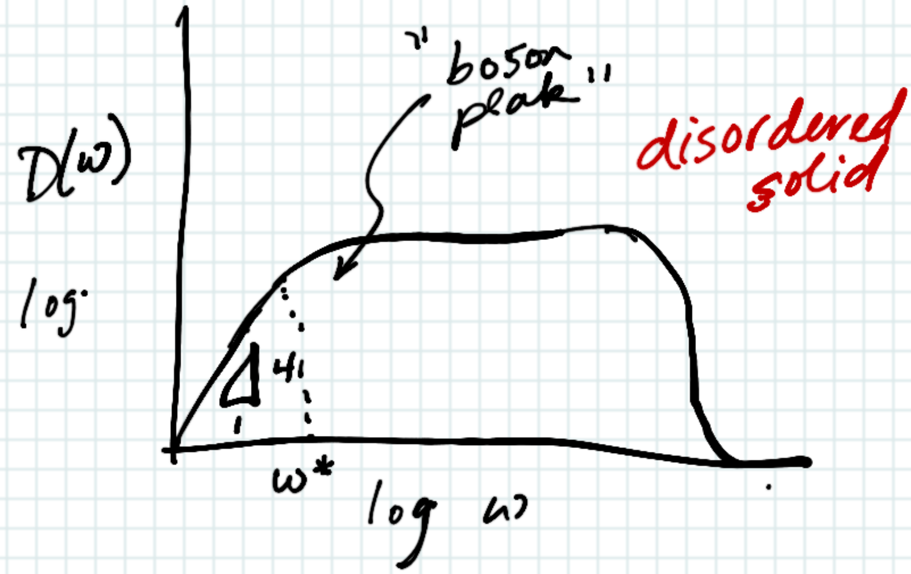
and

$$\mathcal{M}_{i\alpha i\beta} = -\sum_j \frac{\partial^2 V(|r_i - r_j|)}{\partial r_{i\alpha} \partial r_{j\beta}}$$

Note: looks a lot like random graph laplacian
you saw yesterday from Eleni

eigen modes
and eigenvectors
have interesting,
universal properties

$\omega^2 = \lambda$.

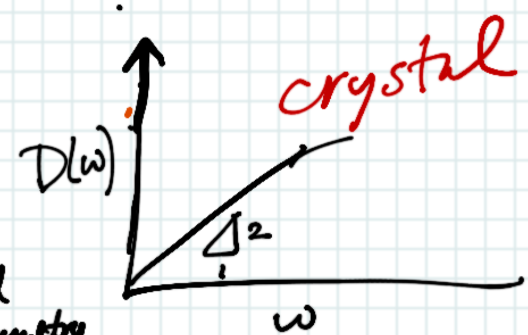


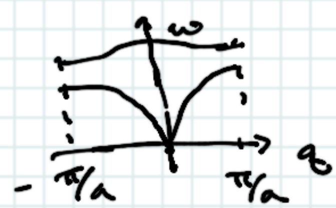
Recall for crystals

$D(\omega) \sim \omega^{d-1}$

because $\omega \sim cq$

Goldstone mode associated with broken translational symmetry





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boson peak modes are disordered, spatially extended.

localized exctions at very low frequencies.

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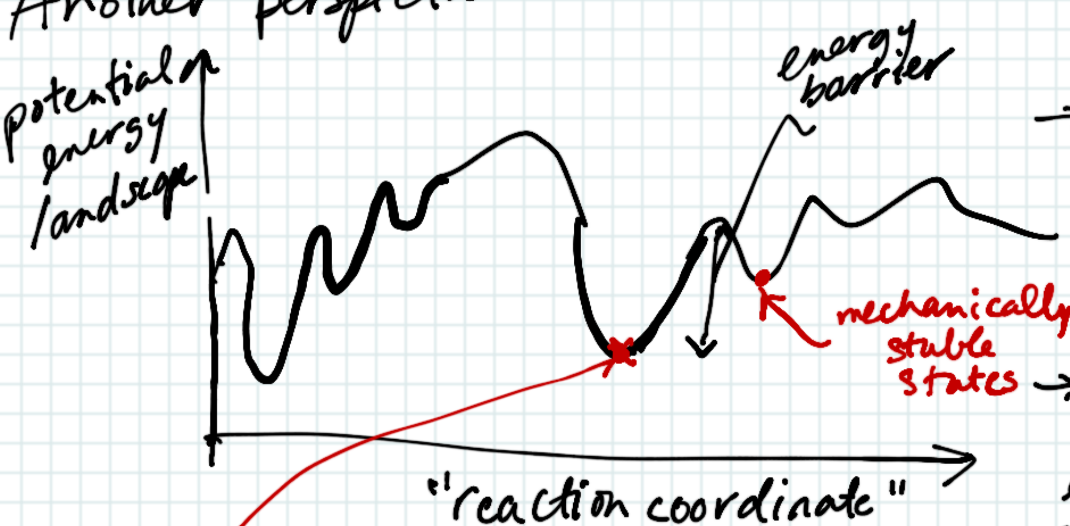
but really, this in an Nd dimensional space.

Another perspective:



→ eigen values describe these curvatures around the minima

→ low frequency excitations are excited in presence of fluctuations

↳ if this was eignvector then curvature would be λ

→ may also be directions of small energy barriers

Recent discovery: Zamponi + collaborators

energy landscape for jammed packings is fractal $\Rightarrow$

a "Gardner" phase, and scaling relations computed analytically using Replica Symmetry Breaking

Glass physics: how are systems trapped in metastable minima in presence of finite temperature fluctuations?

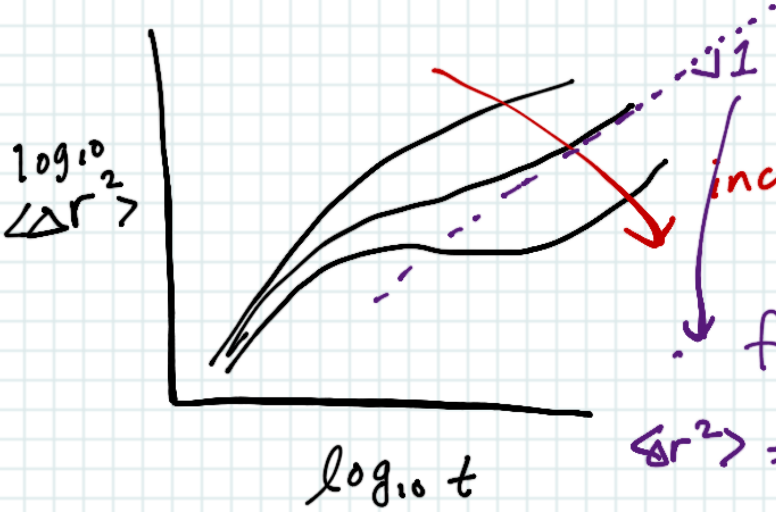
<u>Lots</u> of ways to look for glass transitions in biological systems

MSD:

χ_4: dynamical heterogeneities

$\chi_4(r-r'; t-t') = \langle \rho(r',t')\rho(r',t)\rho(r,t')\rho(r,t) \rangle$

slides:



$\tau \sim \frac{1}{D_r}$

fit the long-time behavior to

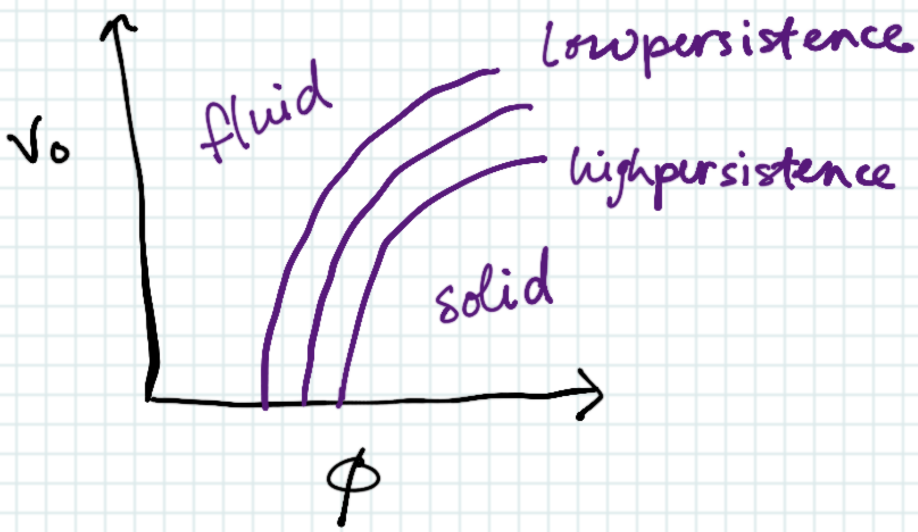
$$\langle\Delta r^2\rangle = 4 D_s(\tau,\phi)\, t$$

long-time diffusion of particle.

Ansatz: $D_s(\tau,\phi) = |\phi_c(\tau) - \phi|^{\gamma(\tau)}$

This is a huge effect!

$\Rightarrow$ ϕ_c changes as a function of $\tau \sim \frac{1}{D_r}$!



one can take a formerly solid state into a fluid state just by changing D_r.

Why are large D_r systems more fluidized?
still not completely clear.

Henkes, Fily, Marchetti PRE 84 2011
Bi, Yang, Marchetti, Manning PRX 2016

$\vec{d}_i(t) = \vec{r}_i - \vec{r}_{0i}$
inherent state

$$\vec{d}_i(t) = \sum_\nu a_\nu(t) \underbrace{\hat{e}_{i,\nu}}$$
eigenector (complete basis set)

or $|d\rangle = \sum_\nu a_\nu |\nu\rangle$ where $\overleftrightarrow{D}|\nu\rangle = \omega_\nu^2 |\nu\rangle$

$\hat{n}_i$ can also be expressed in basis of eigenvectors

$|n\rangle = \sum_\nu b_\nu |\nu\rangle$

eigenvector angle

polarization angle

write $b_\nu = \langle n|\nu\rangle = \cos(\theta_\nu - \Psi)$ b/c $n + \nu$ both unit vectors

then EOM for SPP becomes

$$\dot{\vec{d}} = -\mu \left.\frac{\partial E}{\partial \vec{r}_i}\right|_{\vec{r}_{0i}} + v_0 \hat{n}_i \qquad \frac{\partial E}{\partial \vec{r}_i} = \hat{D}|d\rangle$$
linear response

$$\frac{d}{dt}\langle\nu|d\rangle = -\mu \langle\nu|\hat{D}|d\rangle + v_0 \langle\nu|n\rangle$$

$$\frac{d}{dt} a_\nu(t) = -\mu \omega_\nu^2 a_\nu(t) + v_0 b_\nu(t)$$

So $\frac{d}{dt} a_\nu(t) = -\mu \omega_\nu^2 a_\nu(t) + v_0 \cos(\theta_\nu - \psi)$

$\dot{\psi} = \eta$: SPP tethered to a spring

solution:

$$\langle a_\nu(t) \rangle = a_\nu(t=0) e^{-kt} + v_0 \int_0^t dt' e^{-\overset{\mu\omega_\nu^2}{k}(t-t')} \langle \cos(\theta_\nu - \psi) \rangle$$

average over noise

some details

$$\left[\begin{array}{l} \langle \cos\psi \rangle = \cos\psi(0) e^{-D_r t} \\ \langle \sin\psi \rangle = \sin\psi(0) e^{-D_r t} \\ \cos(\theta_\nu - \psi) = \sin(\theta_\nu) \sin\psi + \cos\theta_\nu \cos\psi \end{array}\right]$$

$$\Rightarrow \langle a_\nu(t) \rangle = a_\nu(0) e^{-kt} + v_0 \cos(\theta_\nu - \psi(0)) \frac{e^{-kt} - e^{-D_r t}}{D_r - k}$$

in limit $D_r \to \infty$ $\langle a_\nu(t) \rangle = a_\nu(0) e^{-kt}$ boring

in limit $D_r \to 0$

$$\langle a_\nu(t) \rangle = a_\nu(0) e^{-\mu\omega_\nu t} + \frac{v_0 \cos(\theta_\nu - \psi)}{\mu\omega_\nu^2}(1 - e^{-\mu\omega_\nu^2 t})$$

so instantaneous response

$\langle a_\nu(0) \rangle \sim a_\nu(0) + \frac{1}{\omega_\nu^2} \Rightarrow$ a_ν is much larger for modes of lower frequencies

?? if lower frequency modes also have lower energy barriers, then this could explain fluidization