Yukawa Institute for Theoretical Physics, Kyoto University, Japan
Physics of Jammed Matter
October 27th (Sat.), 2018
10:30-11:10, 30mins. talk and 10mins. discussion

Vibrational properties of nearly jammed amorphous solids

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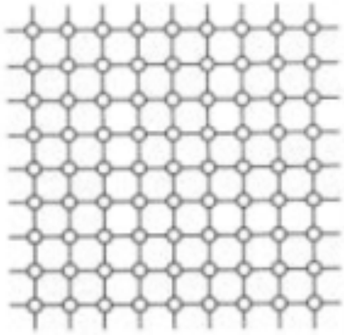
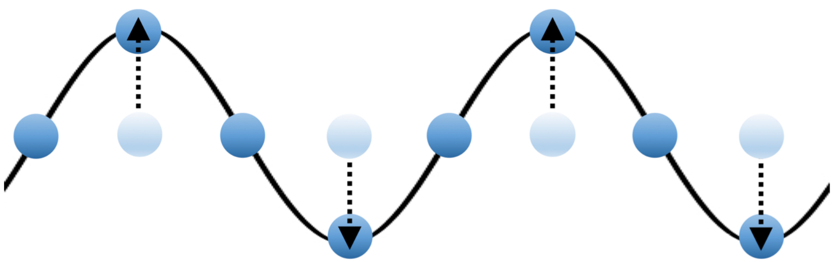
M. Shimada, H. Mizuno, A. Ikeda, M. Wyart, arXiv:1804.08865

Background: Vibrational modes in crystals and amorphous solids

Crystals (lattice structure)

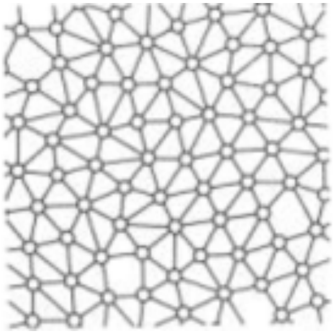


Molecules vibrate around lattice structure

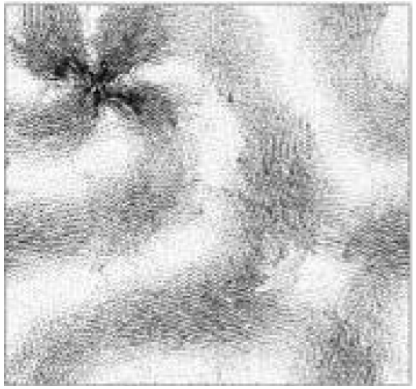


Vibrational modes are phonons

Amorphous solids (amorphous structure)



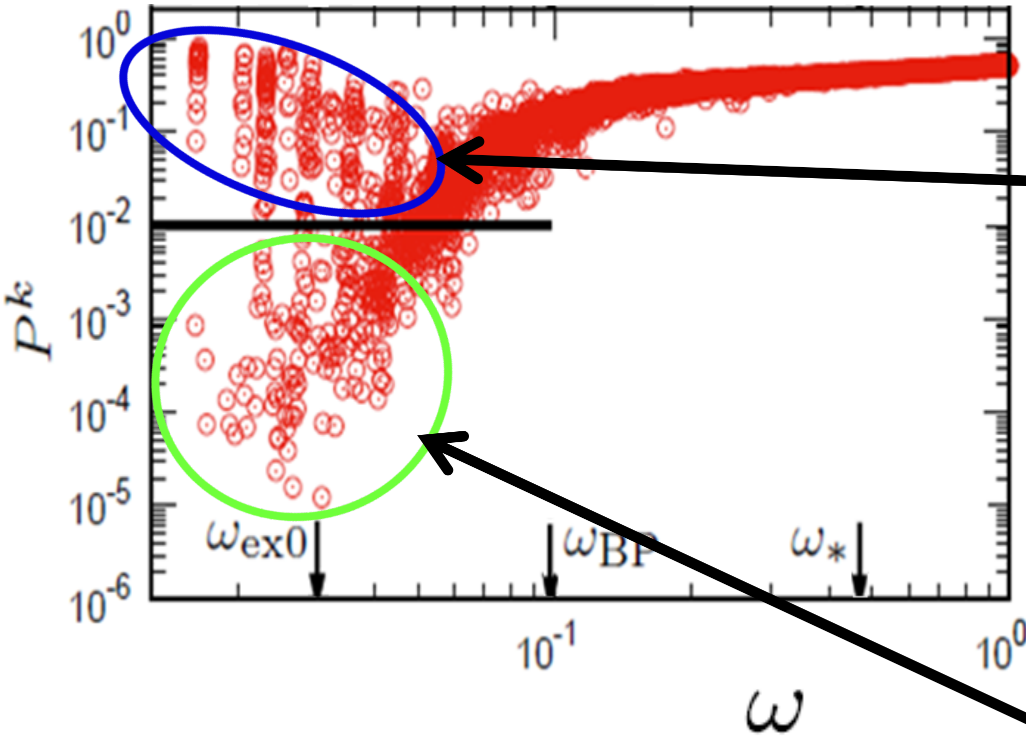
Molecules vibrate around amorphous structure



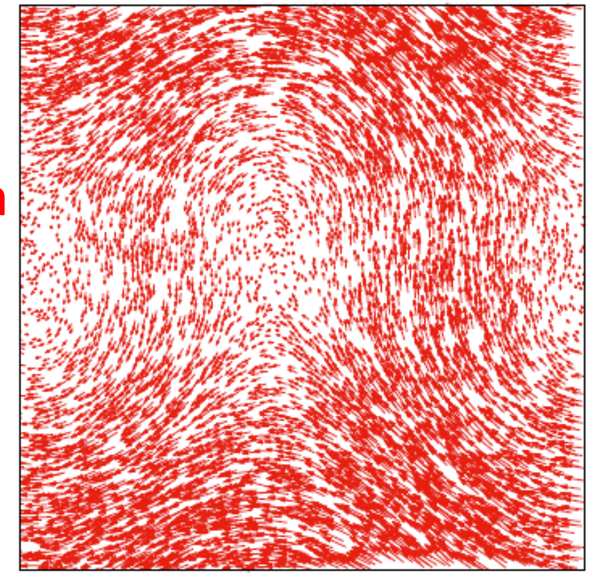
Tanguy et al., EPL 2010

Some modes are spatially heterogeneous
-> These modes are non-phonons

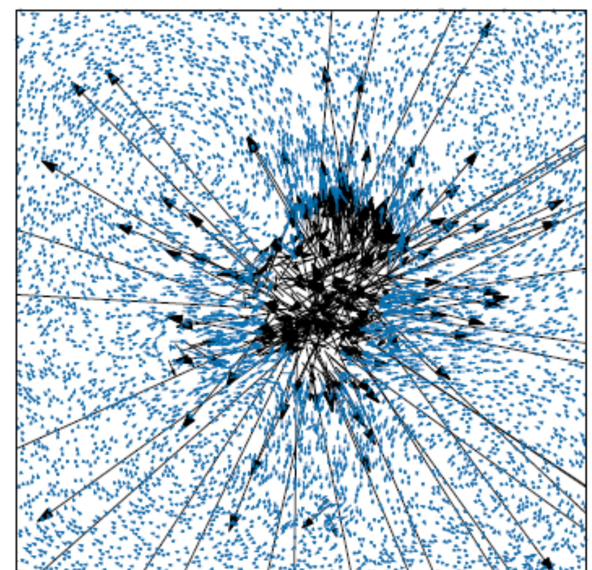
Background:
Phonons and localized modes in amorphous solids



Phonon modes



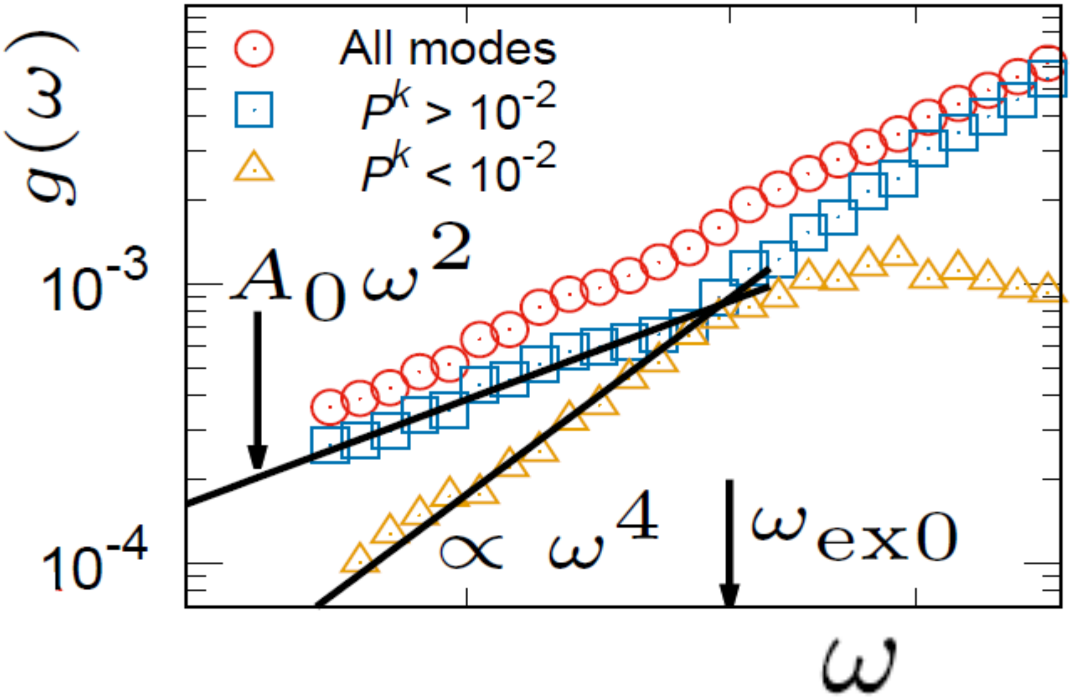
Localized modes



Phonon modes and localized modes coexist in the low-frequency regime

Mizuno, Shiba, Ikeda, PNAS (2017), Shimada, Mizuno, Ikeda, PRE (2018)

Background: Phonons and localized modes in amorphous solids



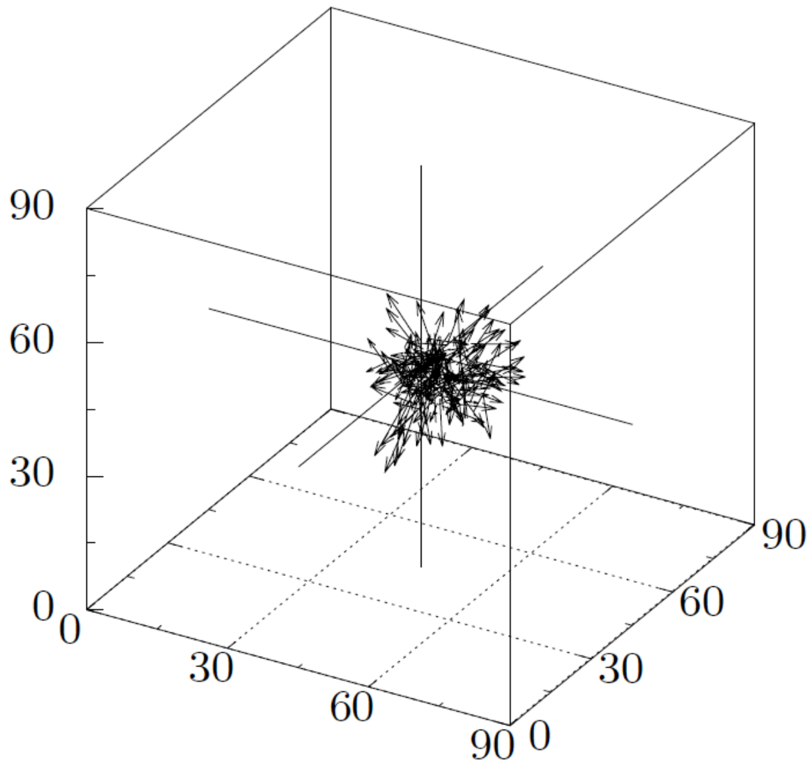
Mizuno, Shiba, Ikeda, PNAS (2017);
Shimada, Mizuno, Ikeda, PRE (2018)

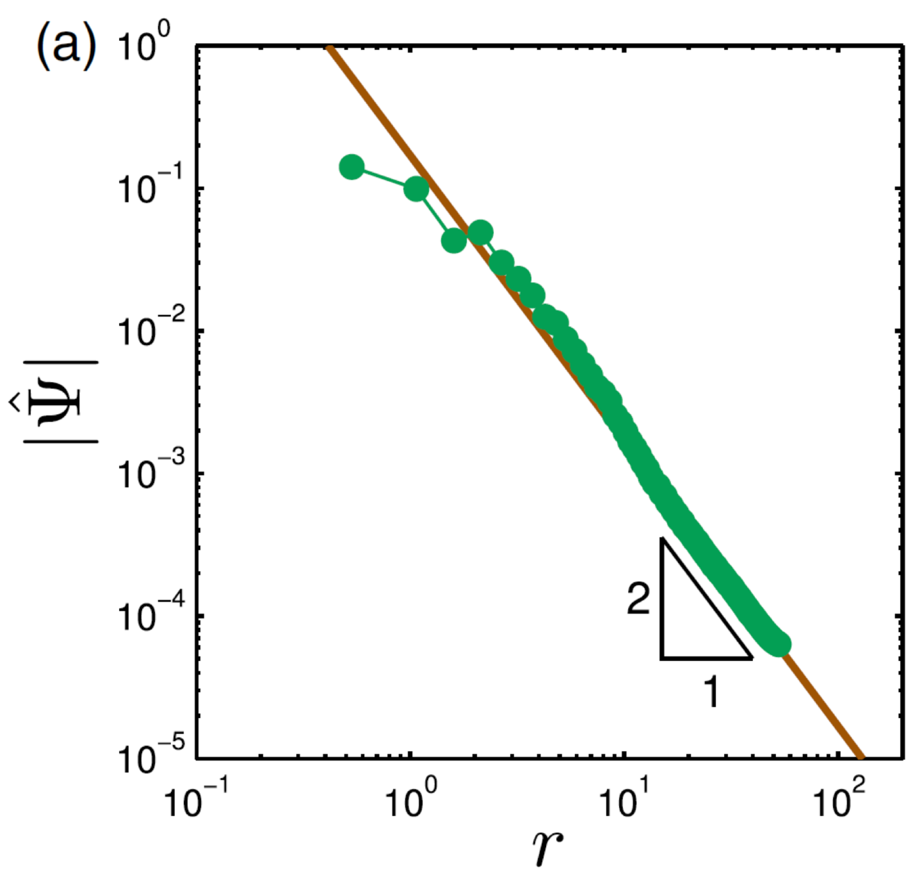
$$g(\omega) = \underbrace{g_{\rm ex}(\omega)}_{A_0\omega^2} + \underbrace{g_{\rm loc}(\omega)}_{\propto\, \omega^4}$$

Debye law of phonon modes

Non-Debye law of localized modes

Background: Localized modes show "quasi"-localized vibrations





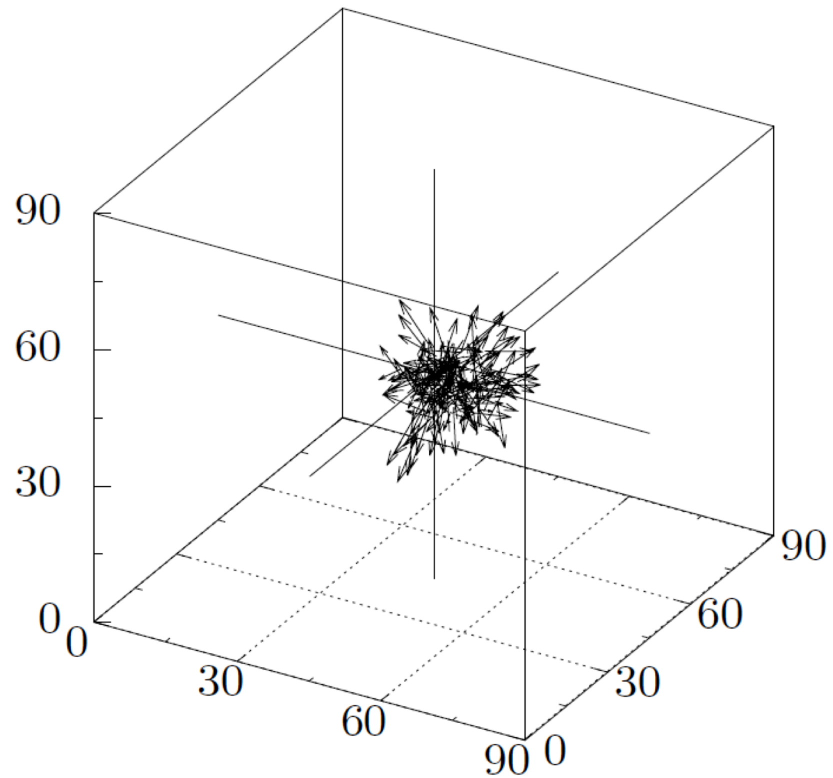
Vibrational amplitude decays with a power law

→ "Quasi"-localized vibrations

Lerner and Bouchbinder et al., PRL (2016)

Questions: Nature of localized modes

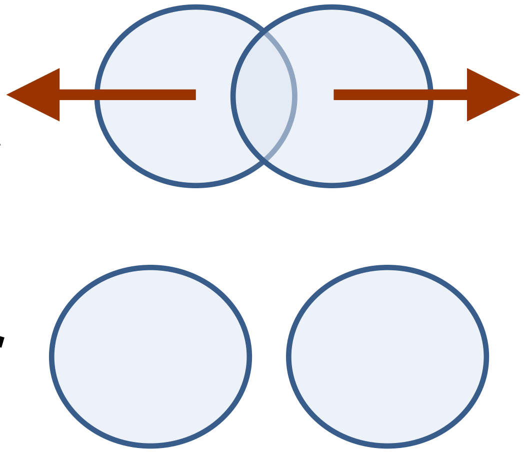
- How do particles vibrate in the core of localized modes?
- What is the size of the core?
- What is the origin?



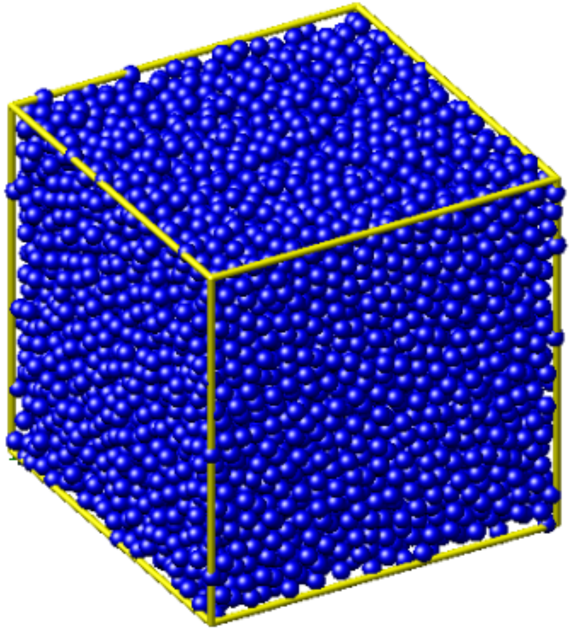
Simple model amorphous solid: Harmonic repulsive potential system

Finite-range, harmonic, repulsive potential

$$\phi(r_{ij}) = \begin{cases} \frac{\varepsilon}{2}\left(1 - \frac{r_{ij}}{\sigma}\right)^2 & (r_{ij} < \sigma) \\ 0 & (r_{ij} \geq \sigma) \end{cases}$$



Quench from liquid state to glass state at *T*=0

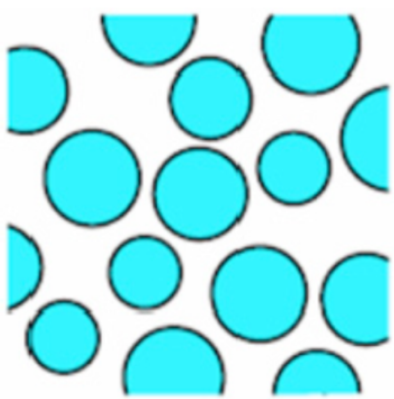


- This system models granular materials, emulsions, etc.
- But, we consider this system as the "simplest" model of glasses

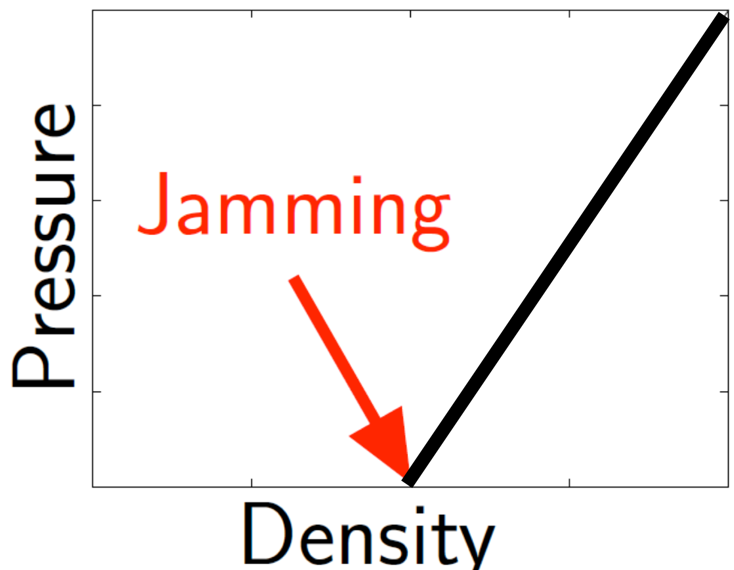
Wyart and co-workers, EPL 2005, PRE 2005, EPL 2010

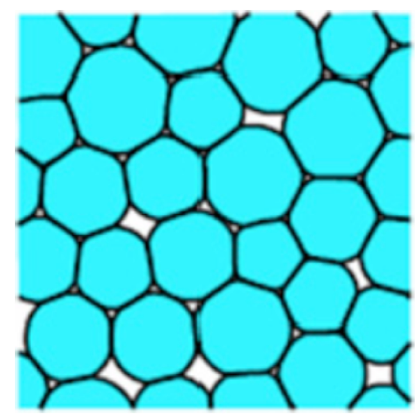
Simple model amorphous solid: Phase diagram

- Temperature is zero -> We study “harmonic” vibrations
- Control parameter is pressure P
- With lowering P, the system undergoes jamming transition
- $P > 0$ above jamming, while $P = 0$ below jamming



Fluid phase
Below jamming

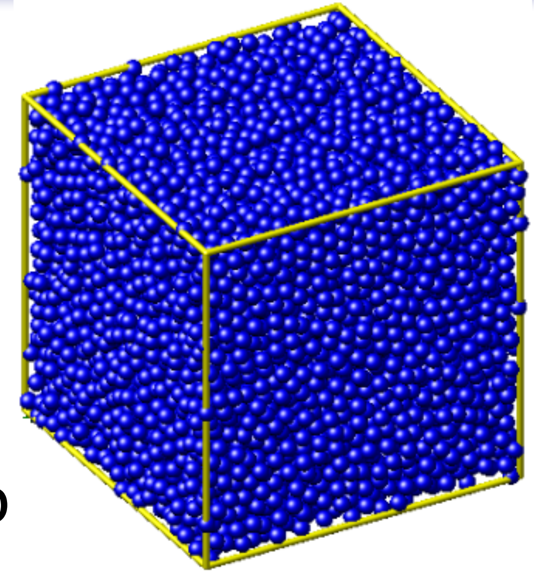




Solid phase
Above jamming

van Hecke, J.Phys.: Condens. Matter (2010)

Simple model amorphous solid: MD simulation and vibrational mode analysis



MD simulation

- Mono-disperse, 3D system
- N=1,000,000 particles
- P is from 0.05 to 0.001
- Quench liquid state configuration to zero temperature state, $T=0$, by FIRE algorithm

Vibrational mode analysis

- Diagonal Hessian matrix to obtain eigen-frequency ω^k and eigen-vector $\boldsymbol{e}^k$
- Analyze localized modes below the lowest phonon band

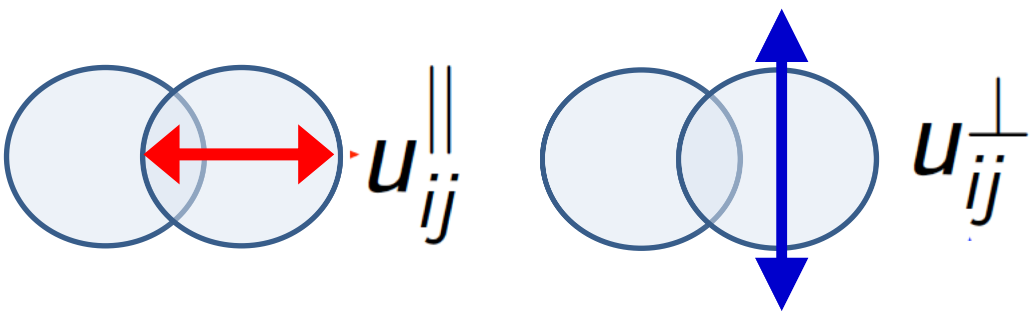
Vibrational energy of localized mode

For a vibrational mode $\mathbf{e}^k$ (an eigenvector), the energy between interacting particles *i* and *j* is given as

$$\delta E_{ij}^k = \left(u_{ij}^{\parallel}\right)^2 + \frac{-f_{ij}}{r_{ij}}\left(u_{ij}^{\perp}\right)^2$$

parallel perpendicular

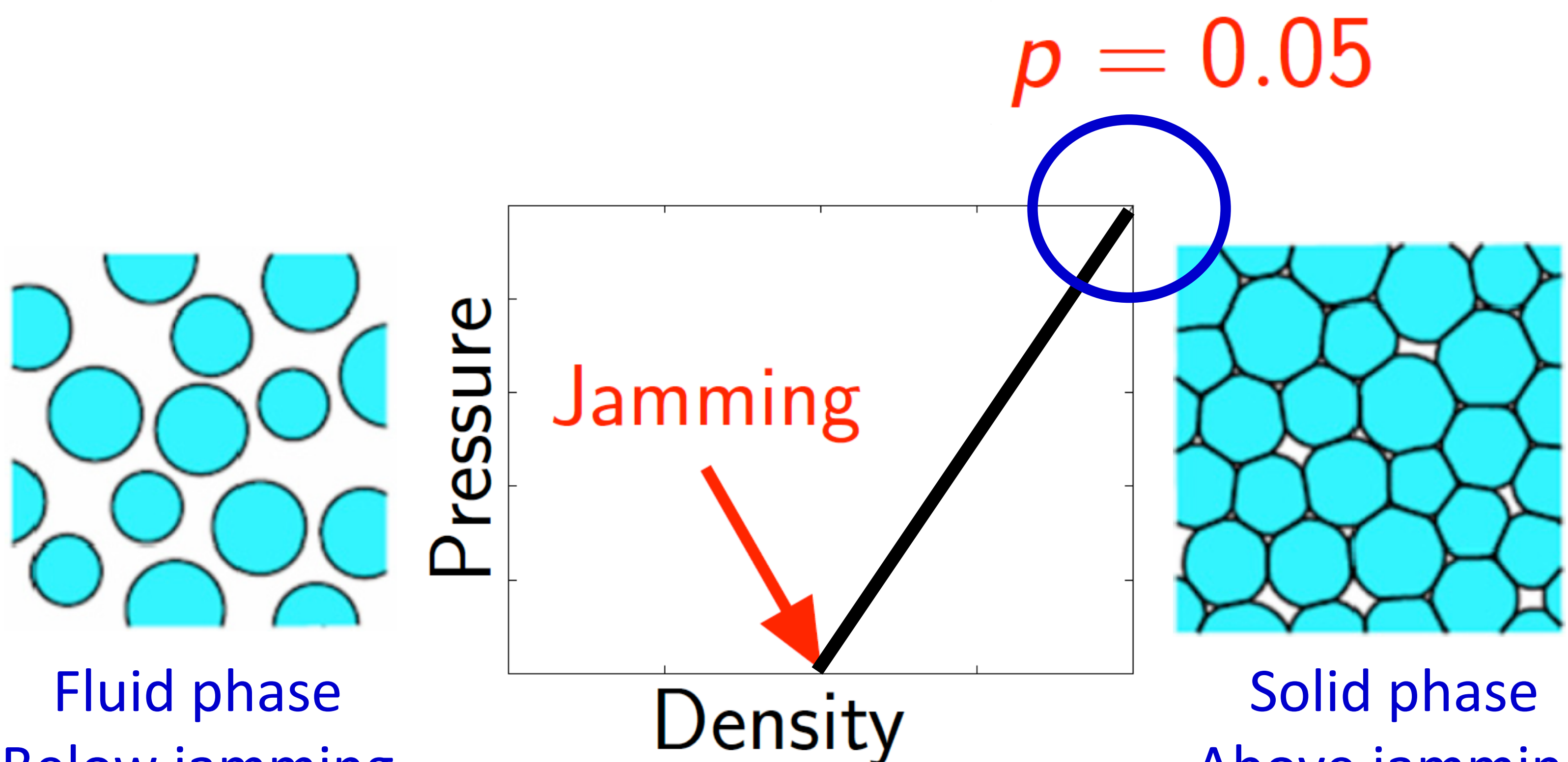
> 0 < 0



fij is force between particles *i* and *j* (*fij* >0 : repulsive)

DeGiuli et al., Soft matter 2014

Simulation results at ***P* = 0.05**



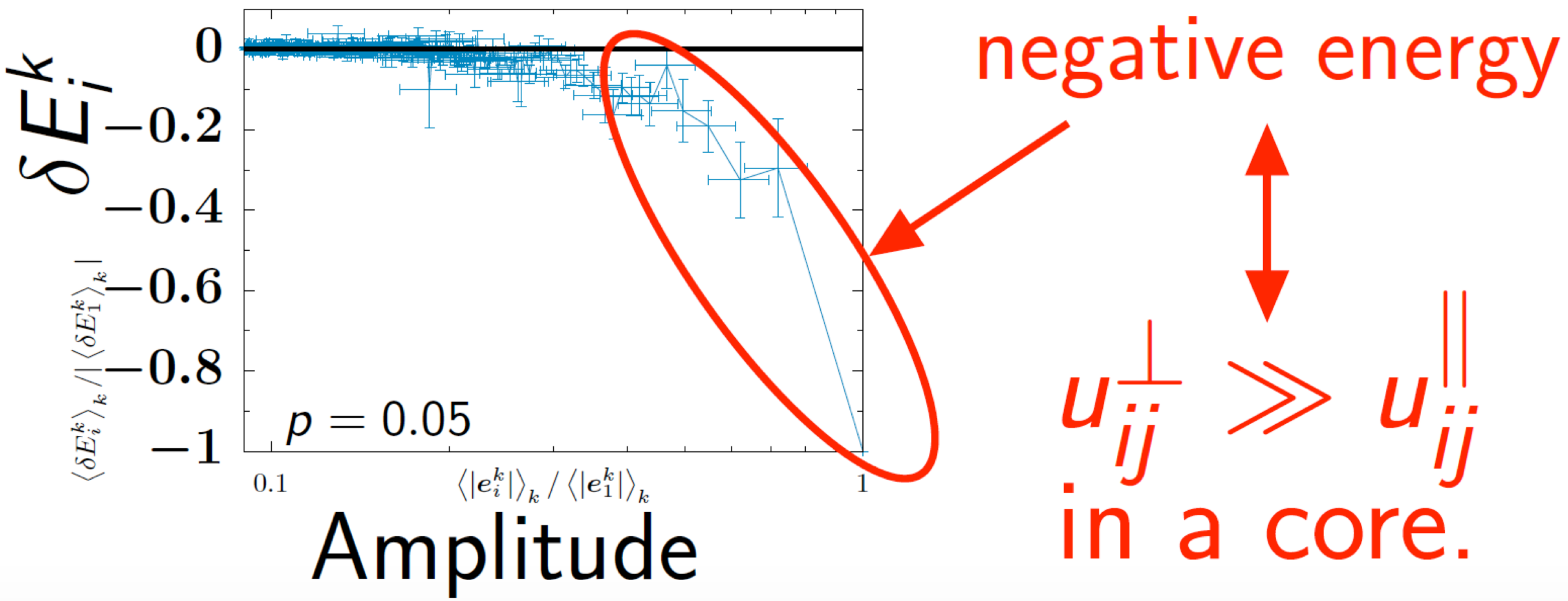
Fluid phase
Below jamming

Solid phase
Above jamming

van Hecke, J.Phys.: Condens. Matter (2010)

Simulation results at P = 0.05: Vibrational amplitude vs energy

Vibrational energy for particle i: $$\delta E_i^k = \frac{1}{2}\sum_{j\in\partial i}\delta E_{ij}^k.$$

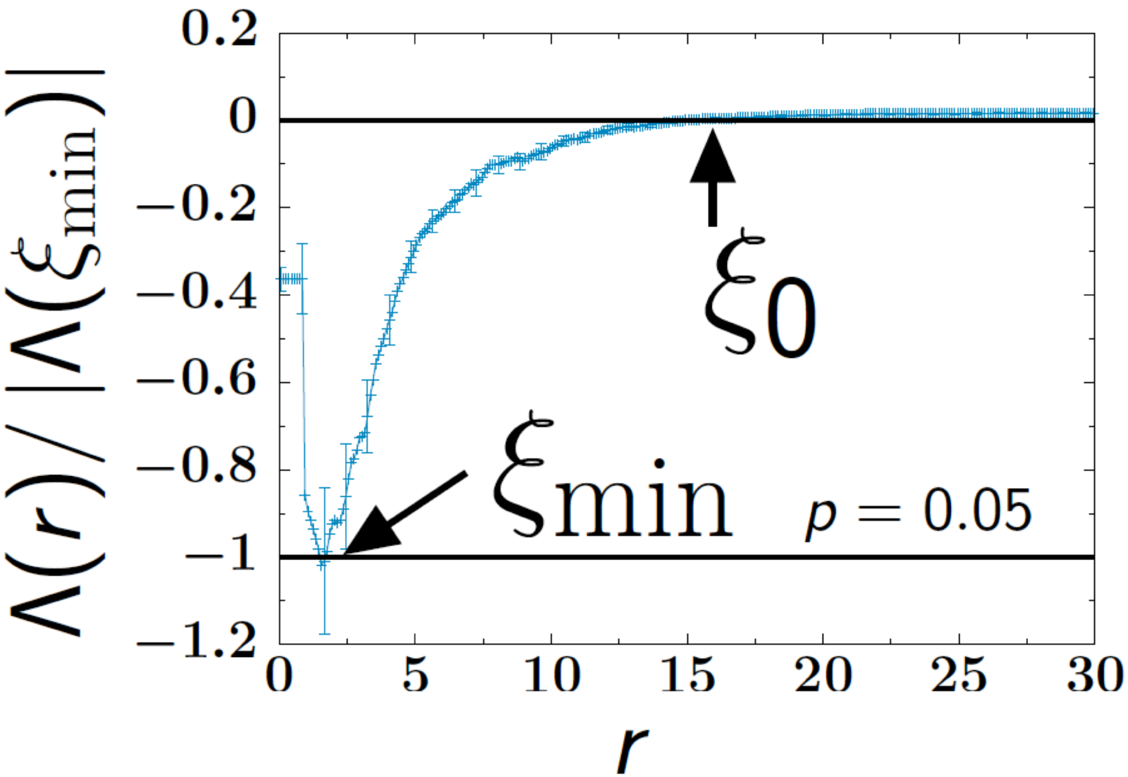


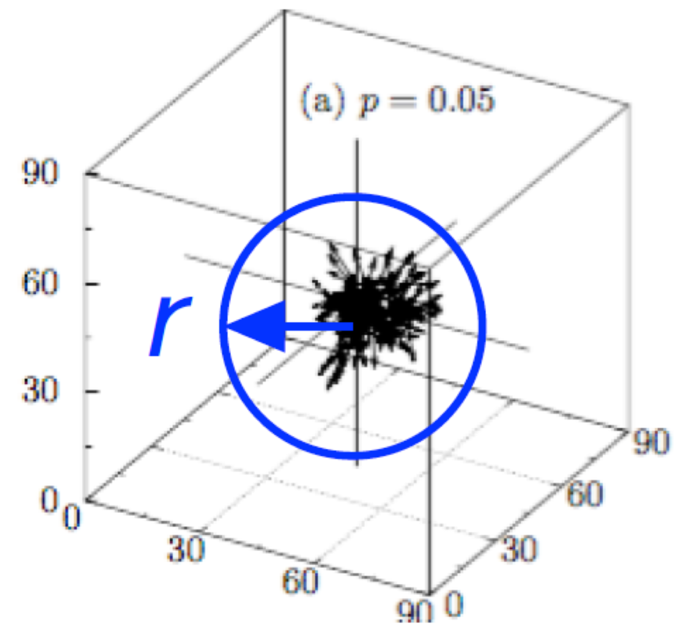
In the core, vibrational energy is negative

-> vibrational motions are unstable

Simulation results at *P* = 0.05: Integrated radial energy distribution function

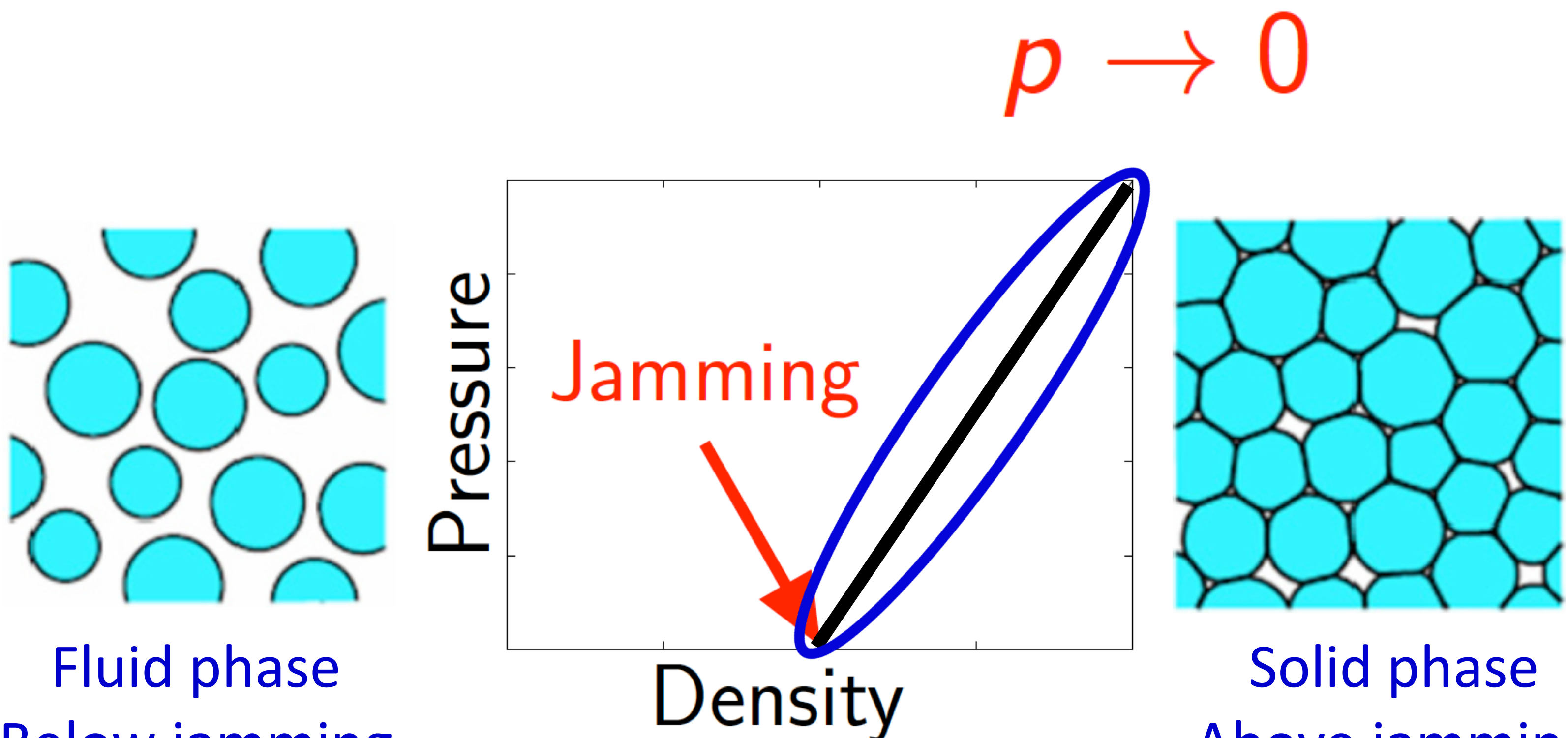
$$\Lambda(r) \equiv \left\langle \sum_{r_i \le r} \delta E_i^k \right\rangle_k .$$





Partial system is unstable up to $r \lesssim \xi_0$

Simulation results at ***P* -> 0** (approach to jamming)



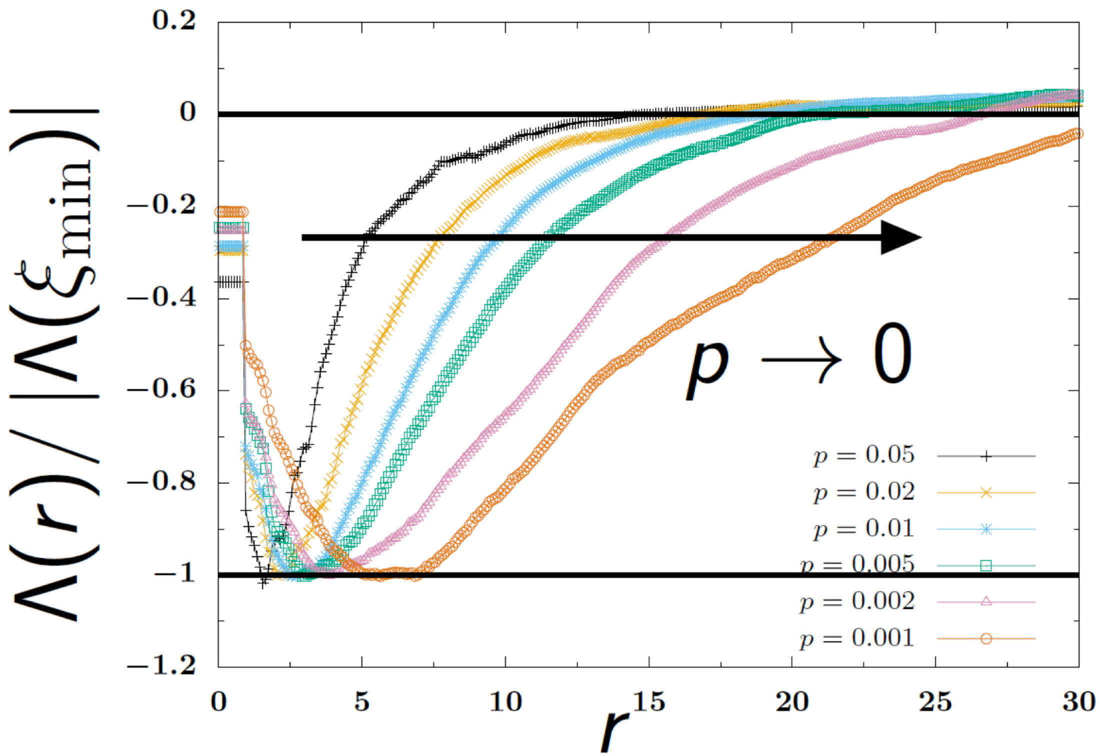
Fluid phase
Below jamming

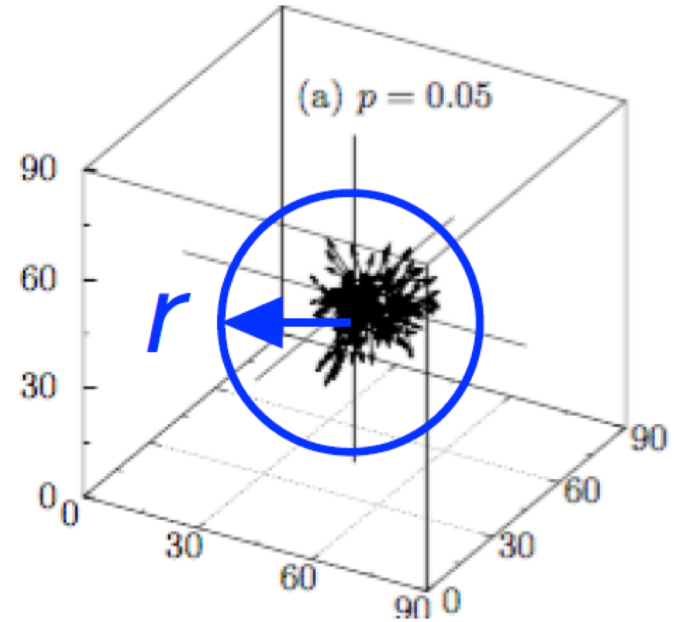
Solid phase
Above jamming

van Hecke, J.Phys.: Condens. Matter (2010)

Simulation results at *P* -> 0 (approach to jamming): Integrated radial energy distribution function

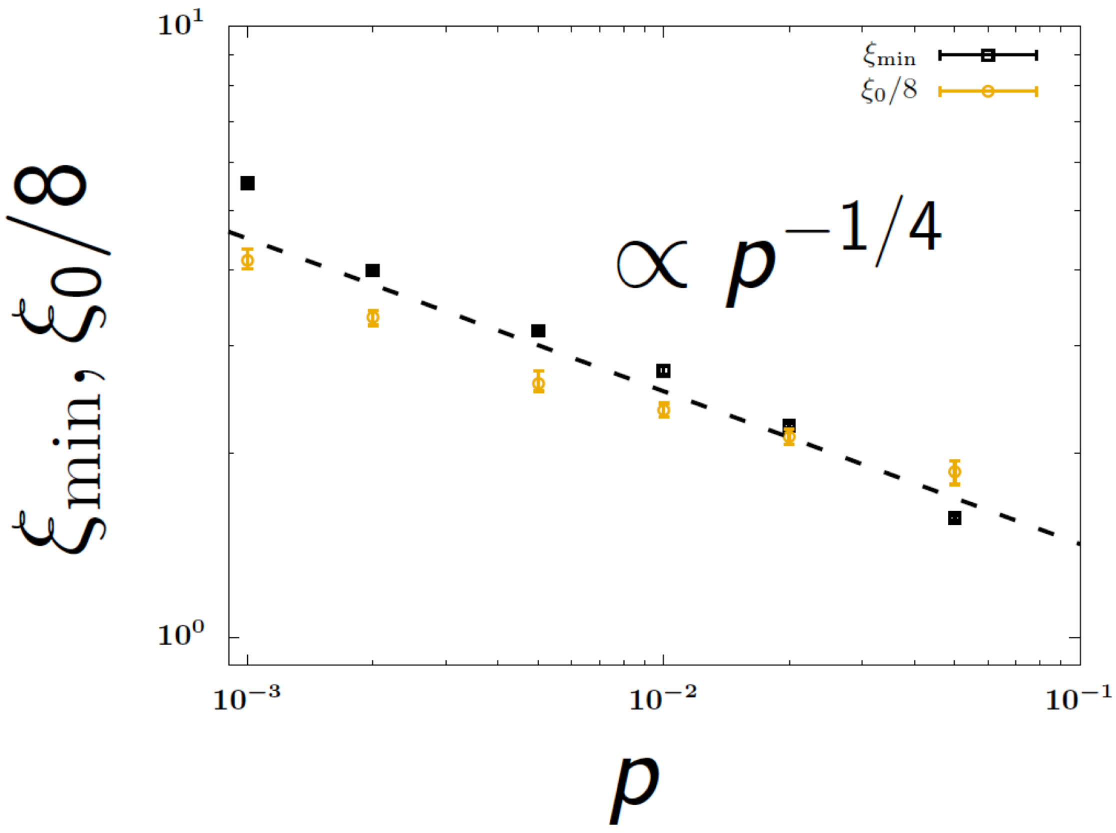
$$\Lambda(r) \equiv \left\langle \sum_{r_i \leq r} \delta E_i^k \right\rangle_k .$$





Negative unstable region becomes large with *P* -> 0

Simulation results at *P* -> 0 (approach to jamming): Pressure dependences of two length scales



Two length scales show a same power-law scaling with *P*:

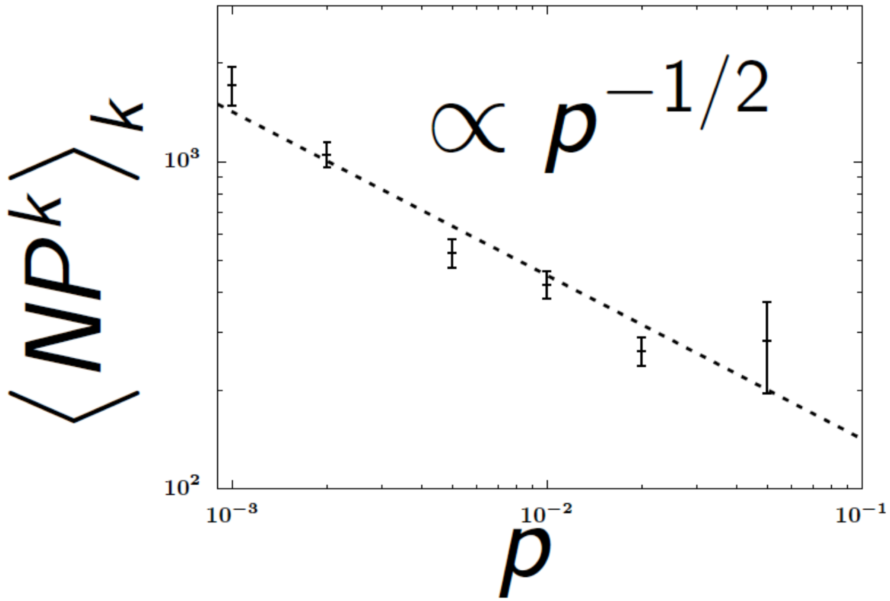
$$\xi_{\min}, \xi_0 \propto p^{-1/4}$$

Simulation results at ***P* -> 0** (approach to jamming): Pressure dependence of characteristic volume

Averaged volume of localized modes: $\langle NP^k \rangle_k$

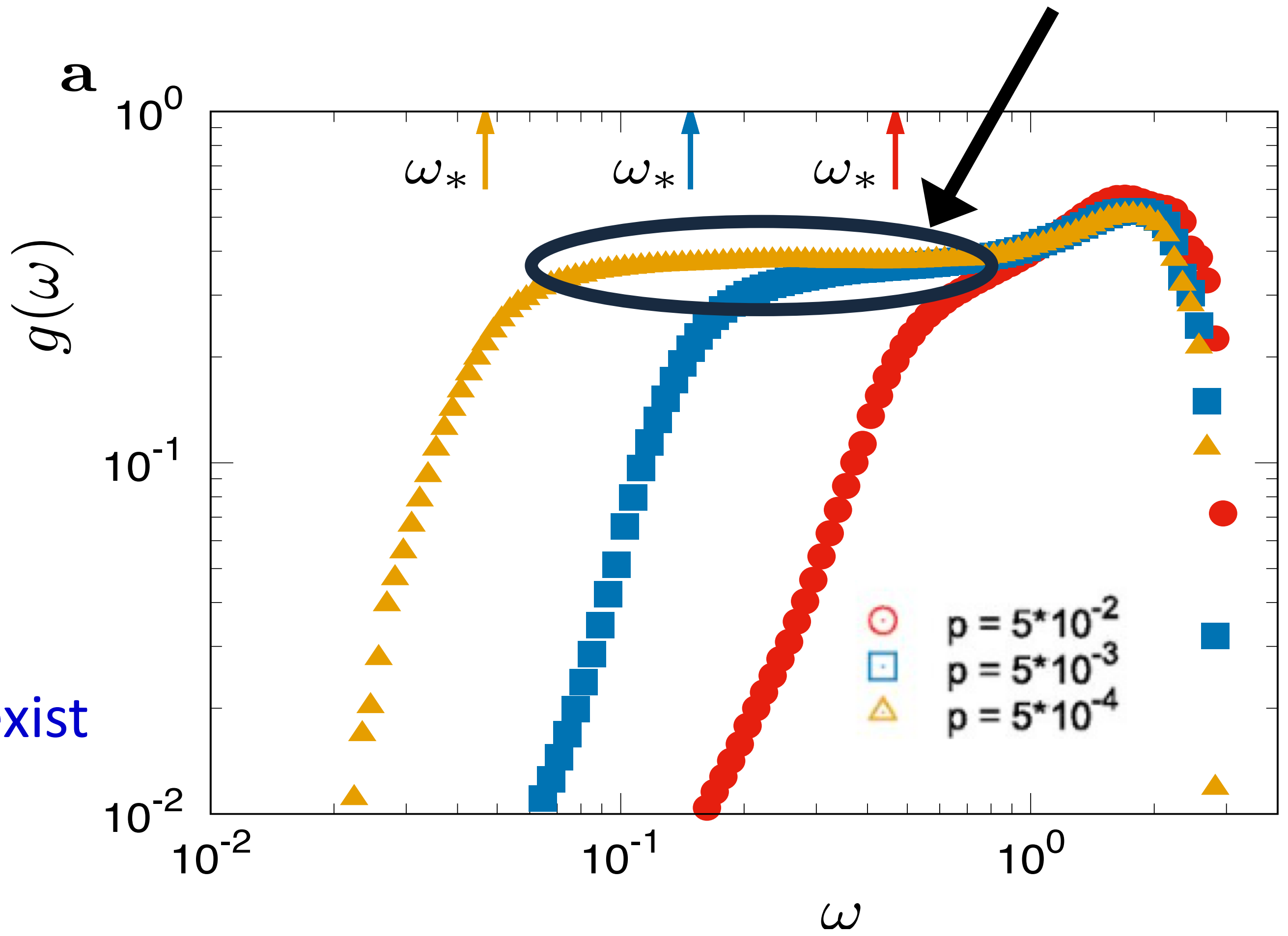
$$P^k = \frac{1}{N}\left[\sum_i \left(\mathbf{e}_i^k \cdot \mathbf{e}_i^k\right)^2\right]^{-1}$$: participation ratio

$$\langle NP^k \rangle_k \propto p^{-1/2}$$



Comparison with anomalous modes

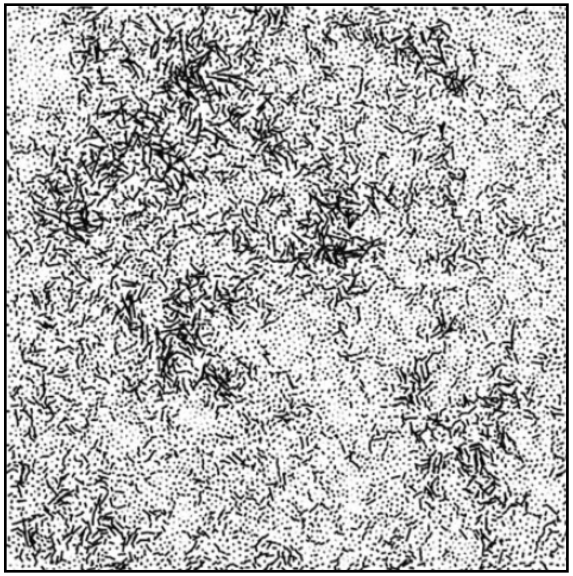
- vDOS shows a characteristic plateau above ω_*
- Modes at the plateau are called "**Anomalous modes**"



Localized modes exist in much lower frequency regime

Comparison with anomalous modes

Anomalous modes are spatially extended modes:



Silbert et al., PRE 2009

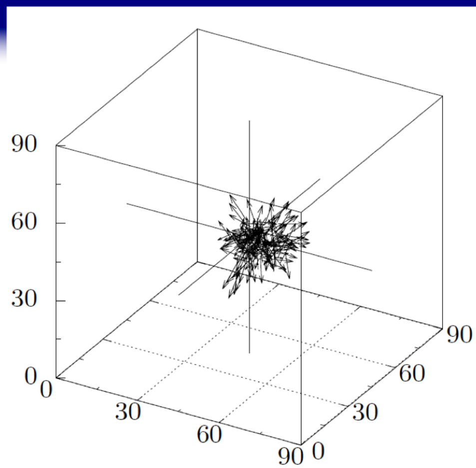
However, spatial correlation of displacements shows

- Characteristic length $\ell_c \sim p^{-1/4}$
- Characteristic volume $V \sim p^{-1/2}$

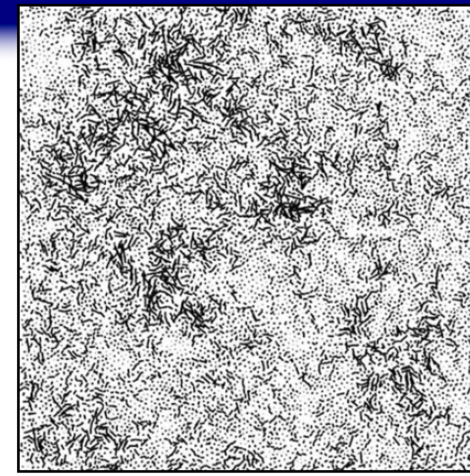
Ikeda et al., JCP 2013
Silbert et al., PRL 2006

-> Localized modes show the same scaling laws as anomalous modes !!!

Comparison with anomalous modes

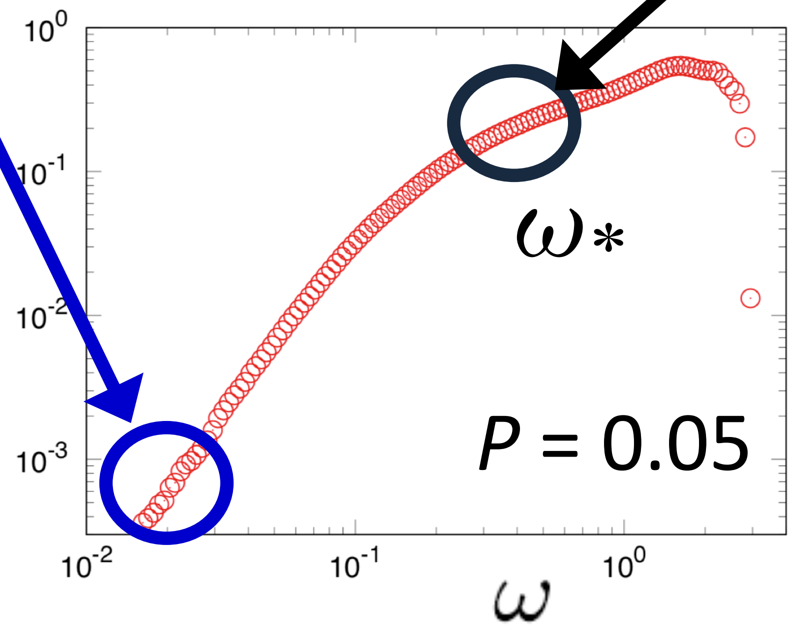


?



Localized modes
(lower frequency regime)

Anomalous modes
(higher frequency regime)



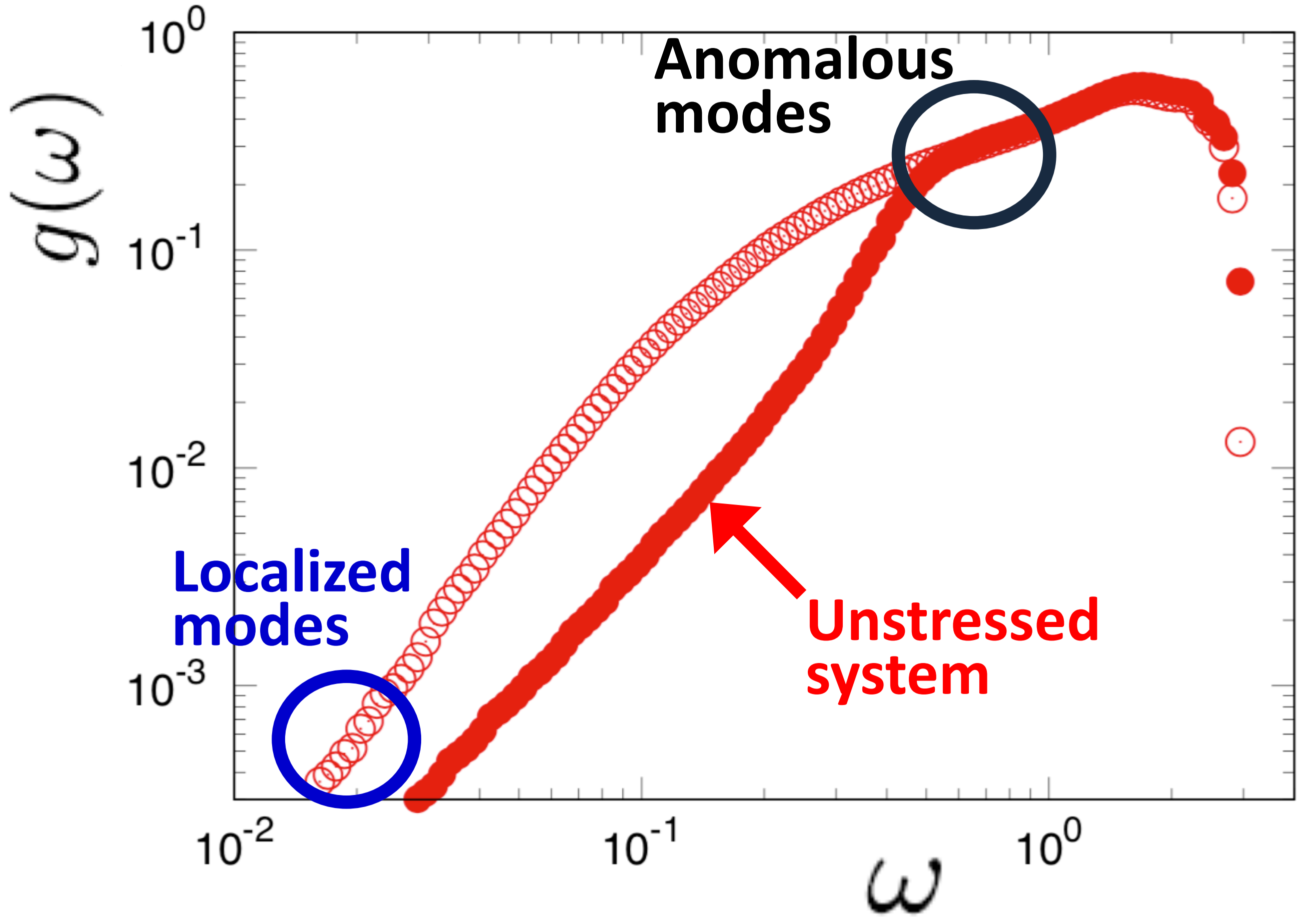
Discussion on origin of localized modes: Introduce "unstressed" system

- **Unstressed system** = the system with zero interparticle forces *fij* = 0 for all the pairs of particles *i* and *j*
- Vibrational modes in the unstressed system have higher vibrational energies than those in the original system

$$\delta E_{ij}^{k} = \underbrace{\boxed{\left(u_{ij}^{\parallel}\right)^2}}_{\text{parallel}} + \underbrace{\cancel{\boxed{\frac{-f_{ij}}{r_{ij}}\left(u_{ij}^{\perp}\right)^2}}}_{\text{perpendicular}}$$

$$> 0 \qquad\qquad < 0$$

Discussion on origin of localized modes: Introduce "unstressed" system



$P = 0.05$

Unstressed system has anomalous modes

but does NOT have localized modes !!!

Mizuno, Shiba, Ikeda, PNAS (2017)

Discussion on origin of localized modes: Theoretical argument for anomalous modes

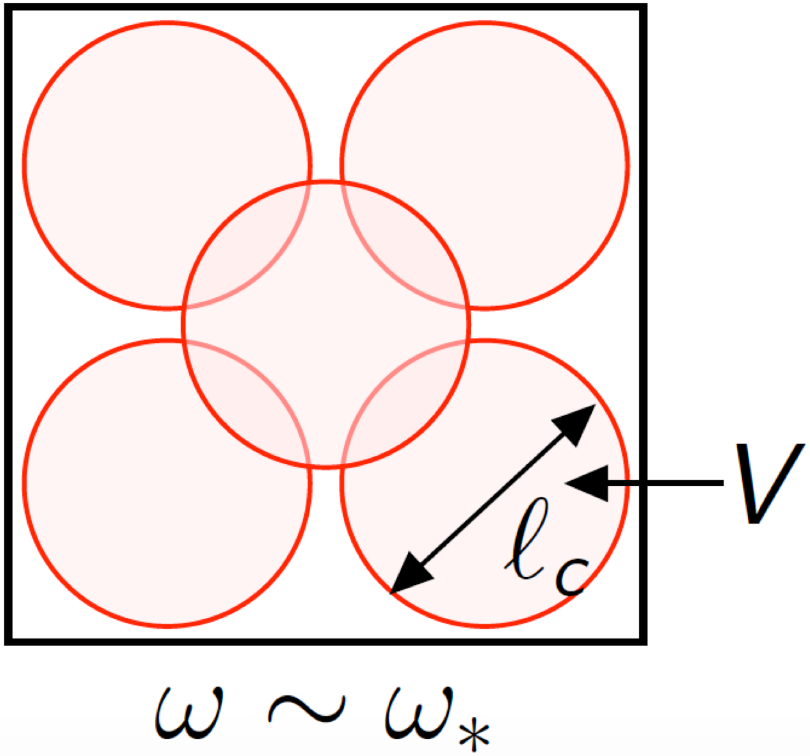
Anomalous modes in the unstressed system can be constructed from the localized vibrations with

the length scale $\ell_c \sim p^{-1/4}$

the volume scale $V \sim p^{-1/2}$

Yan and Wyart, EPL 2016

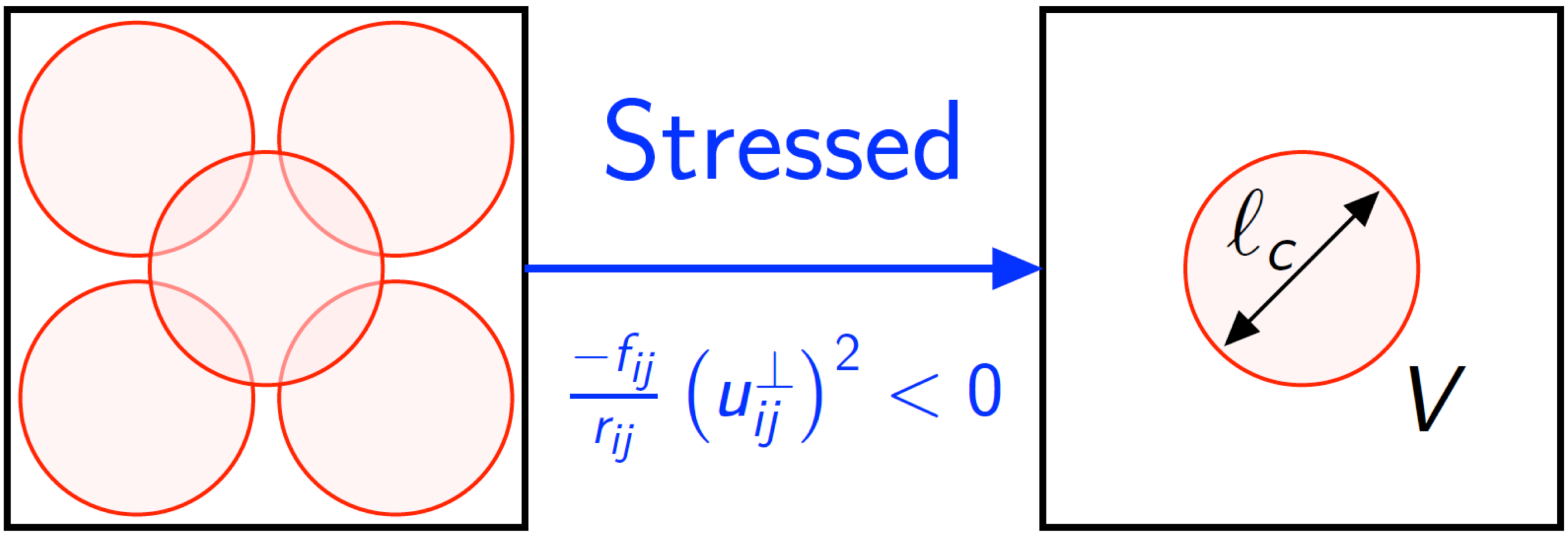
Anomalous modes
in
the unstressed system



Discussion on origin of localized modes

Anomalous modes
in the unstressed system

Localized modes
in the original system



$\omega \sim \omega_*$

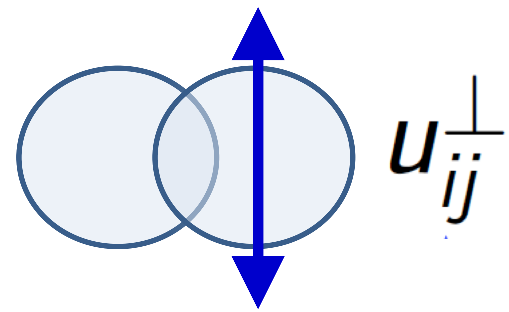
$\omega \ll \omega_*$

Localized modes are anomalous modes destabilized by the second term of vibrational energy *fij*

Conclusion

- How do particles vibrate in the core of localized modes?

-> Particles move perpendicularly to bonds



- What is the size of the core?

-> It shows the characteristic size of anomalous modes that diverges at the jamming transition

- What is the origin?

-> Localized modes are the anomalous modes destabilized by the perpendicular motions in the cores (buckling-like mechanism)

Shimada, Mizuno, Ikeda, Wyart, arXiv:1804.08865