Vibrations in jammed solids: Beyond linear response

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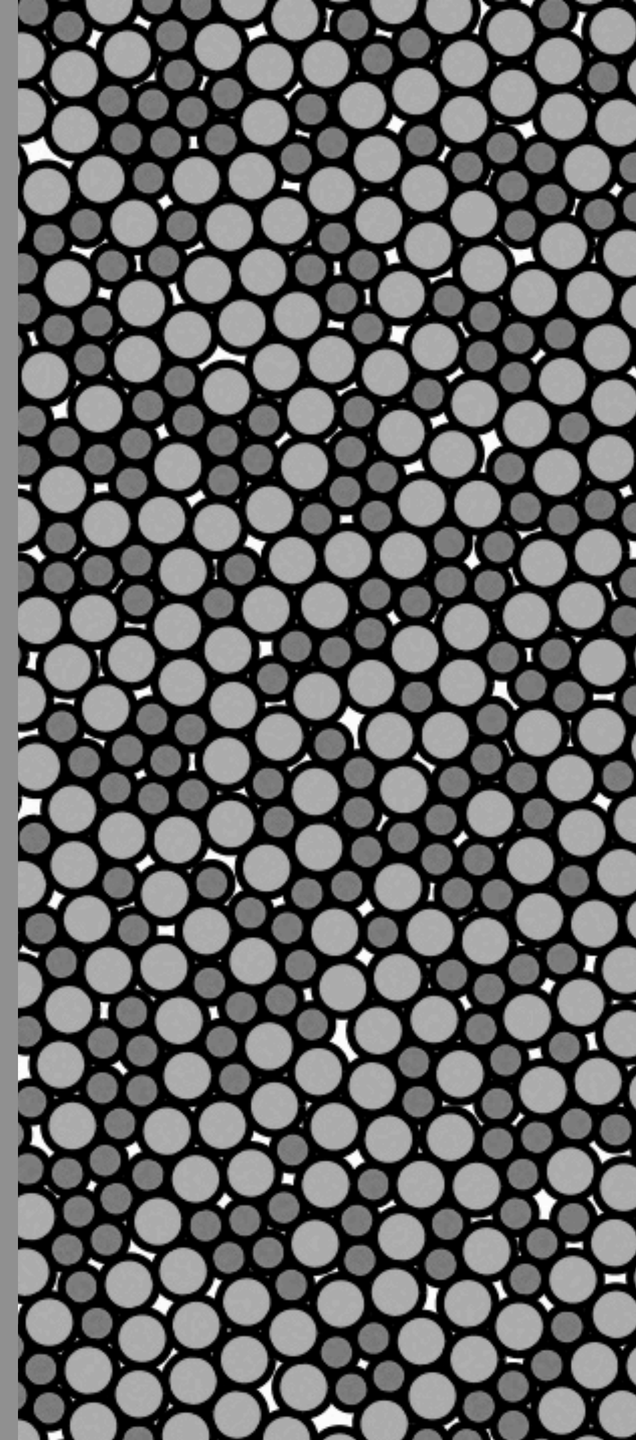
Physics of Glassy and Granular Materials
YITP 2013



Nonlinear Effects in Granular Solids

Nonlinear vibrational properties of granular solids –
Vibration dampening, solitary modes, dispersion,
deviations from elasticity theory

Non-linear effects in real granular packings:

- Breaking existing and forming new contacts
- ~~Non linear interactions (Hertzian)~~
- ~~Sliding and rolling friction~~
- ~~Energy dissipation~~

See Carl Schreck's poster for details on Hertzian interactions

Isolate the effects of fluctuations in the network of contacts!

Absence of Linear Response

Dynamical Matrix:

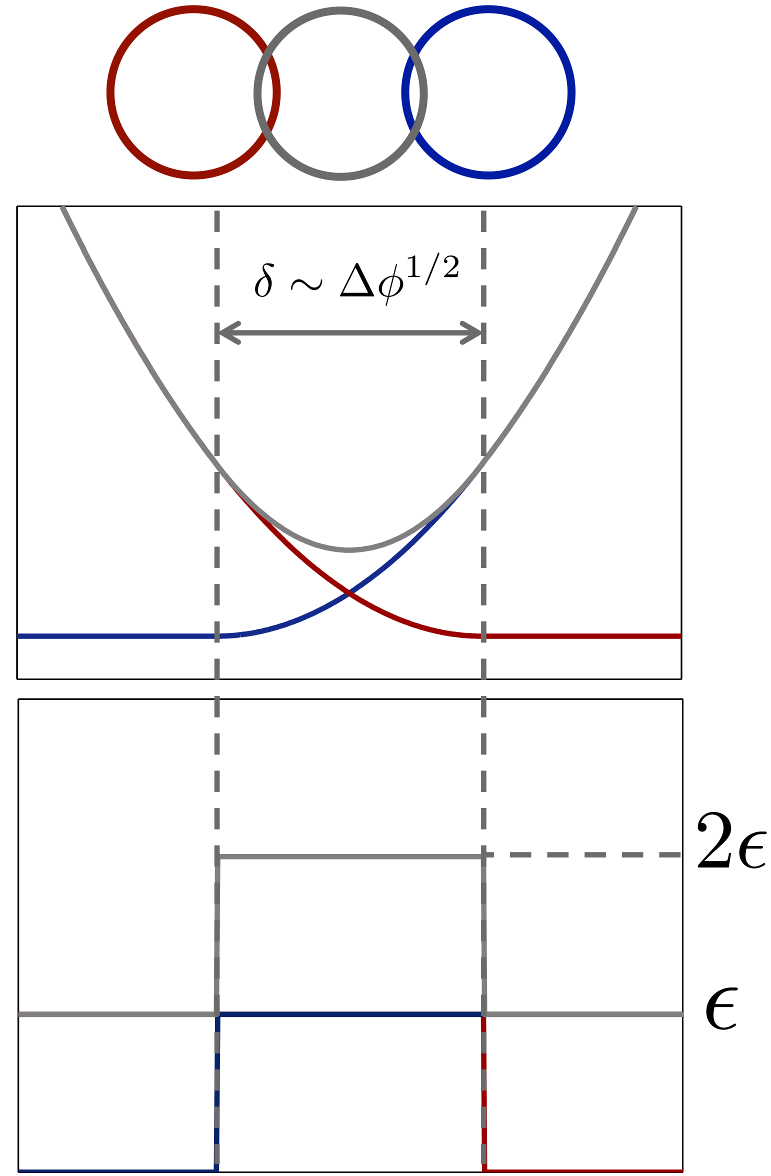
$$V(r_{ij}) = \frac{\epsilon}{2}\left(1 - \frac{r_{ij}}{\sigma_{ij}}\right)^2 \Theta\left(1 - \frac{r_{ij}}{\sigma_{ij}}\right)$$

$$M_{\alpha,\beta} = \left(\frac{\partial^2 V}{\partial r_\alpha \partial r_\beta}\right)_{\vec{r}=\vec{r_0}}$$

Diagonalize the dynamical matrix
to access eigenfrequencies:

$$\hat{e_i}, i \in \{1, \ldots, 2N\}$$

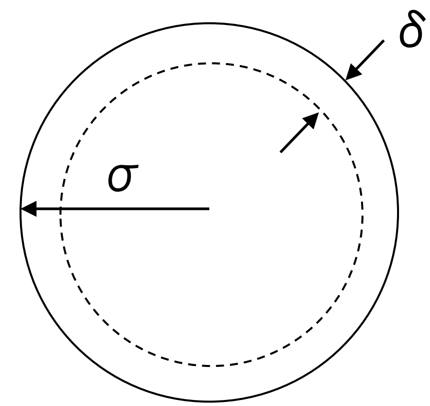
$$\lambda_i = m\omega_i^2$$



Absence of Linear Response

Temperature allow particle to explore its surrounding on a distance δ :

$$\frac{1}{2}k\delta^2 = T \qquad \delta = \sqrt{\frac{2T}{k}}$$



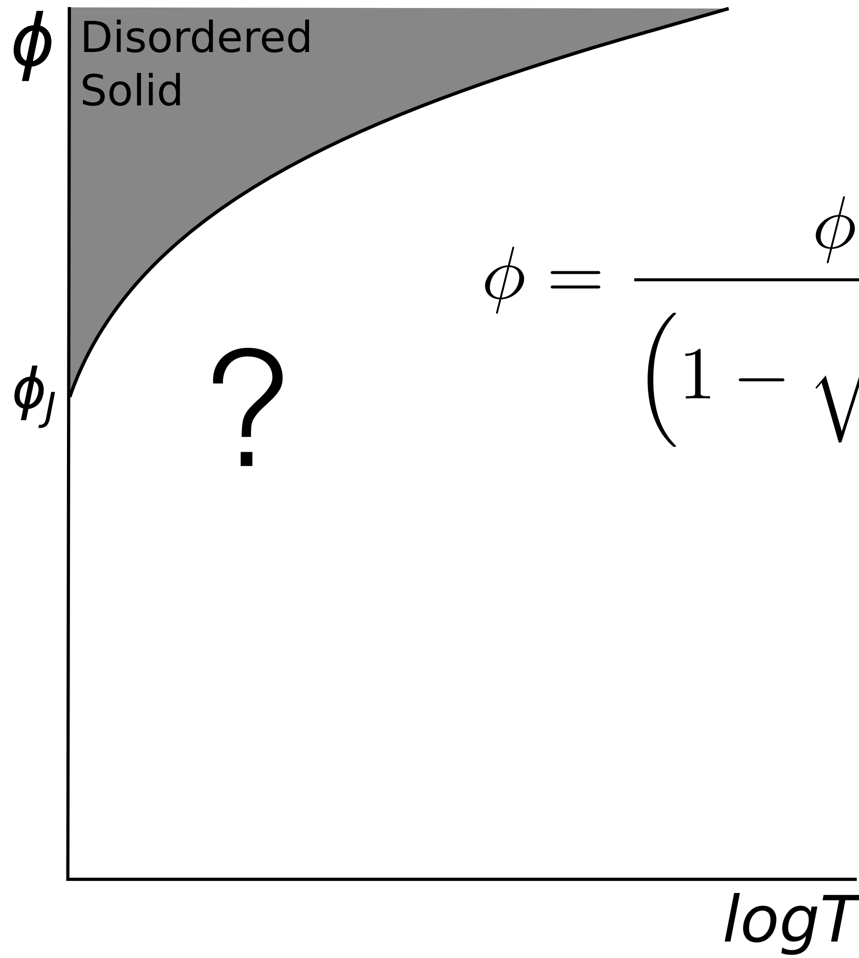
Apparent diameter of a particle: $\sigma^{\mathrm{eff}} = \sigma - \delta$

$$\phi^{\mathrm{eff}} = \phi\left(1 - \frac{\delta}{\sigma}\right)^2$$

Need to increase the volume fraction to rejam the system at a given T:

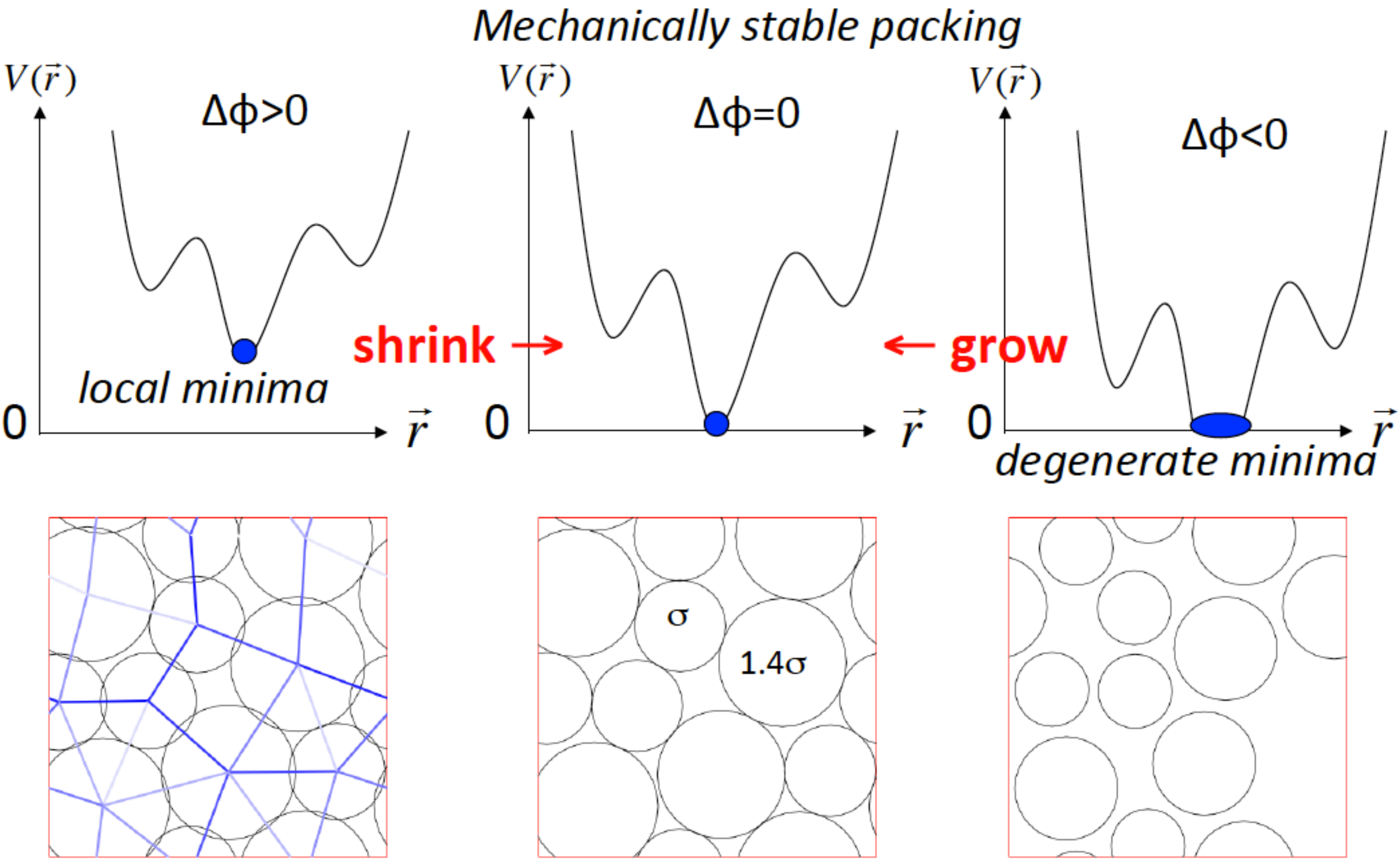
$$\boxed{\phi = \frac{\phi_J}{\left(1 - \sqrt{\frac{2T}{k\sigma^2}}\right)^2}}$$

Absence of Linear Response

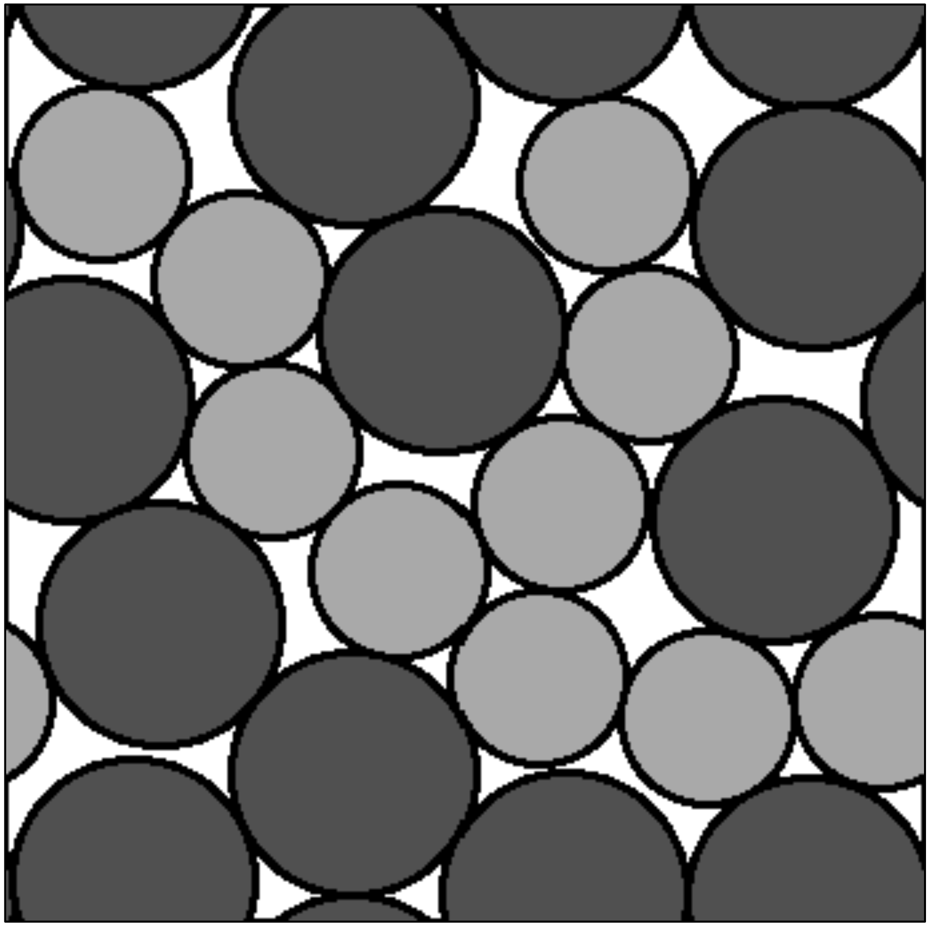


$$\phi = \frac{\phi_J}{\left(1 - \sqrt{\frac{2T}{k\sigma^2}}\right)^2}$$

Generating Jammed Packings



Beyond the Harmonic Approximation…



$N = 20$

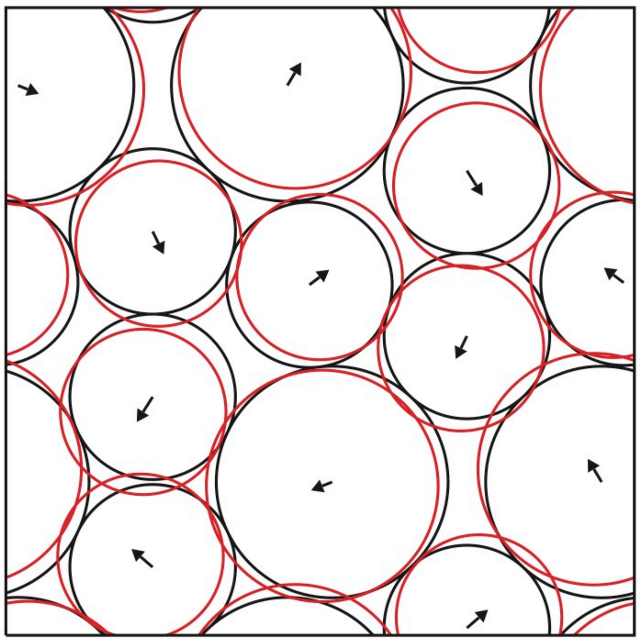
- Molecular Dynamics Simulation
- Constant energy
- Linear Spring Repulsion
- Frictionless
- No dissipation
- At t=0, add temperature

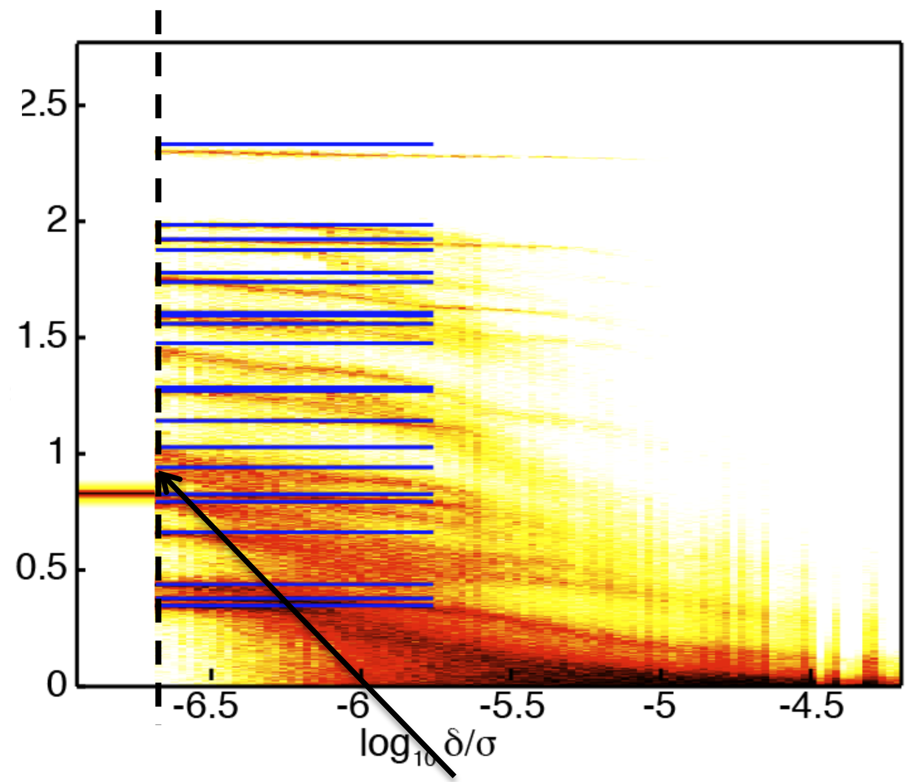
Non-harmonicity in Disordered Solids

Protocol:

- Perturb along eigenmode by δ
- Let the system evolve at constant energy
- Study the FT of the particle motion

N = 12
$\Delta\phi = 10^{-5}$
mode = 6





Schreck, Bertrand, Shattuck, O'Hern, *Phys. Rev. Lett.* 107 (2011) 078301

Beyond the Harmonic Approximation…

Under *harmonic approximation:*

$$\mathbf{M} = k_B T \mathbf{C}^{-1}$$

$$\mathbf{V} = \frac{1}{N}\langle v v^{\mathrm{T}} \rangle \qquad \mathbf{V} = k_B T \mathbb{I}$$

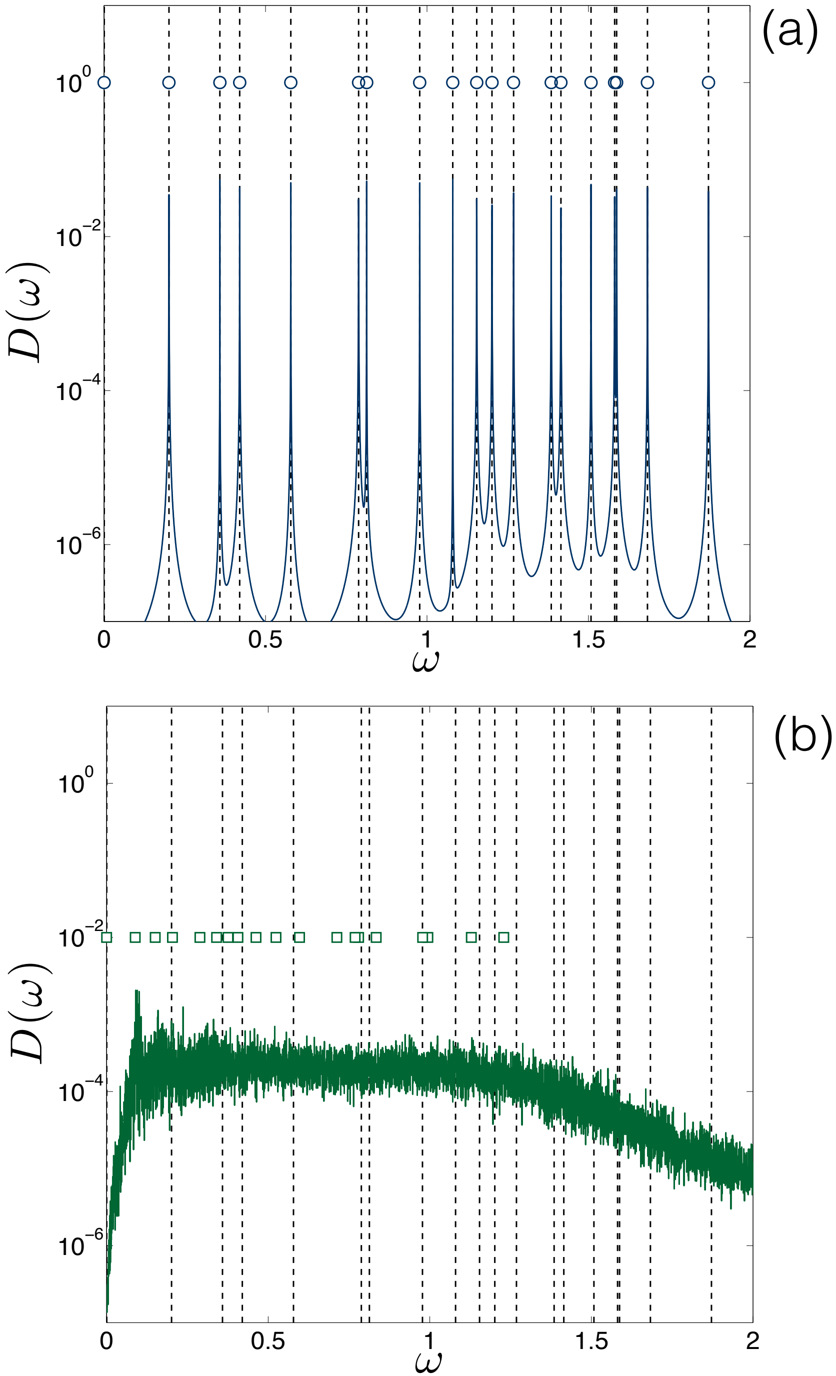
Solution 1: probing the correlation of particles displacements via

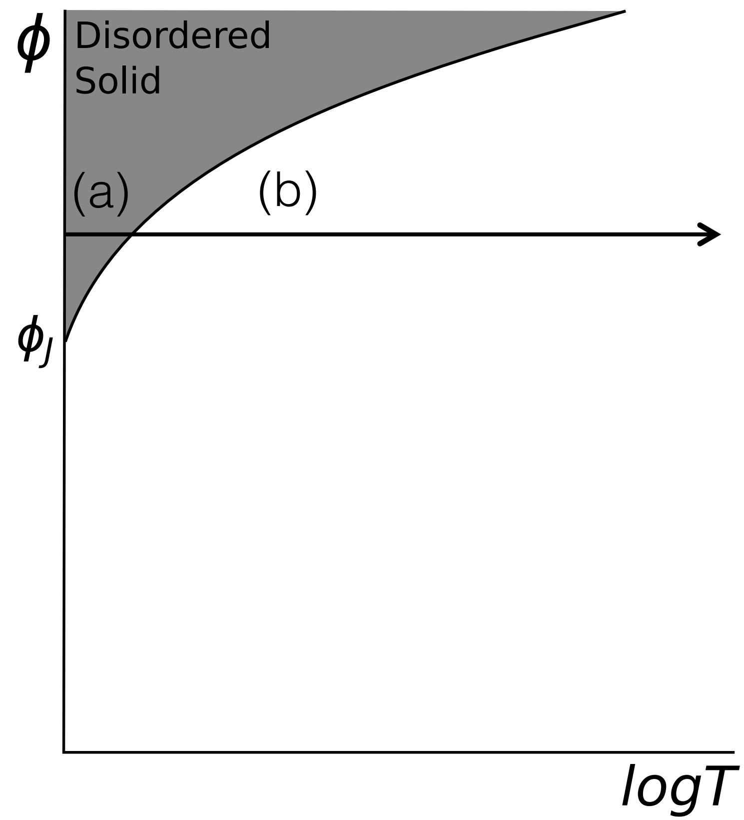
$$\boxed{\mathbf{M} = \mathbf{V}\mathbf{C}^{-1}}$$

Solution 2: looking for vibrational frequencies emerging in the Fourier Transform of the velocity autocorrelation function via

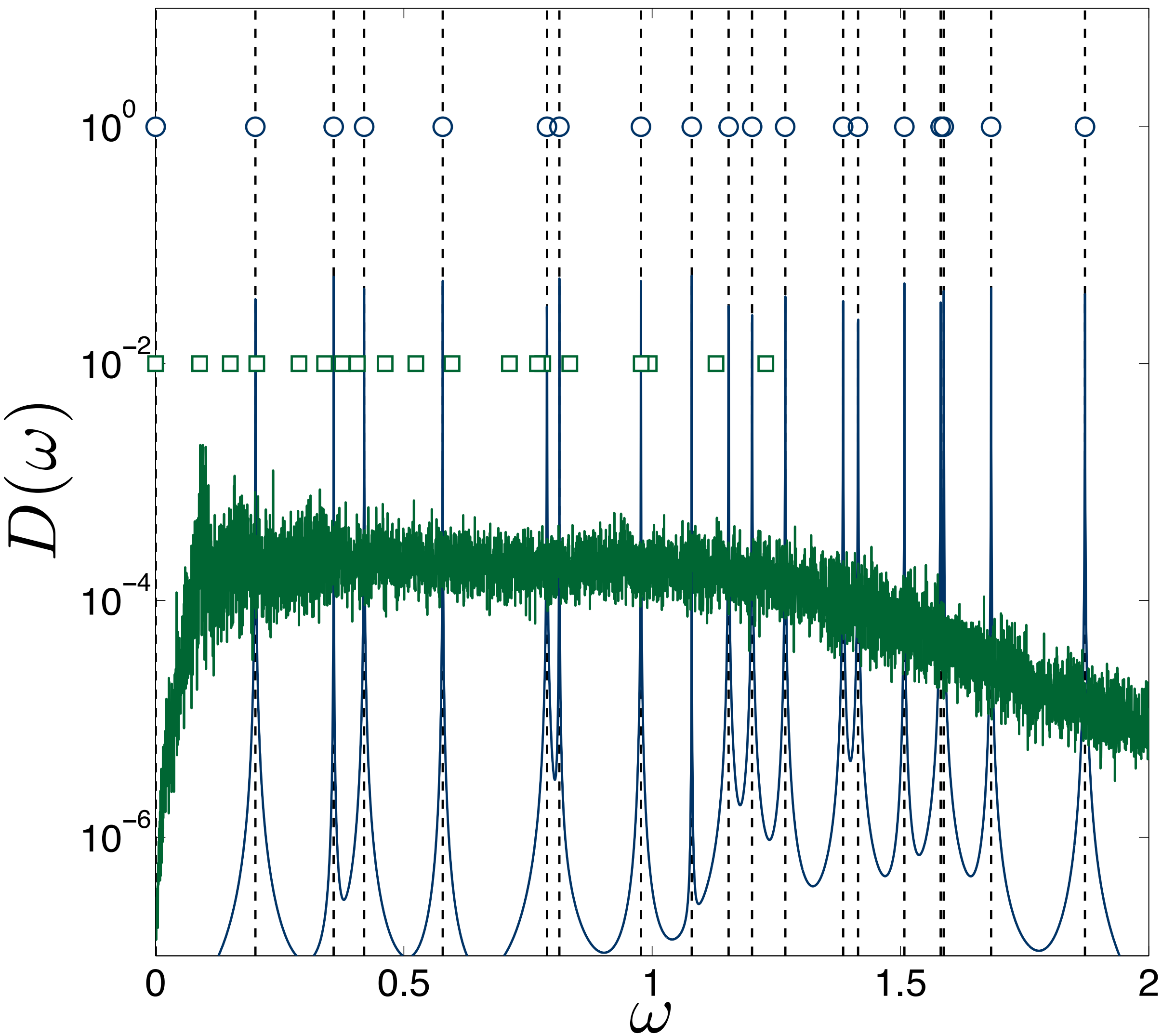
$$d(t) = \frac{\sum_{i=1}^{N} \langle \mathbf{v}_i(t).\mathbf{v}_i(0) \rangle_0}{\sum_{i=1}^{N} \langle \mathbf{v}_i(0).\mathbf{v}_i(0) \rangle_0} \qquad \boxed{\tilde{d}(\omega) = \mathcal{F}[d(t)]}$$

Assessing the Vibrational Frequencies



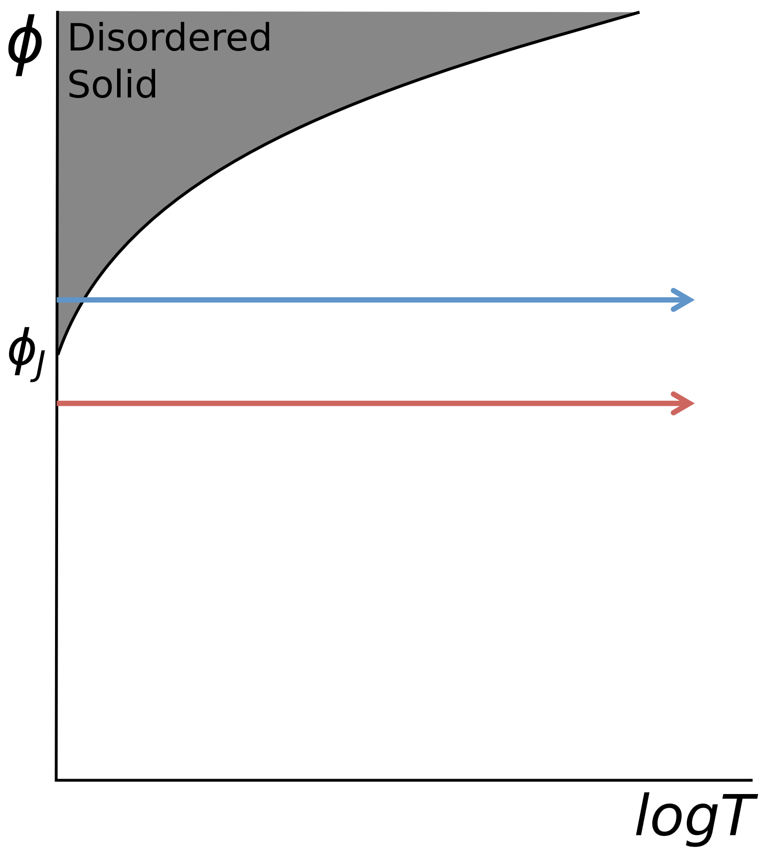


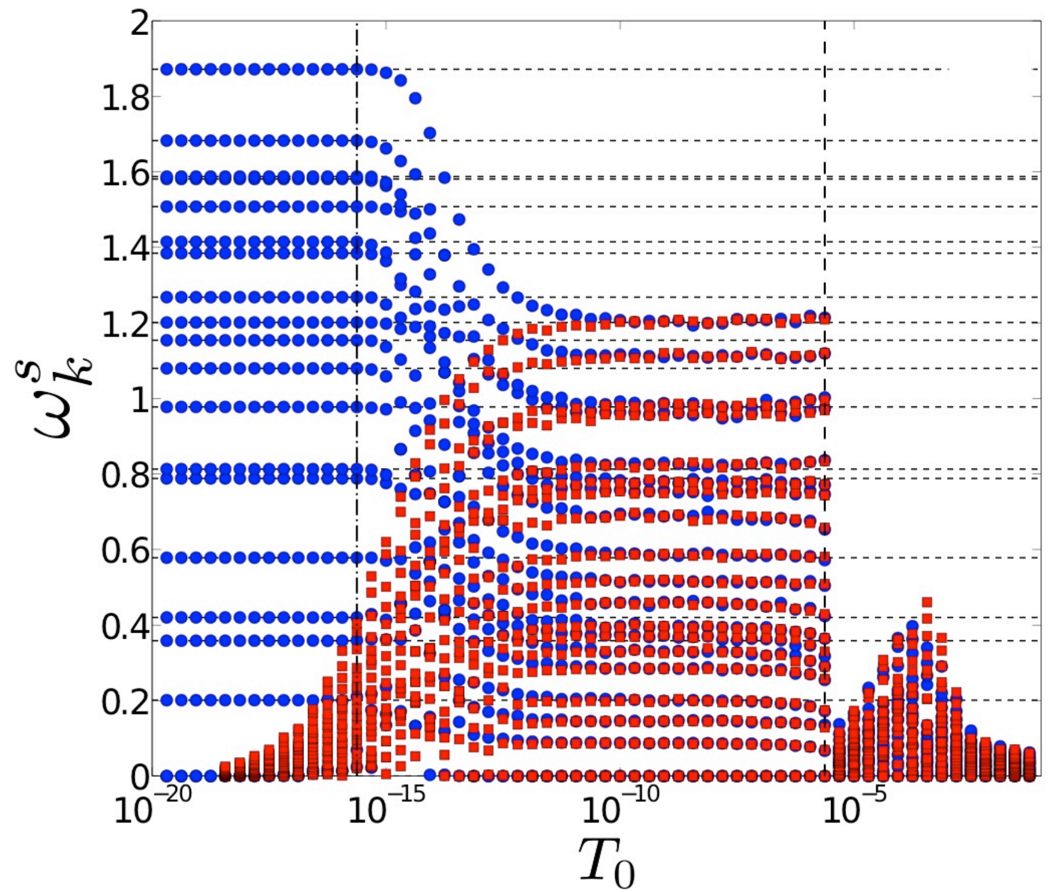
Assessing the Vibrational Frequencies



Non trivial evolution of the covariance matrix prediction and Fourier transform of Velocity autocorrelation function w/ T

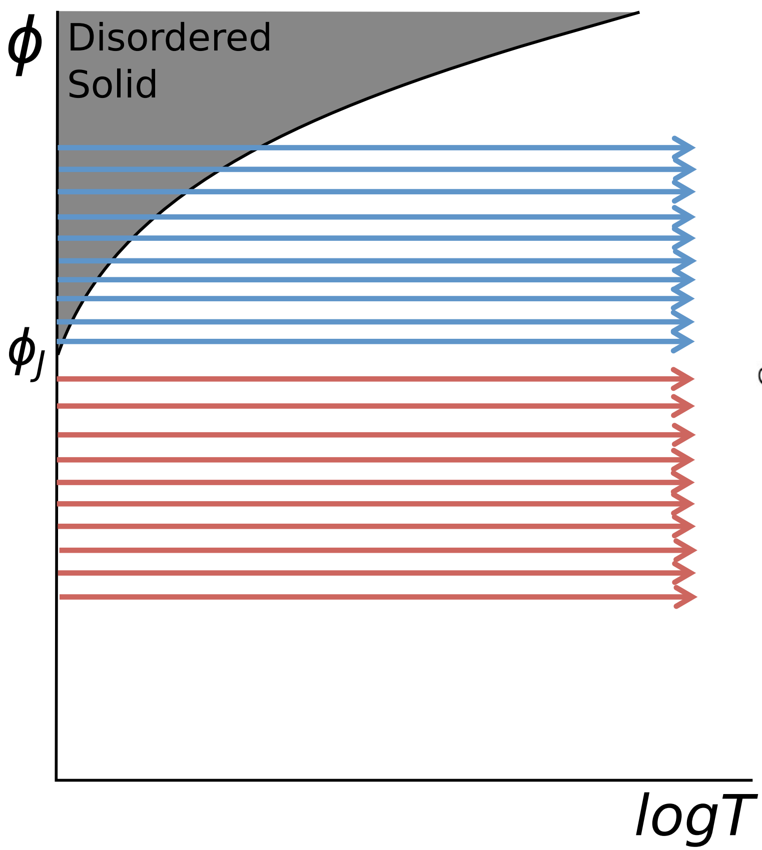
Temperature Dependence of the Frequencies

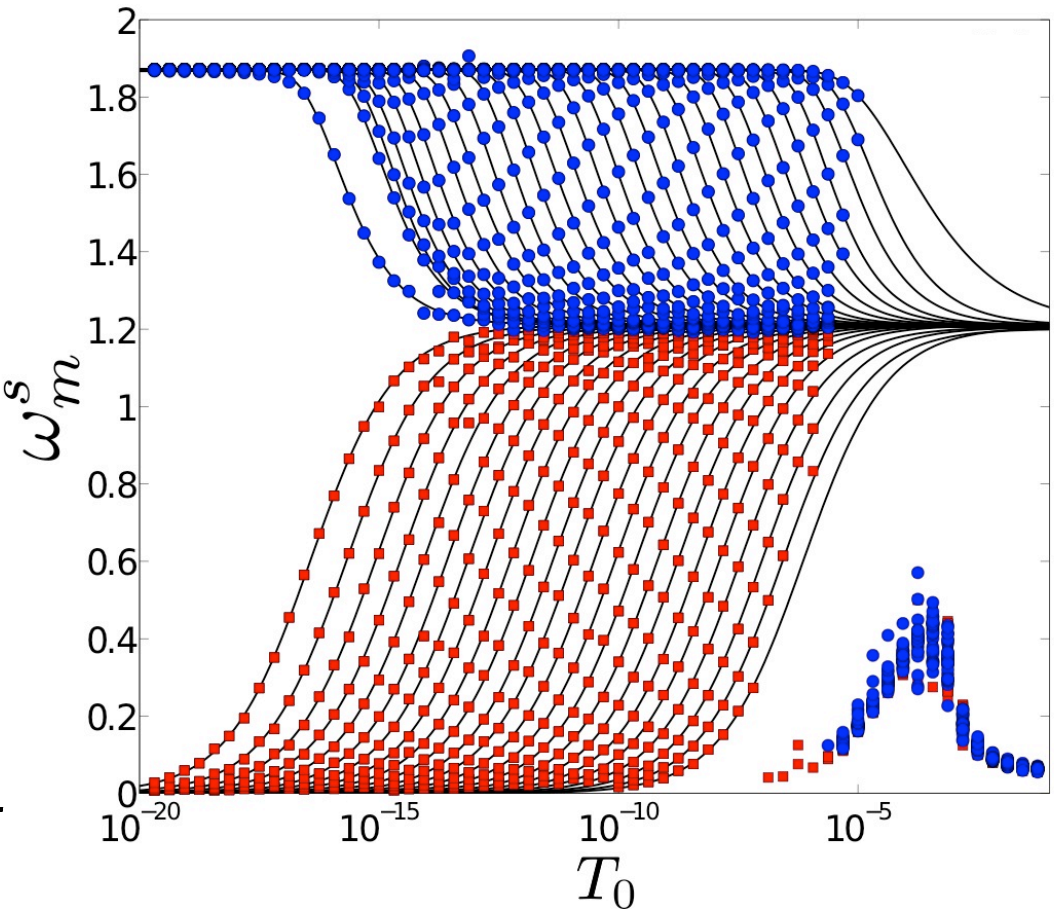




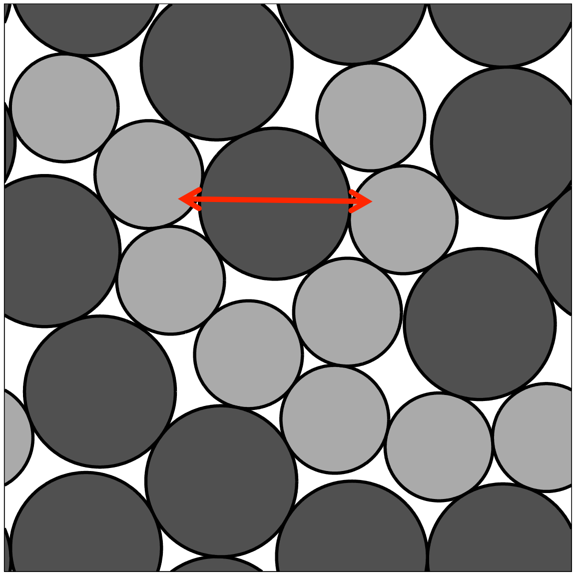
$$\omega_k(T) = \omega_k^d + \frac{\omega_k^* - \omega_k^d}{\left(1 + l_c(\Delta\phi)/\sqrt{T}\right)^{\nu}}$$

Temperature Dependence of the Frequencies

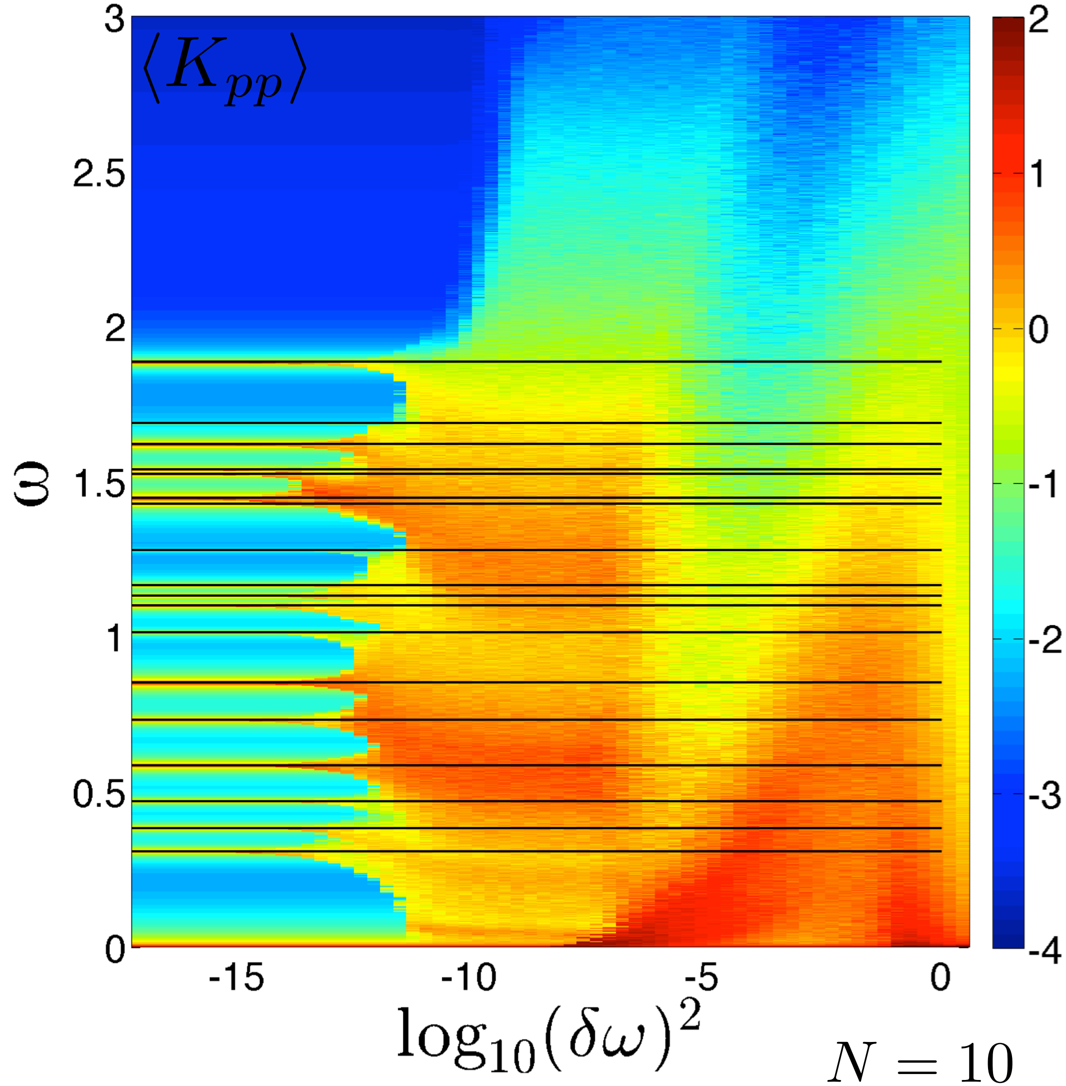




Testing Resonance in the Modes



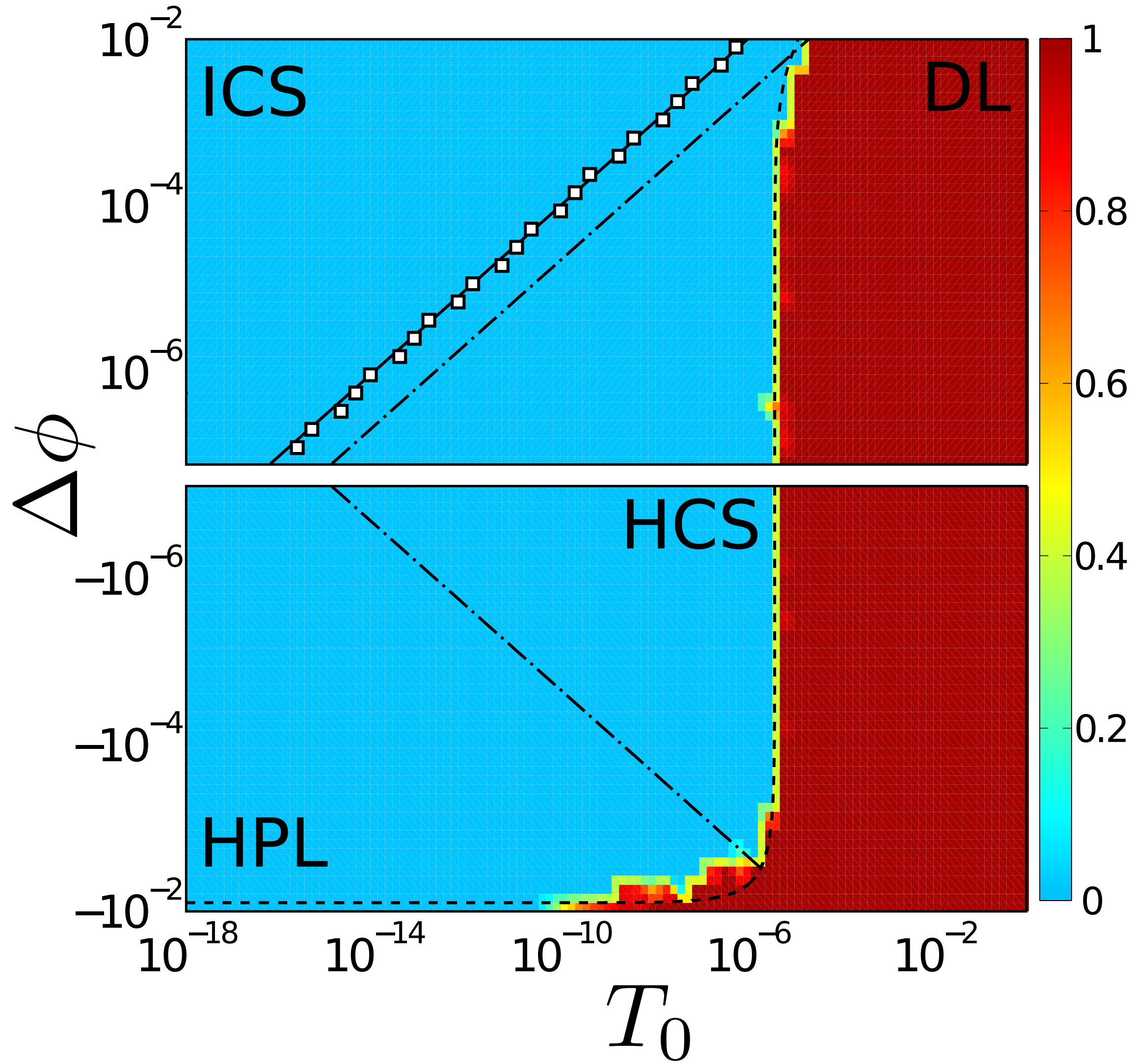
- Drive one particle
- Record average kinetic energy per particle in steady state



$N = 10$

$\Delta\phi = 10^{-8}$

Rearrangement probability

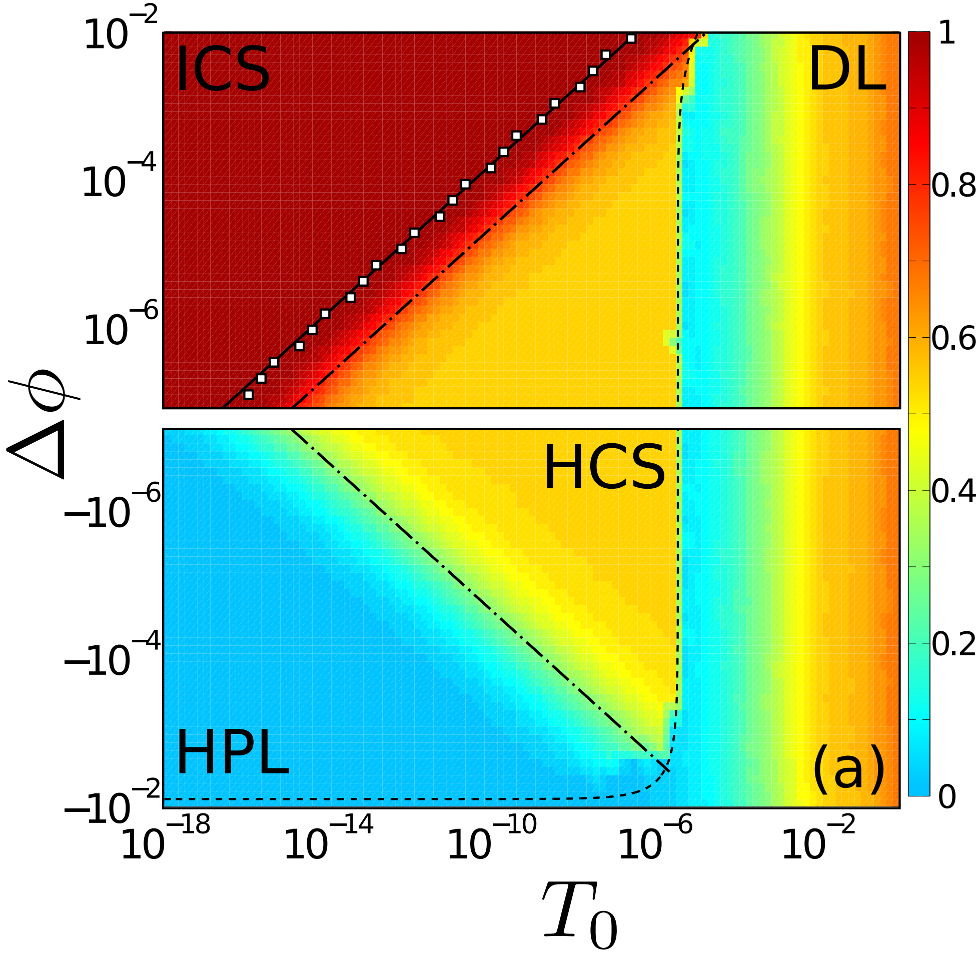


Packing ***did not rearrange***, relate to the same inherent structure

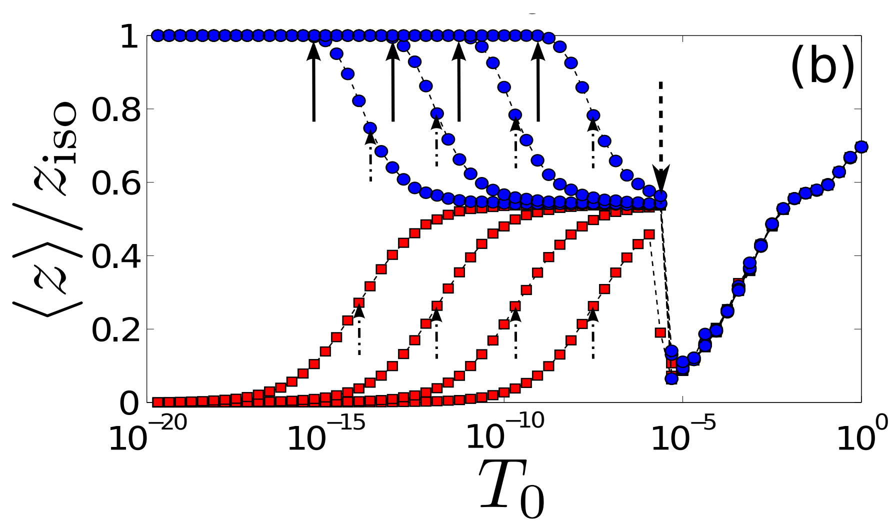
Packing ***rearranged***, relate to a different inherent structure

100 snapshot over the course of the simulation

Introducing a new Phase Diagram

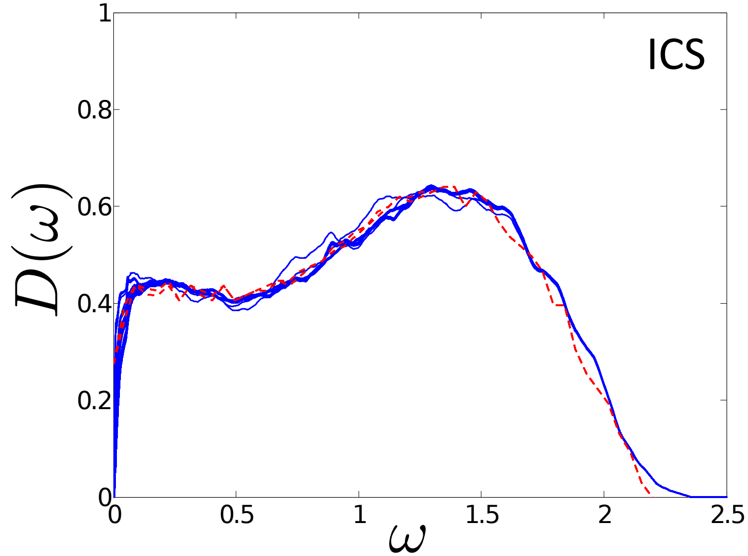


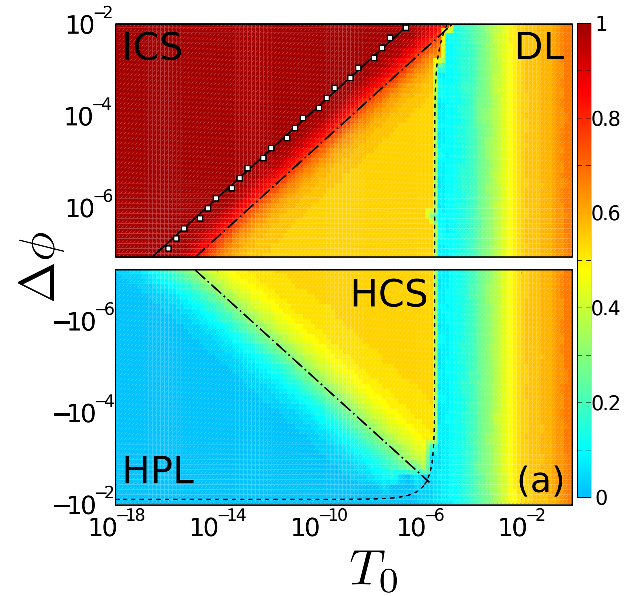
$$z_{\text{iso}} = dN - d + 1$$

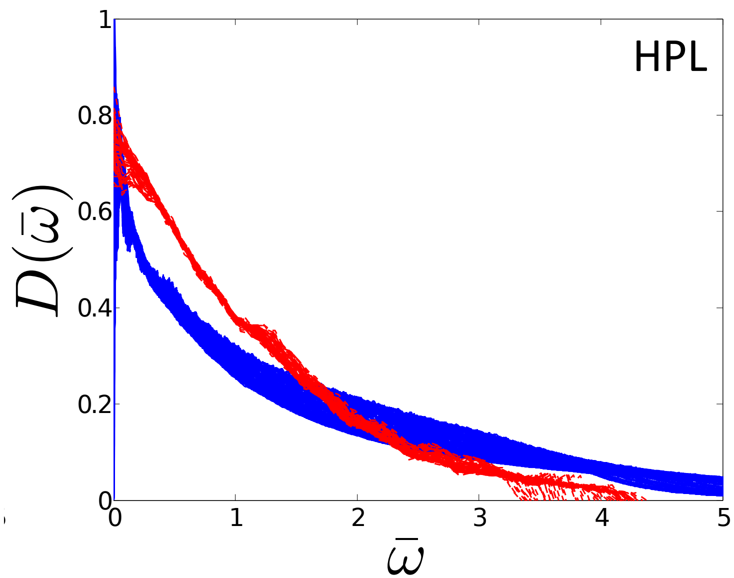


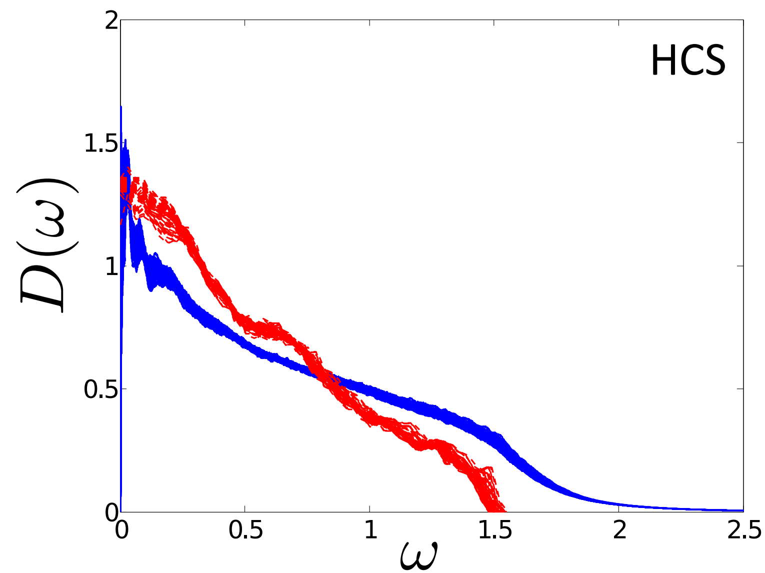
ICS = Iso-coordinated Solid
HCS = Hypo-coordinated Solid
HPL = Hard Particle Liquid
DL = Dense Liquid

Density of States

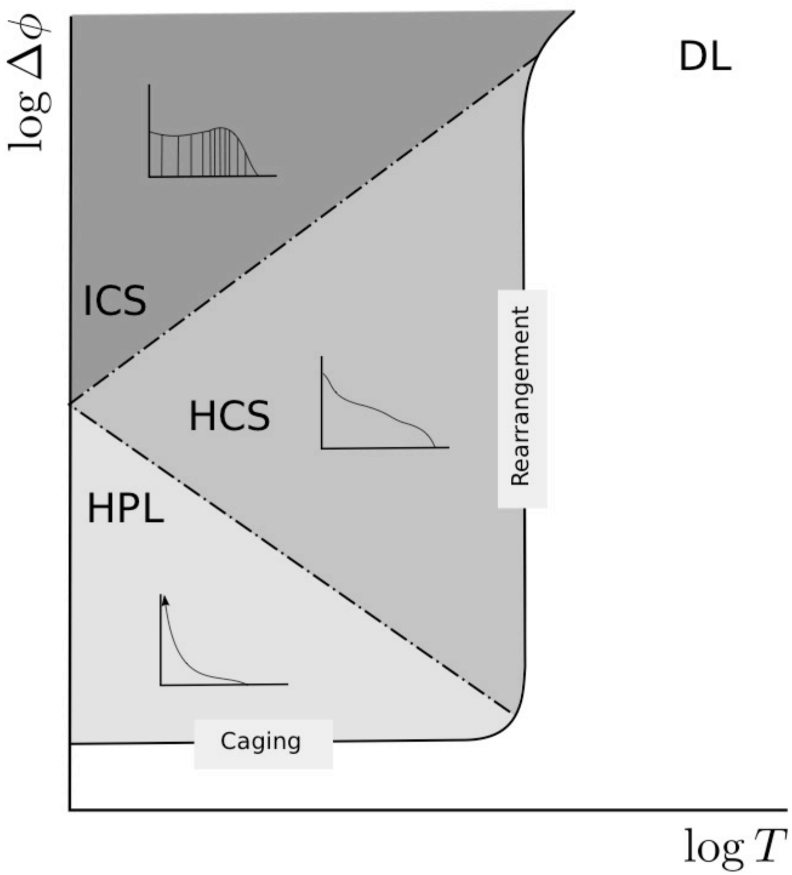






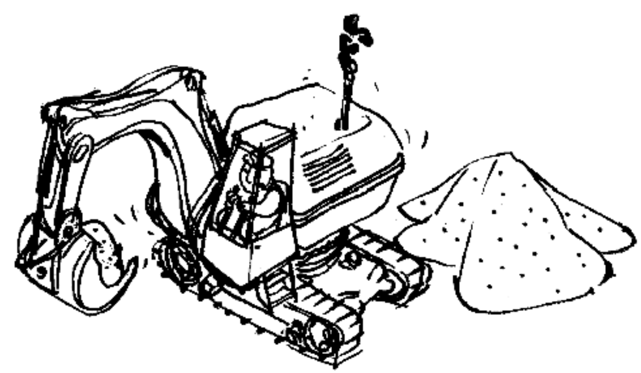


Conclusions & Future directions



- No linear response for a wide range of parameters
- Need of a new description for the vibrational dynamics of jammed packings
- Transition from resonant to non-resonant modes
- Investigating effect of friction, particle shape and order

"Vibrations in jammed solids: Beyond linear response", T.Bertrand, C.F.Schreck, C.S.O'Hern and M.D.Shattuck, submitted to PRL (arXiv:1307.0440)



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