Relevance of jamming to the mechanical properties of solids

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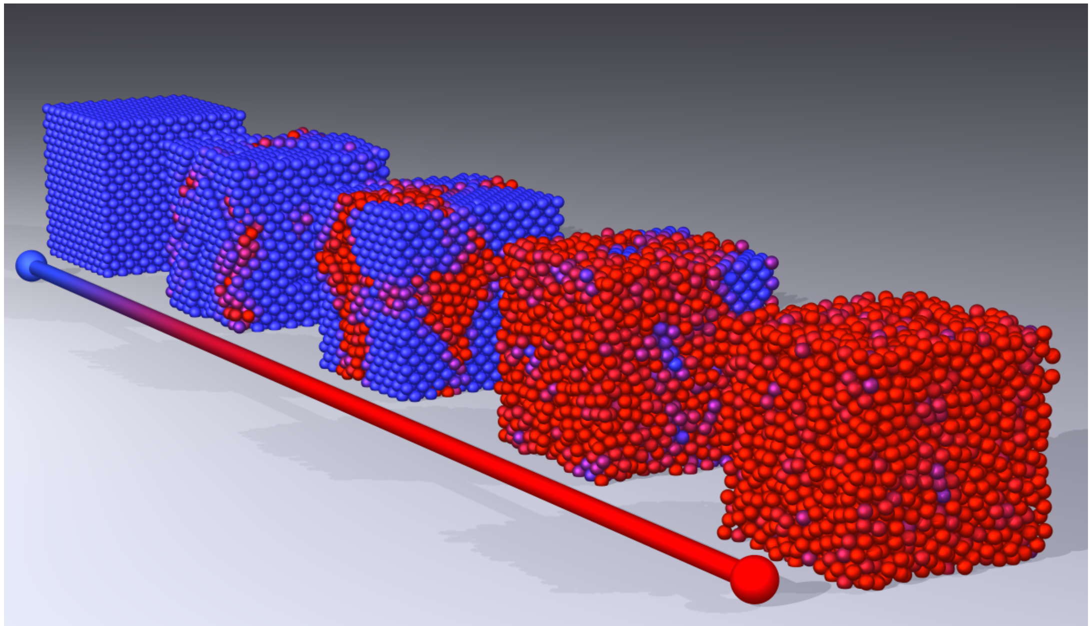
University of Chicago

Capri; September 12, 2014



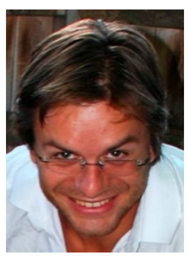
What is role of (dis)order for mechanical behavior?

Andrea J. Liu

Carl Goodrich

Justin Burton

Ning Xu



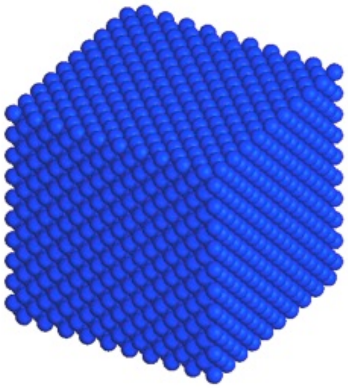
Matthieu Wyart

Leo Silbert

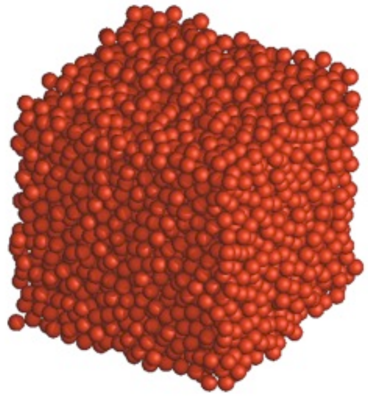
Vincenzo Vitelli

Corey O'Hern

Department of Energy, Office of Basic Energy Sciences,
Division of Materials Sciences and Engineering



Crystals are essence of order
What is essence of disorder?



Why ask that?

Cannot perturb crystal (*i.e.*, add defects) to get physics of glasses

Need other limit - complete disorder

Prototype of an*other* way of making solids:

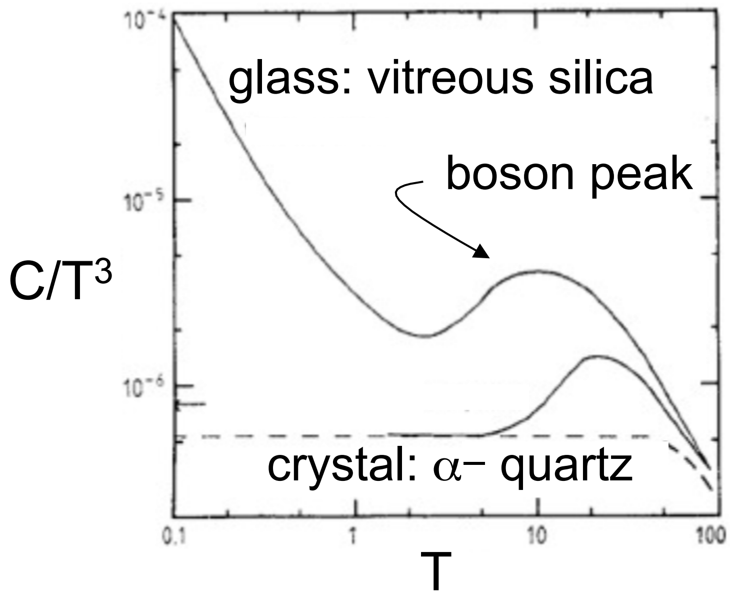
- Crystallization: 1st-order nucleation
- What (non-equilibrium) process creates complete disorder?

Do all ways of creating rigidity produce same behavior?

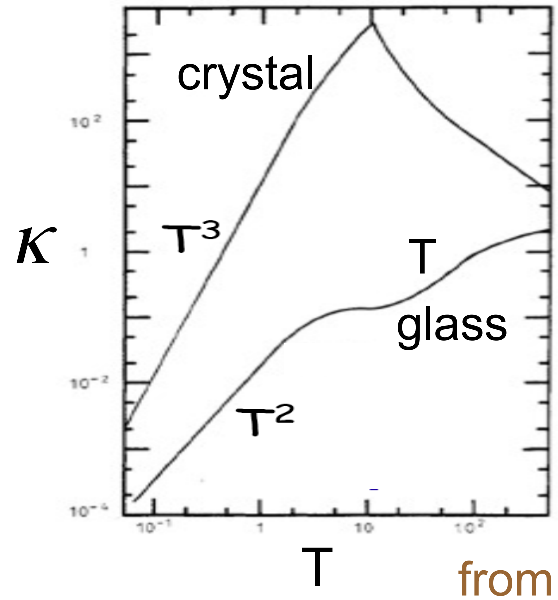
Example: phenomena created by disorder

Qualitatively different from crystals

specific heat: excess low-T excitations

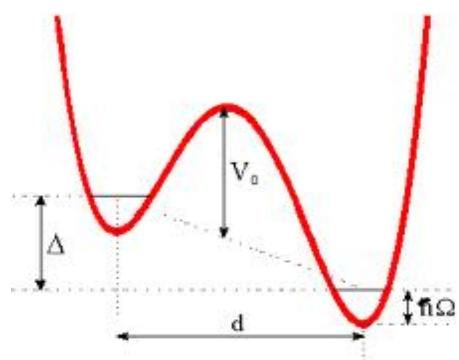


thermal conductivity



from: W.A. Phillips

Quantum-mechanical two-level (tunneling) systems have been postulated to explain low-temperature properties of glasses



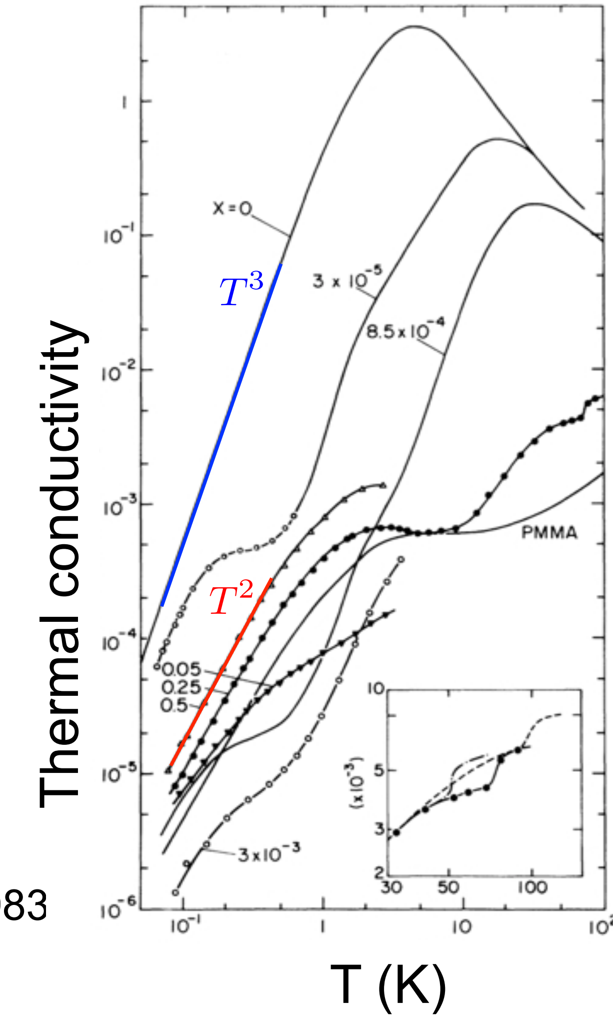
Orientational glass: $(KBr)_{1-x}(KCN)_x$

$x = 0$ → crystal

$x \approx 0.5$ → orientational glass

Crossover from ordered to disordered behavior occurs at *very low* disorder

$$x_{crossover} \approx 0.01$$

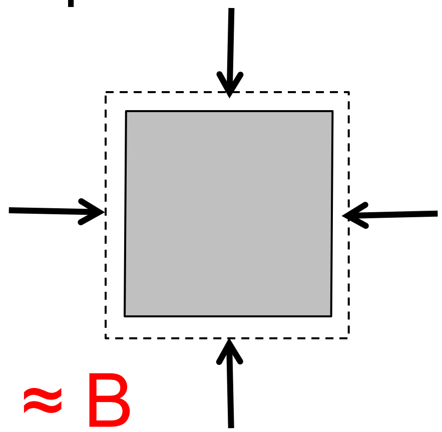


De Yoreo *et al.* PRL (1983

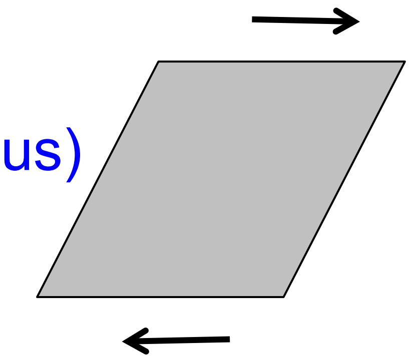
Nature of rigidity and excitations

Response to compression and to shear:

B
(bulk modulus)



G
(shear modulus)



In crystals, G ≈ B

Excitations: Normal modes of vibration
density of states; spatial properties; heat transport; anharmonicity

Does disorder matter?

Jamming:

Compress random collection of spheres in a box

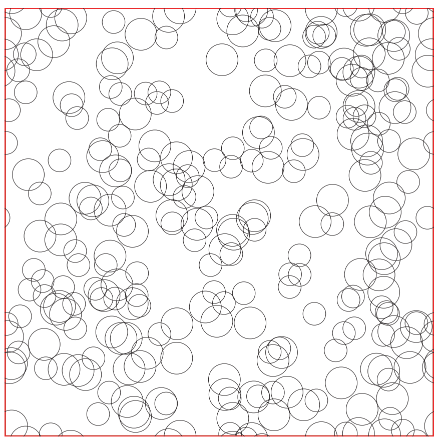
Does this protocol produce different physics from crystals?

Simulate finite-range, repulsive potentials:

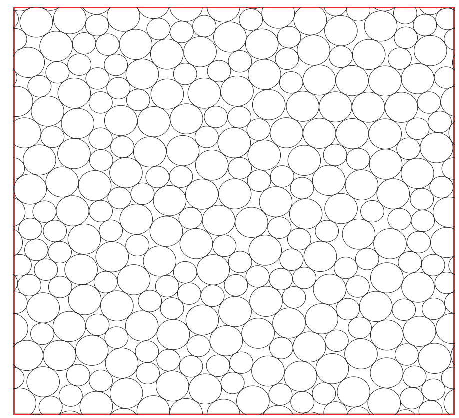
$V(r) = V_0 (1 - r/\sigma)^{\alpha} \quad r < \sigma \quad D = 2,\ D = 3$

$\quad\;\; = 0 \quad\quad\quad\quad\quad\; r > \sigma$

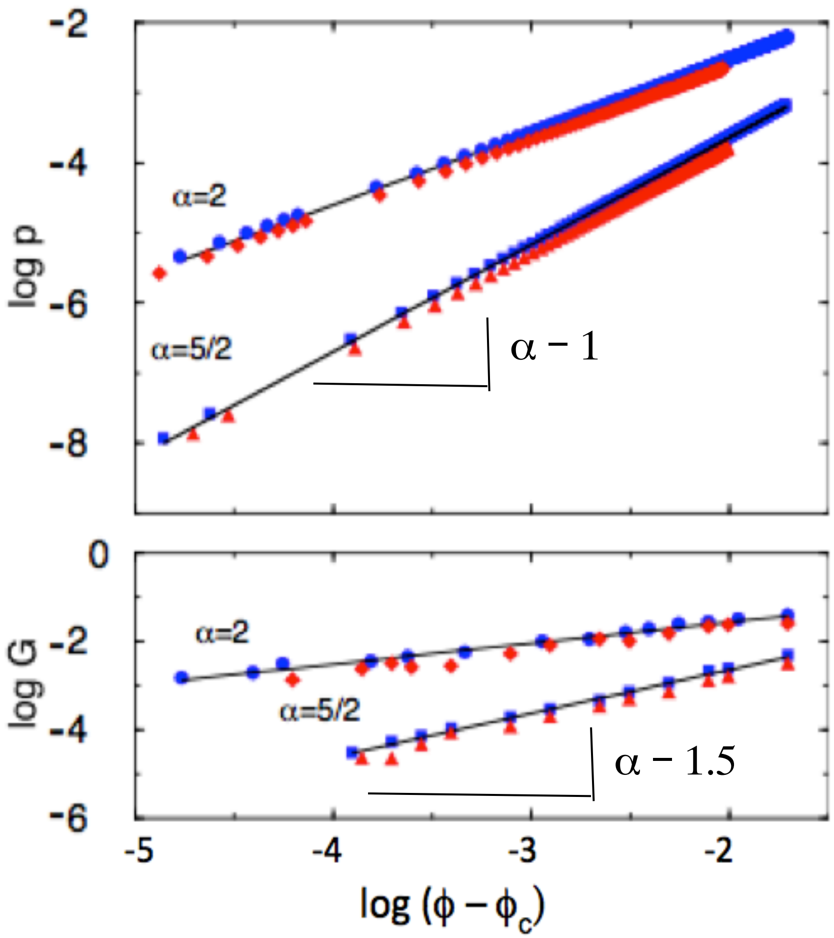
ϕ_c -- onset of jamming at $T = 0$



Quench to local energy minimum



Jammed solids different from crystals



Shear and compression become constrained at same ϕ_c

Jamming
G/B → 0 at ϕ_c (like liquid)

Crystal
G/B ~ 1

Shear infinitely weaker than bulk modulus at transition

Durian, O'Hern, Liu

Maxwell criterion for rigidity

Minimum number of overlaps needed for mechanical stability

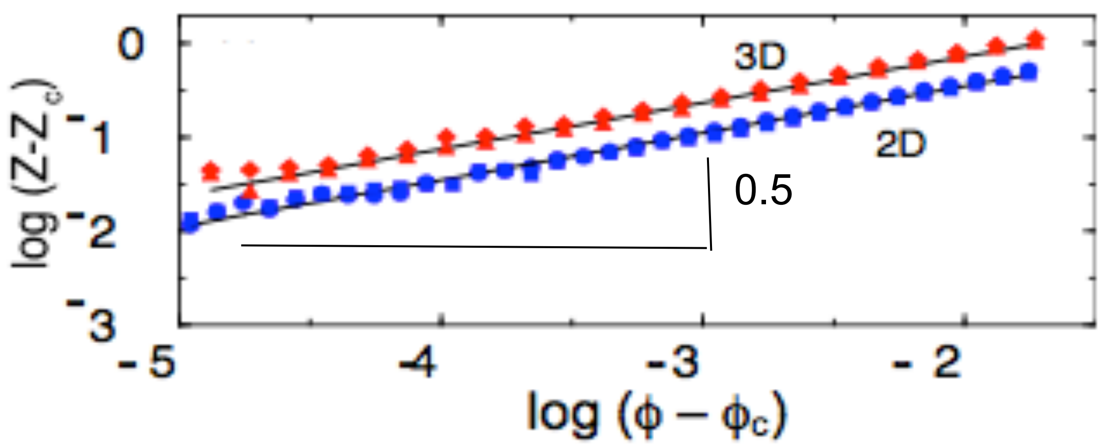
N frictionless spheres in D dimensions:

Match # equations (# non-trivial degrees of freedom) = ND
to # unknowns (# interparticle normal forces) = NZ/2

$\Rightarrow Z_c = 2D$

Criterion for rigidity: *global* condition - not *local*

Physics governed by connectivity (Thorpe, Phillips, Alexander)



O'Hern, Liu

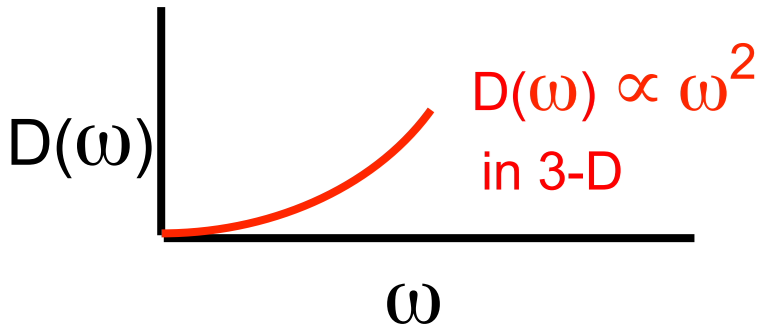
Normal modes in "normal" solid

Low-frequency normal modes

$\Longrightarrow$ long-wavelength plane waves.

Density of modes, $D(\omega)$, from counting waves:

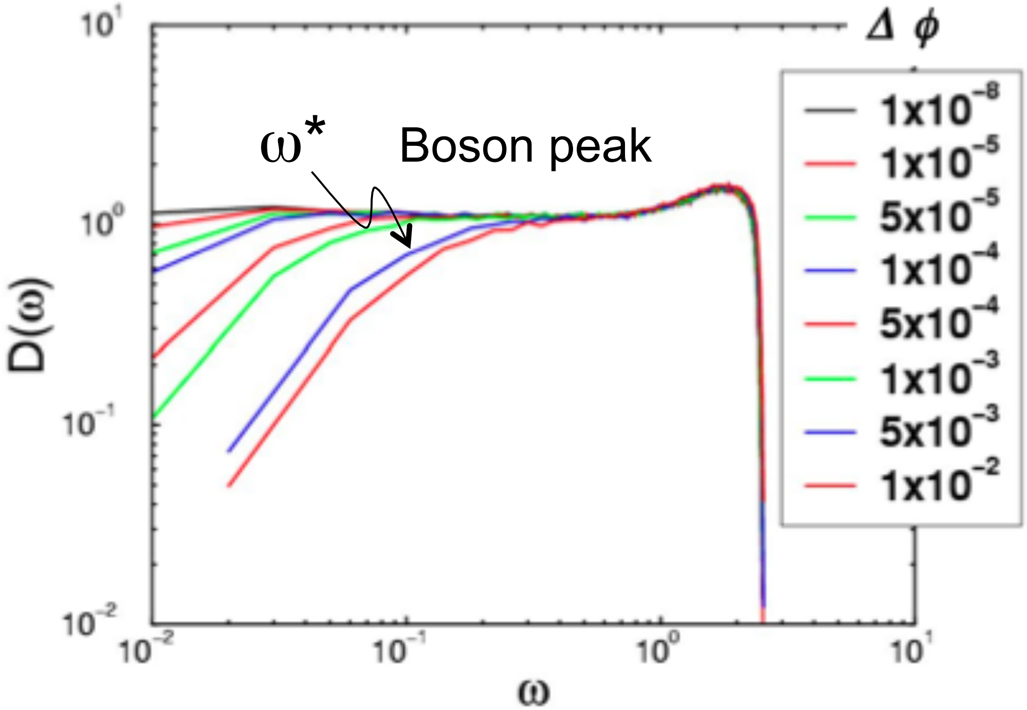
$D(\omega) \propto \omega^{d-1}$ in d-dimensions.



Long wavelengths "average" over disorder.

All solids *should* behave this way.

Density of states near jamming:
no Debye behavior at ϕ_c



ω^* is characteristic onset-frequency of new excitations

$\omega^* \rightarrow 0$ as $\Delta\phi \rightarrow 0$

Jamming is epitome of disorder
(no length on which one can average to recover elasticity)

New class of excitations

Silbert, Liu

Concrete example of new class of excitations:
emerge from critical point
What are they?

Created from soft modes:

Cutting argument (Wyart)

Structure (not plane waves):

"Quasi-localized" at low frequencies

Heat transport at low T:

Poor conductors -- nearly-constant diffusivity

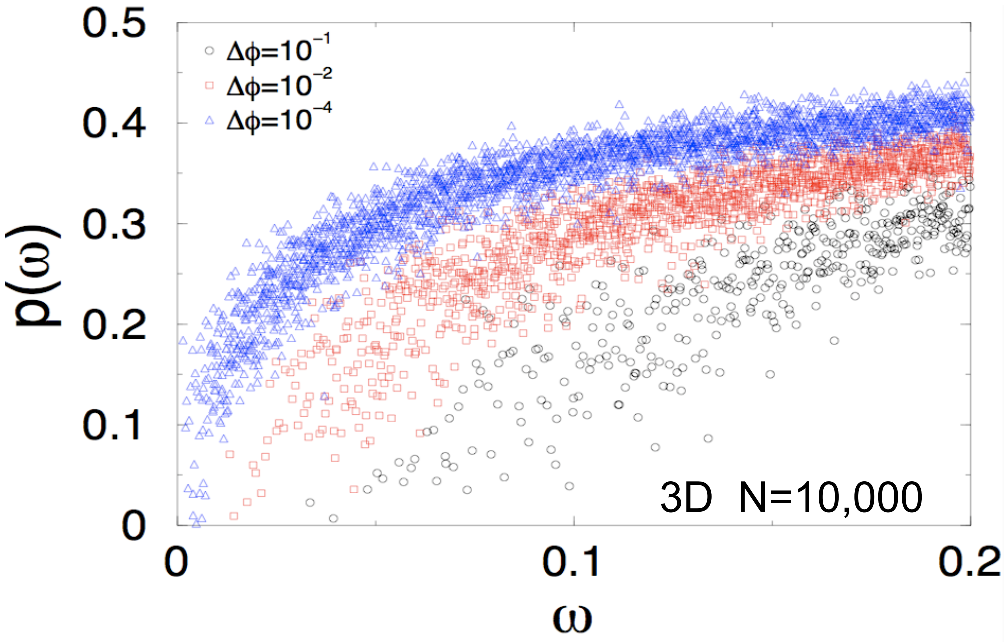
Highly anharmonic:

Dynamic heterogeneities?

Properties tuned by varying $\Delta\phi = (\phi - \phi_c)$

Spatial properties of modes

Participation ratio (measures localization): $p(\omega) = \dfrac{(\Sigma_\alpha |\varepsilon_\omega(\alpha)|^2)^2}{N\, \Sigma_\alpha |\varepsilon_\omega(\alpha)|^4}$



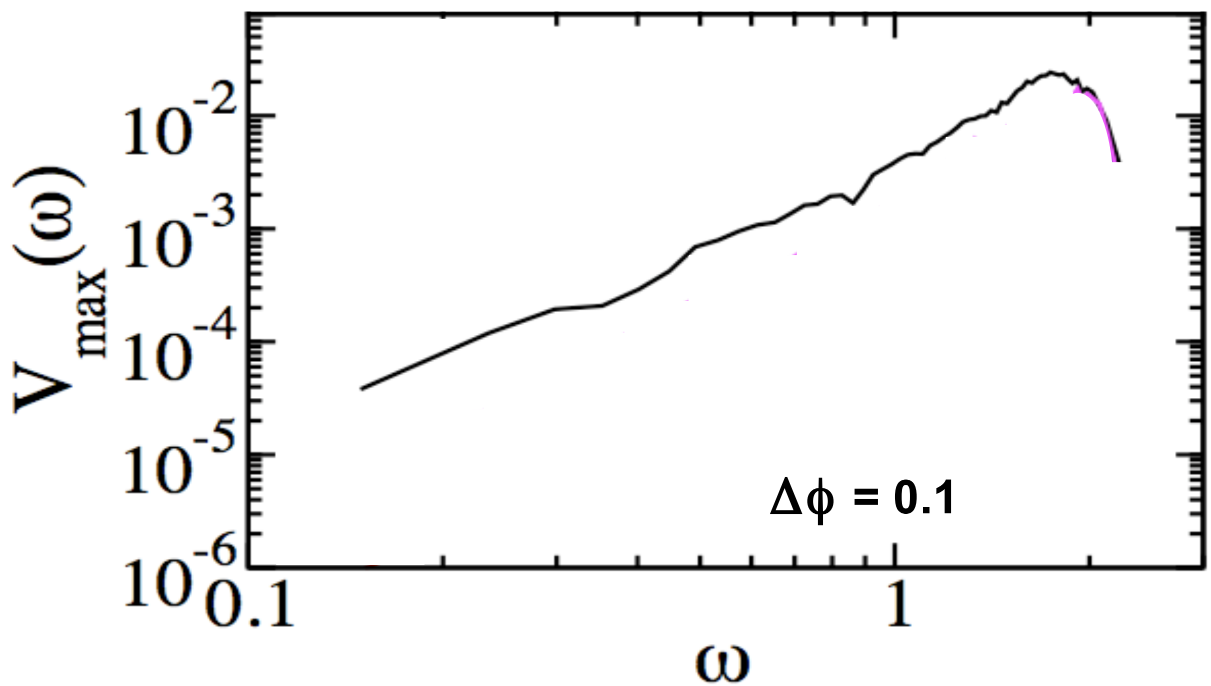
For all $\Delta\phi$, quasi-localized (resonant) modes near ω = 0

(from band tail of anomalous modes)

N. Xu, V. Vitelli, A. Liu

Basins and energy barriers

V_{max} = energy barrier to new ground state.



Lowest - ω modes $\Rightarrow$ smallest barriers

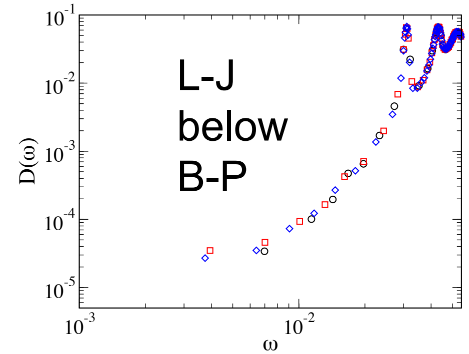
Most anharmonic

N. Xu, V. Vitelli, A. Liu

Can modes explain low-T properties of glasses?

Must reproduce predictions of tunneling model:

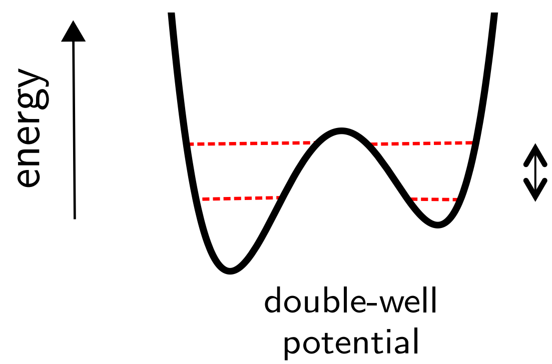
Linear specific heat: $\mathcal{D}(\omega) \sim$ const.
T^2 thermal conductivity
Saturation
Time dependent specific heat



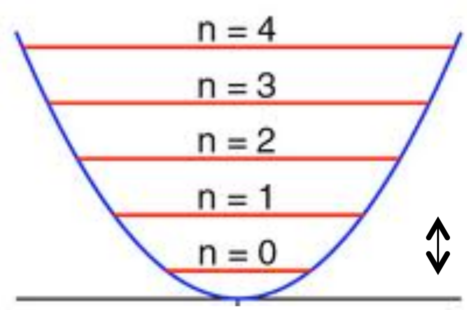
⟹ Phonon echoes (similar to spin echoes in NMR)

Need Quantum 2-level systems   Not thought possible from vibrations

Two-level system



Harmonic oscillator



Acoustic echoes in anomalous modes?

At low ω, modes highly anharmonic + localized

CLASSICAL echoes in simulations (w/o quantum 2-level systems).

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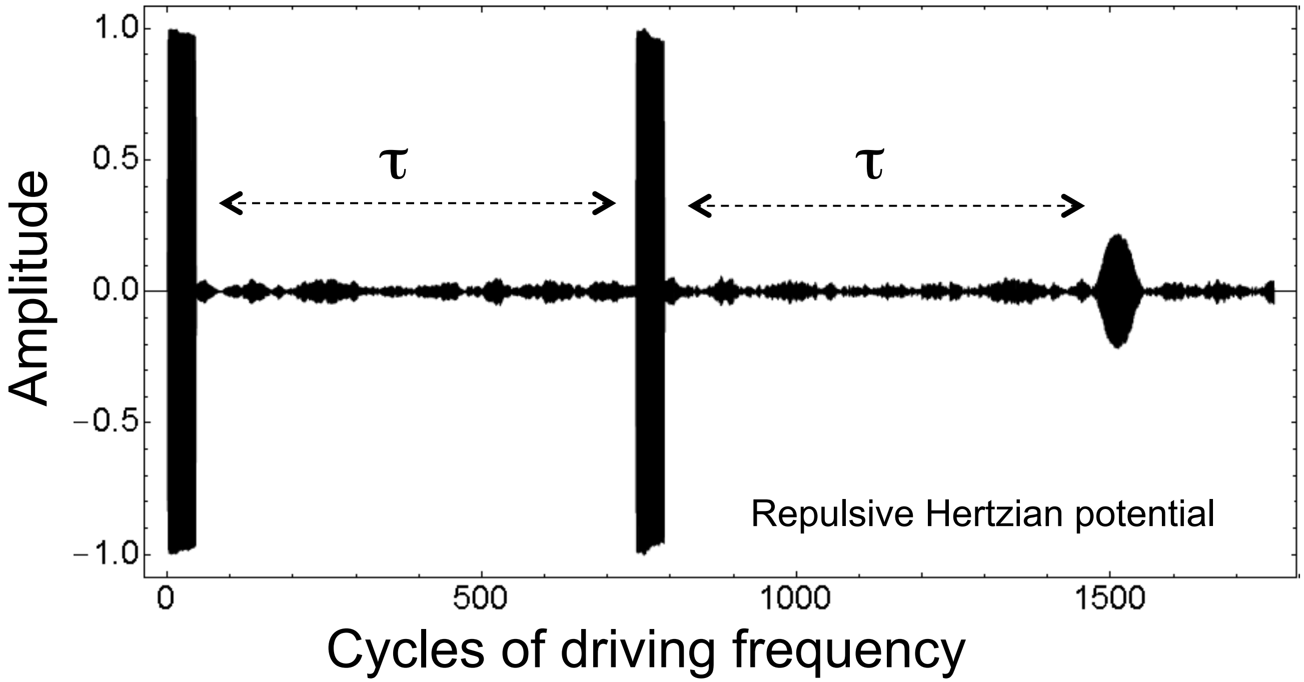


Time of echo = τ

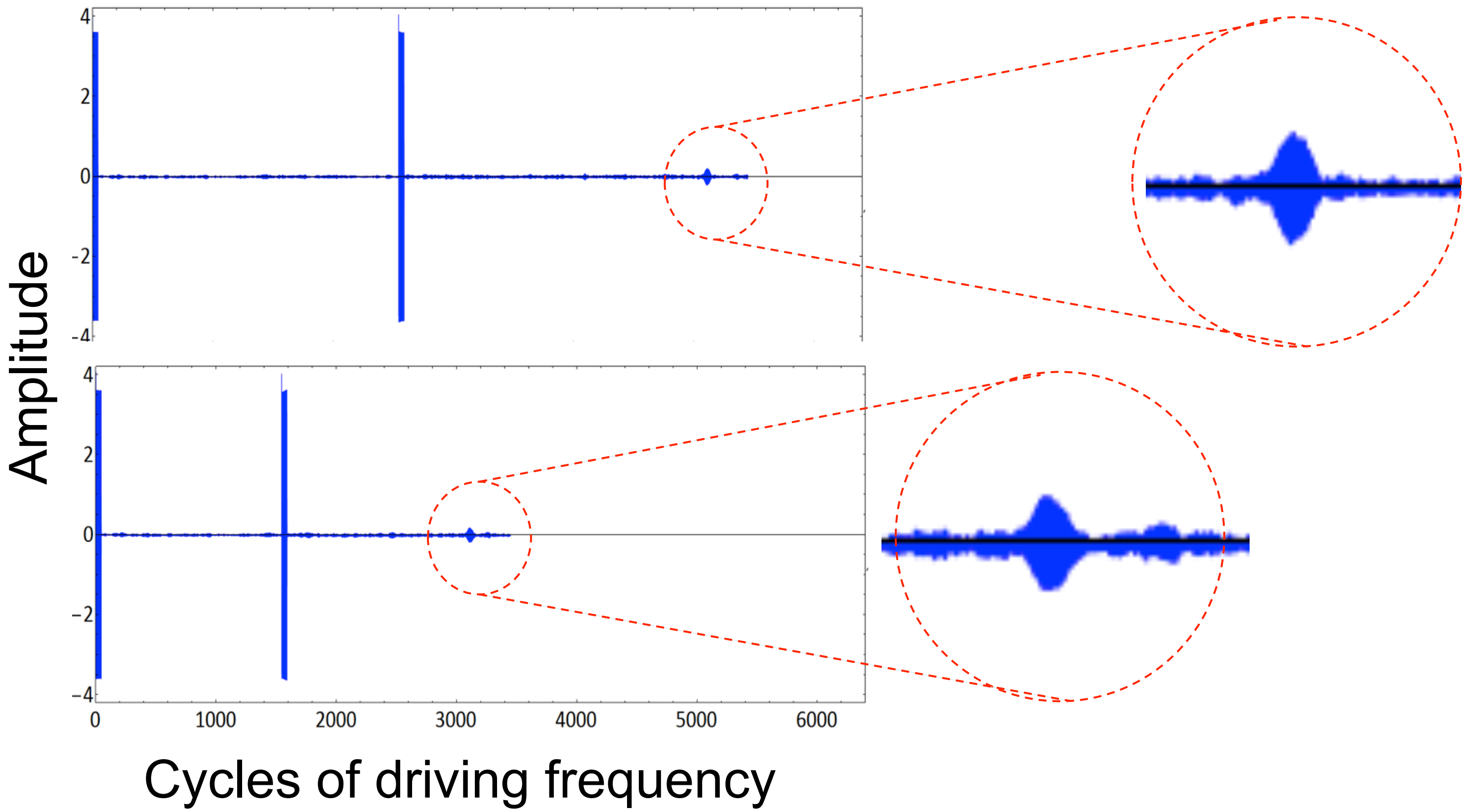
Justin Burton

Acoustic echoes

appears at time τ

Repulsive Hertzian

Average over 10,000 $N = 10^3$



Justin Burton

Acoustic echoes

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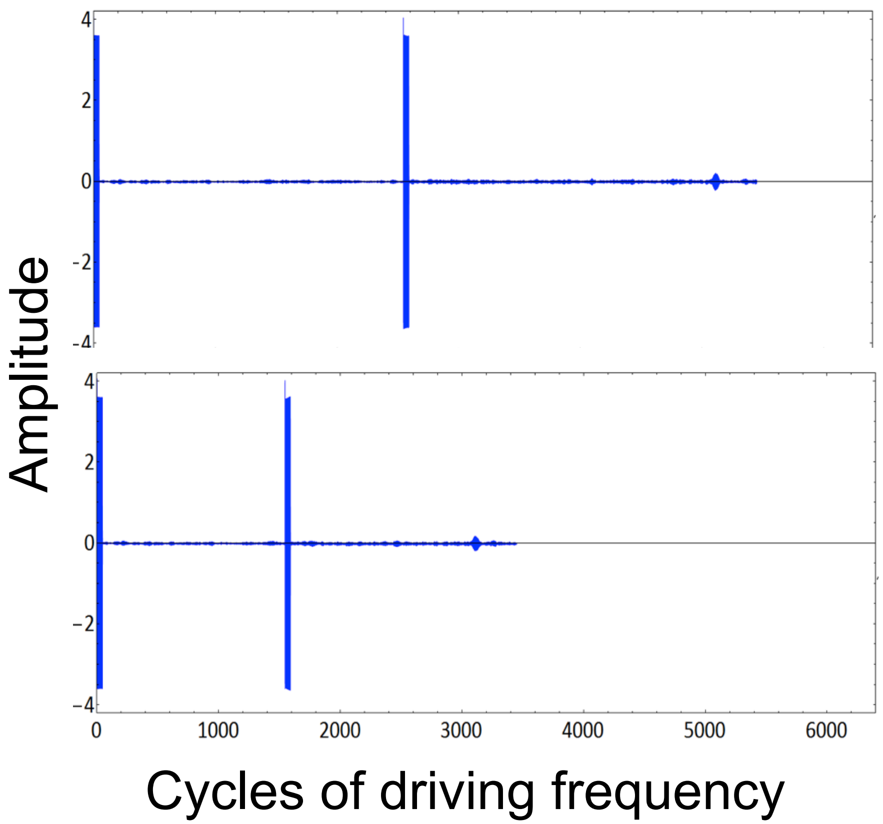
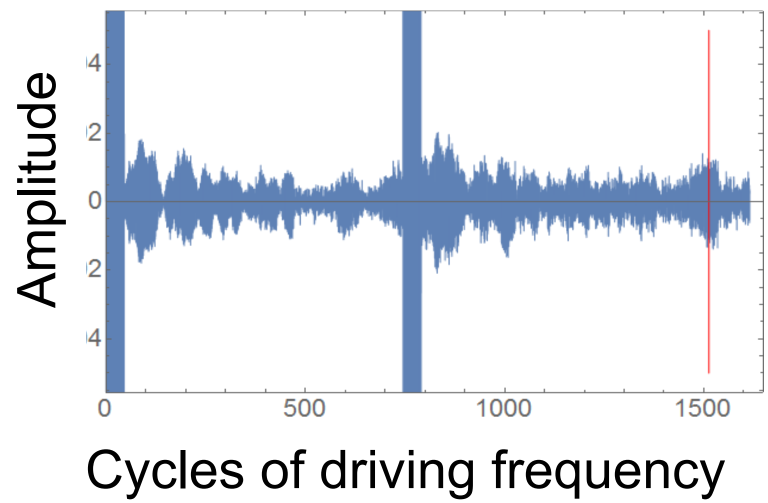
Repulsive Hertzian
Average over 10,000 N = 10^3



12 systems, N = 10^6



Justin Burton

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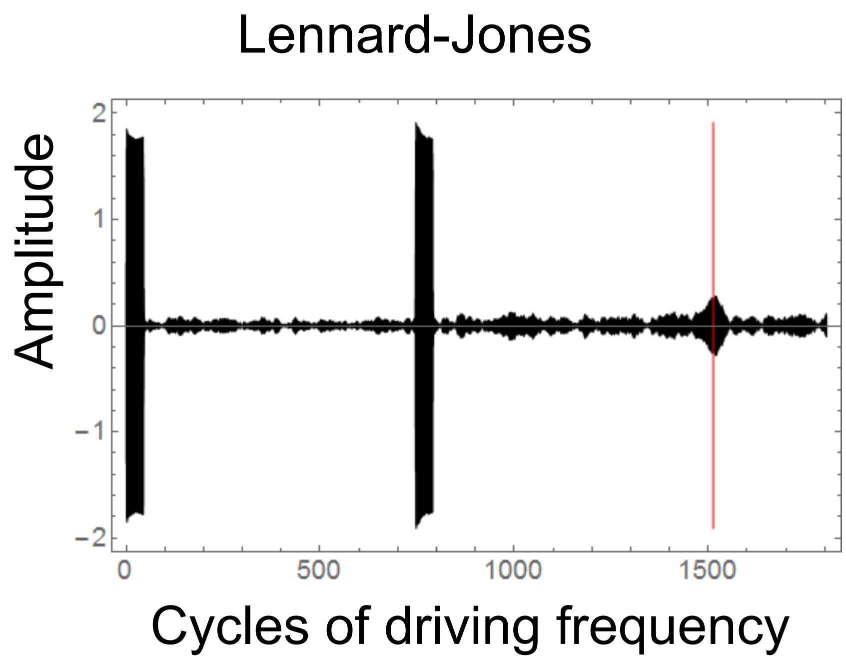
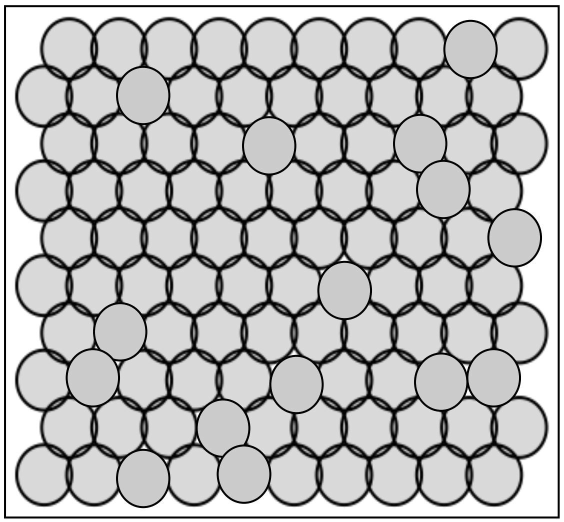


Echoes independent of inter-particle potential.
Needs: anharmonicity & weak coupling between modes (localization)

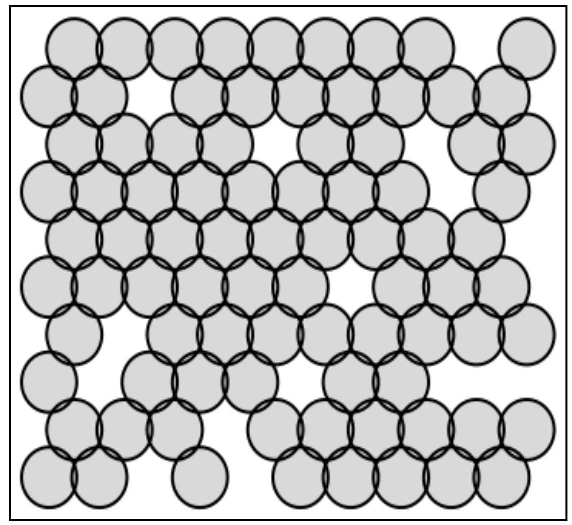
Justin Burton

Tune from perfect order to complete disorder

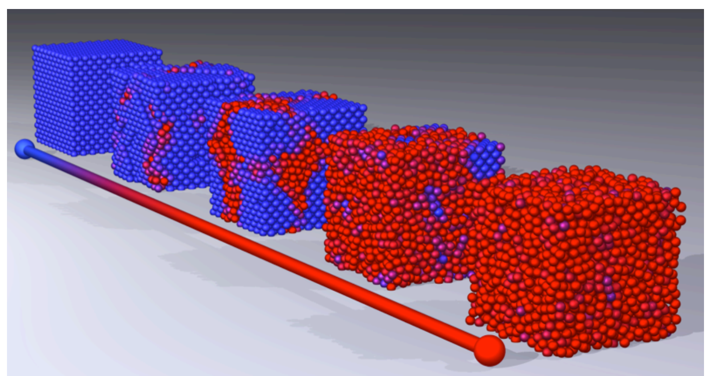
Start w/ perfect crystal



Create m random vacancies (or vacancy/interstitial pairs)



Relax positions, vary pressure



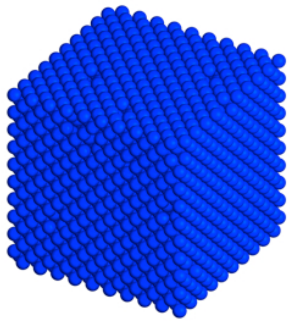
Goodrich, Liu

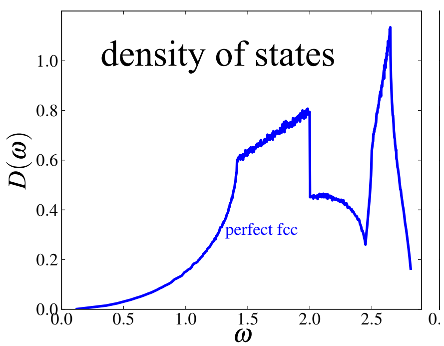
From order to disorder:

When does (dis)order dominate response?

ordered

$F_6=1$





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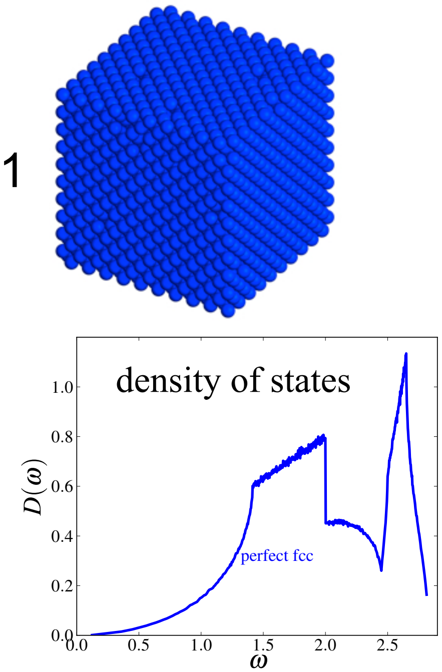
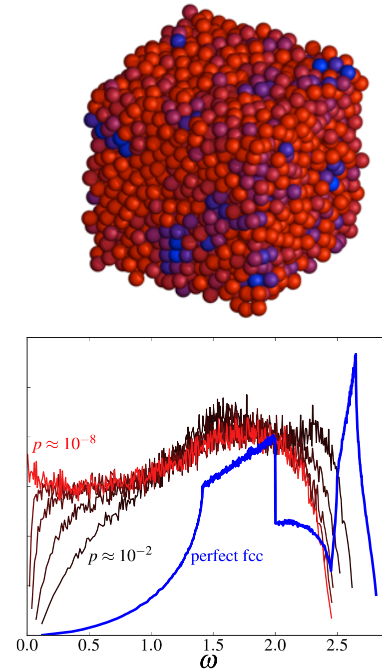


disordered

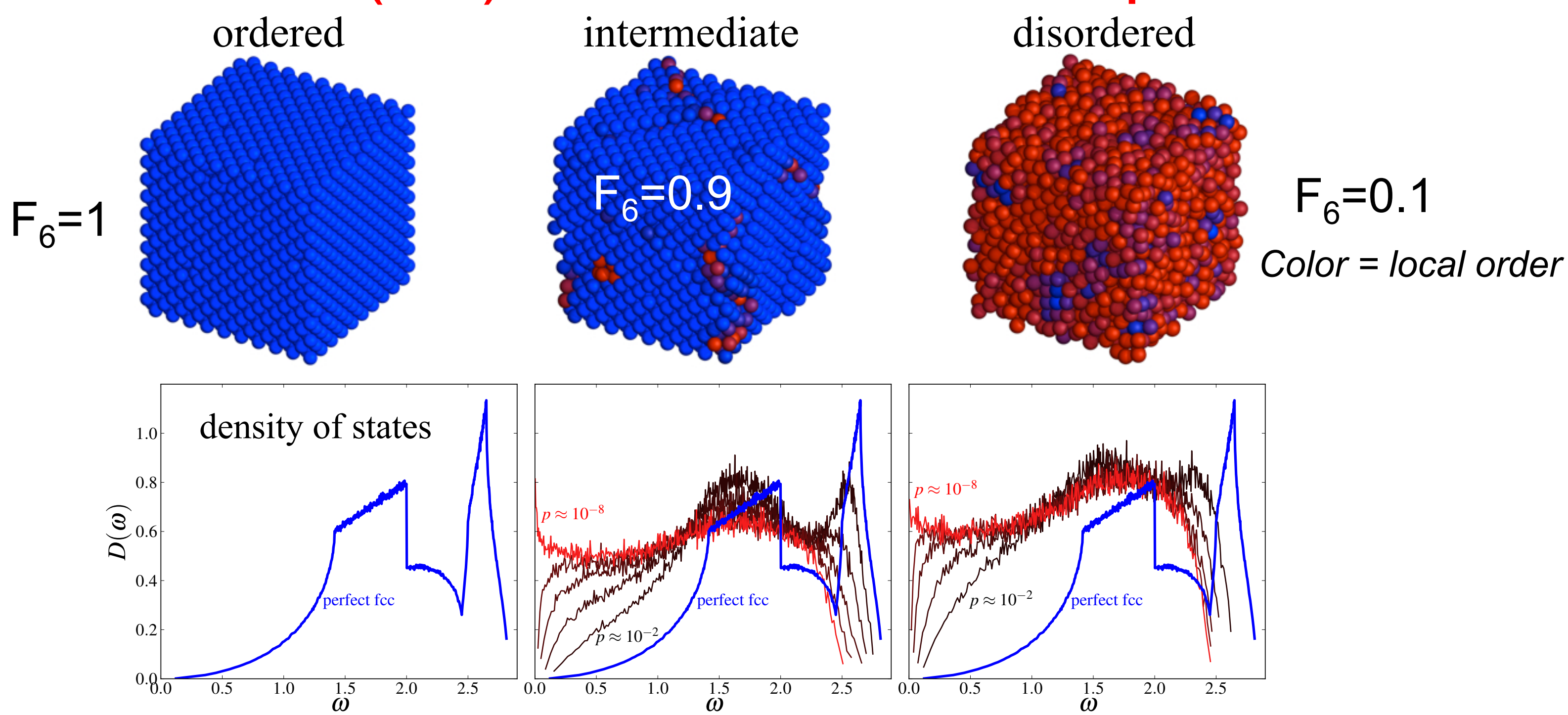
F_6=0.1

Color = local order



From order to disorder:

When does (dis)order dominate response?



Little disorder makes it behave like jammed solid

From order to disorder:

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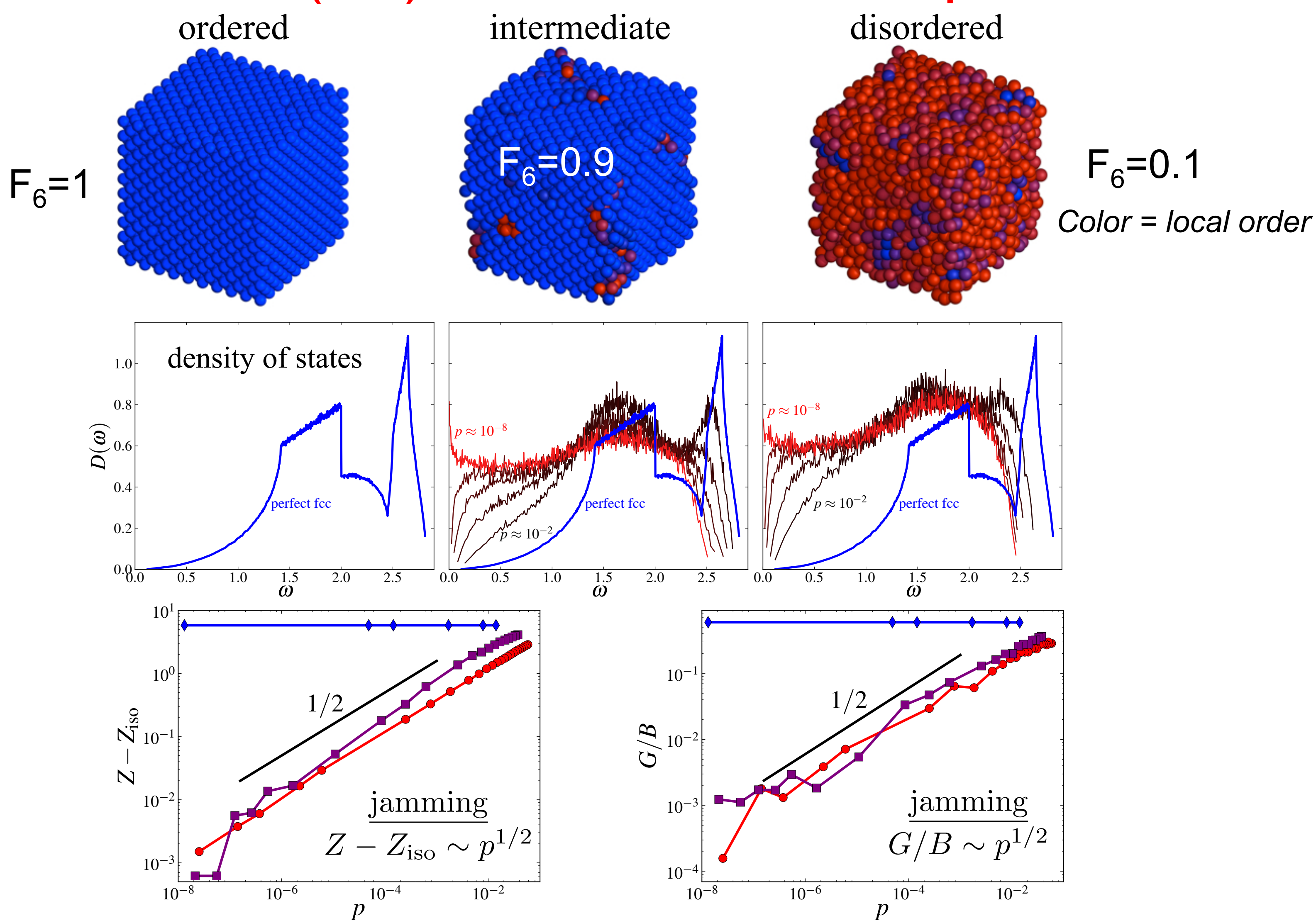

Little disorder makes it behave like jammed solid

Jamming – disordered limit for rigidity

Implication of jamming ⇔ Low-T glasses

Excess low-energy excitations ⇒ Boson peak

Small constant diffusivity ⇒ $\kappa(T) \propto T$ above plateau

Anharmonic & quasi-localized modes ⇒ phonon echoes

Basic results hold for:

Long-range interactions with attractions (*e.g.*, L-J potentials)

New class of excitations

⇒ new way to think about glass properties

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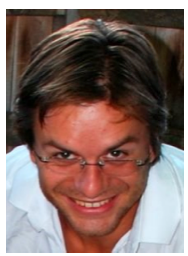

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