Universität Konstanz

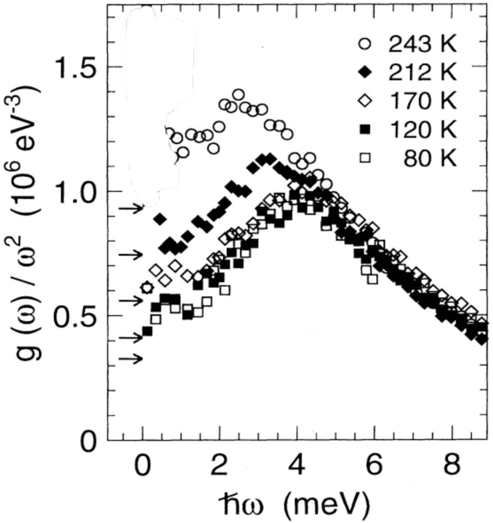
Vibrational phenomena in athermal amorphous solids and the un-jamming transition

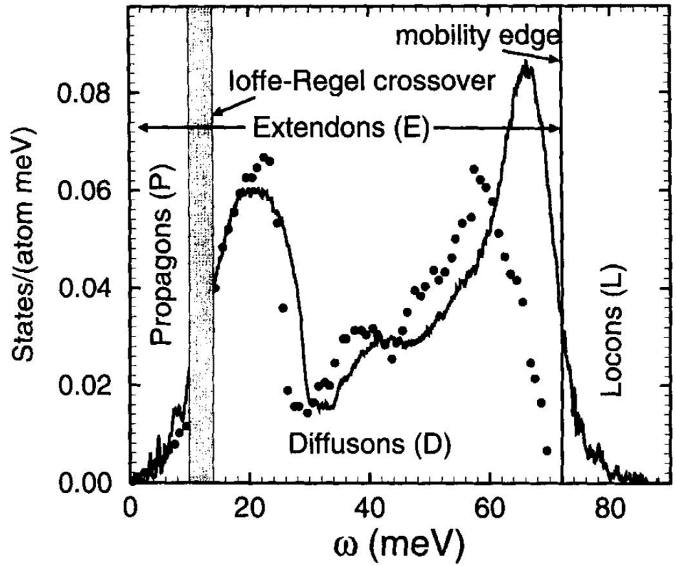
Matthias Fuchs

Universität Konstanz

Yukawa Institute for Theoretical Physics, Kyoto , July 30, 2024

Vibrations in glass: Density of states





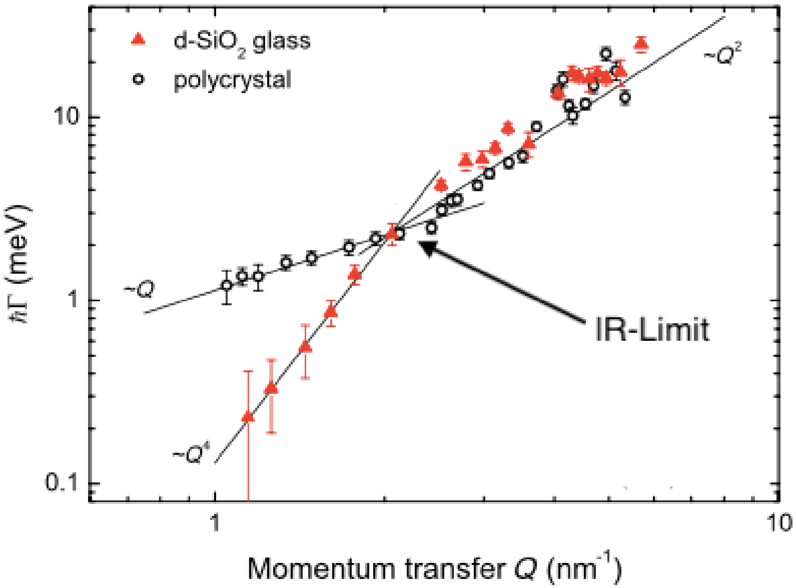
- universal Boson peak in reduced vDOS
- excess above Debye for $T \to 0$

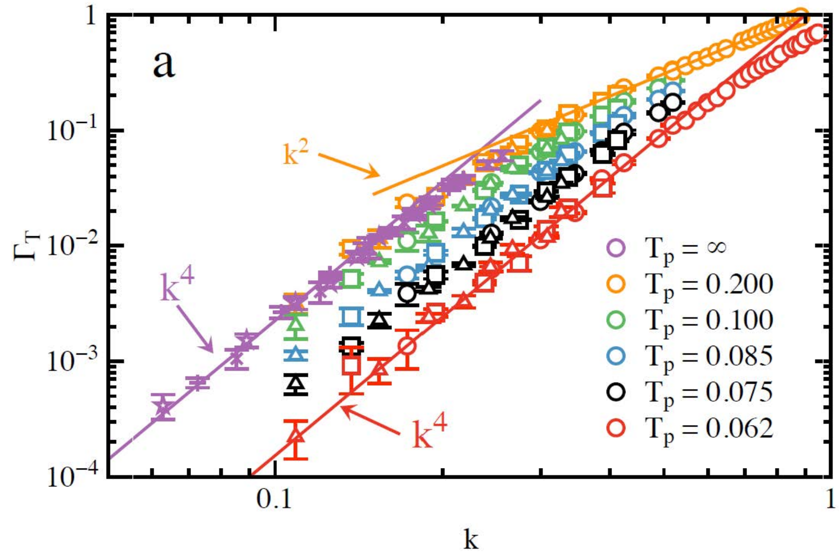
- Wave-like below Ioffe-Regel limit

∗ Wuttke et al., Phys. Rev. E 53, 4026 (1995); glycerol

∗ Allen, Feldmann, Fabian, Phil. Mag 79, 1715 (1999); am Si

Vibrations in glass: Sound damping



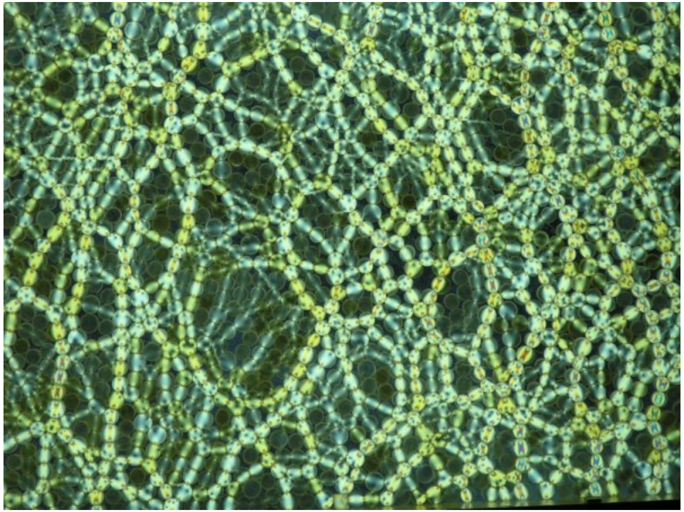


- Rayleigh-damping, $\Gamma \propto q^4$
- history dependent, stable glass: small Γ

∗ Baldi et al., Phys. Rev. Lett 110, 185503 (2013)

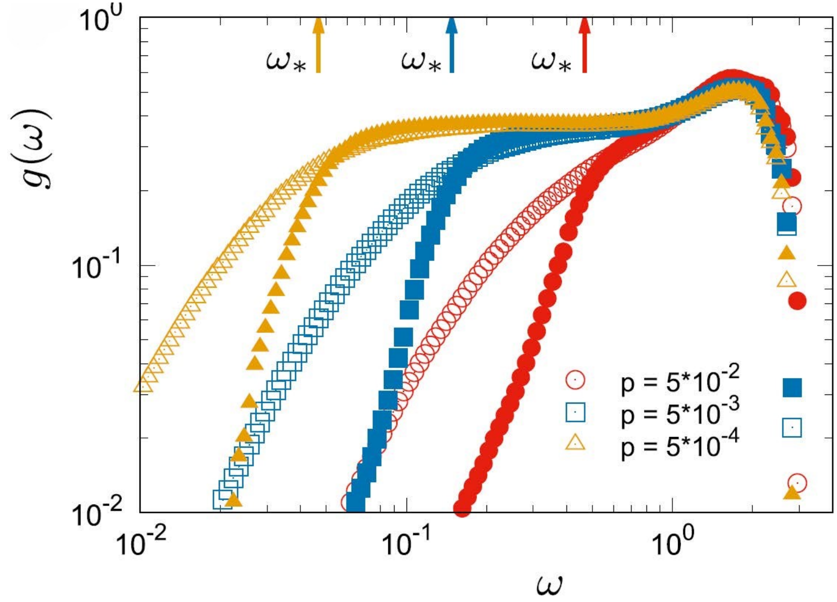
∗ Wang, Berthier, Flenner, Guan, Szamel, Soft Matter 15, 7018 (2019)

Un-jamming of disordered solid



- Force chains in jammed granular media

∗ Majmudar & Behringer, Nature 435, 1079 (2005)



- floppy modes in vDOS for $p \to 0$

∗ Mizuno, Shiba, Ikeda, PNAS 114, E9767 (2017); soft repulsive

Outline

- Vibrational anomalies in glass
- Euclidean Random Matrix (ERM) ensemble
  - Exact diagonalization
    - vibrational density of states (vDOS)
    - sound damping
    - eigenmodes
  - Self-consistent field theory
    - non-planar Feynman diagrams
- Un-jamming in ERM model
  - cut-off spring function
  - Self-consistent transverse response theory

Philipp Stengele

Florian Vogel

The ERM-model

Harmonic oscillators

$$\ddot{\Phi}_i = -\sum_{j=1}^{N} M_{ij}\,\Phi_j\,, \qquad \text{for } i = 1, \ldots, N \to \infty$$

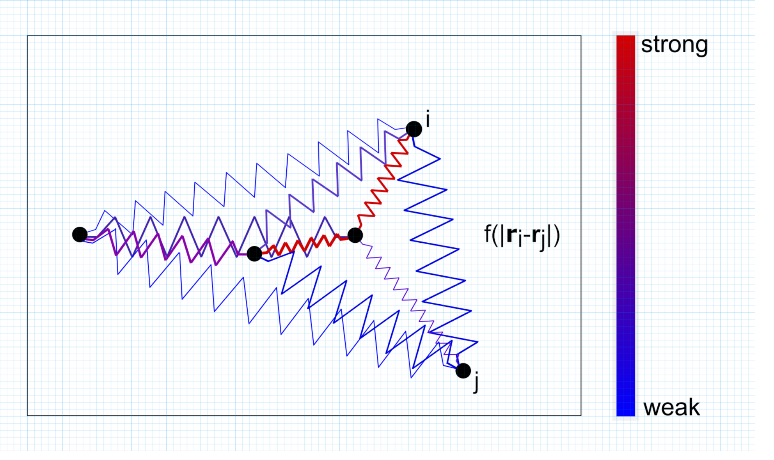
at random positions $\mathbf{r}_j$ with potential

$$U(\boldsymbol{\phi}) = \frac{1}{2}\sum_{i,j} M_{ij}\phi_i\phi_j = \frac{m\omega_0^2}{4}\sum_{i,j} f(|\mathbf{r}_i - \mathbf{r}_j|)(\phi_i - \phi_j)^2$$

spring function $f(r) \geq 0 \Rightarrow$ eigenvalues $\lambda^k \geq 0$

convention: $m = \omega_0 = \sigma = 1$.

Model



∗ Mezard et al., Nucl. Phys. 559B, 689 (1999)

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perform disorder average $\overline{\ldots}$

$\Rightarrow$ Euclidean random matrix (ERM) ensemble*

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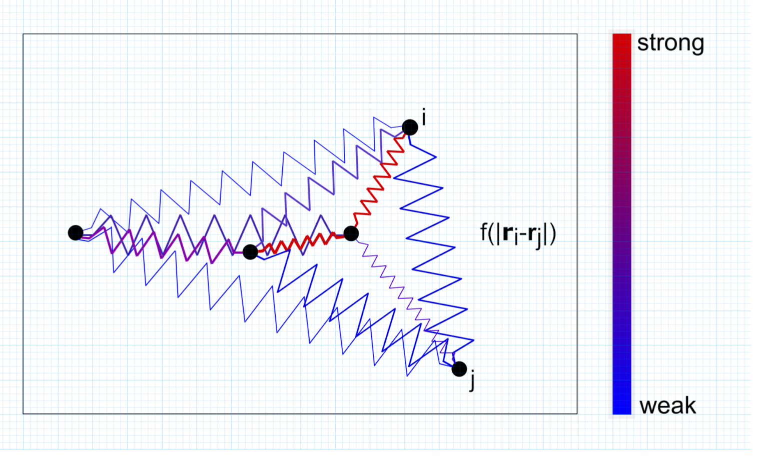

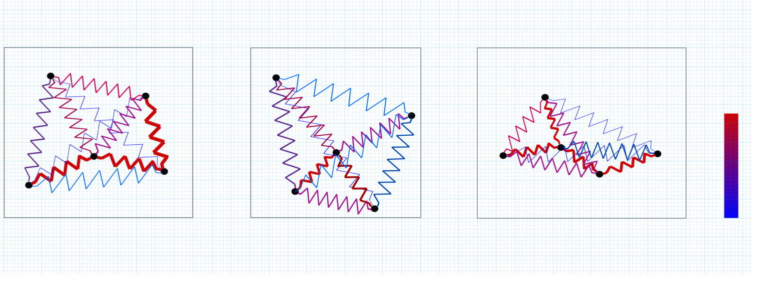

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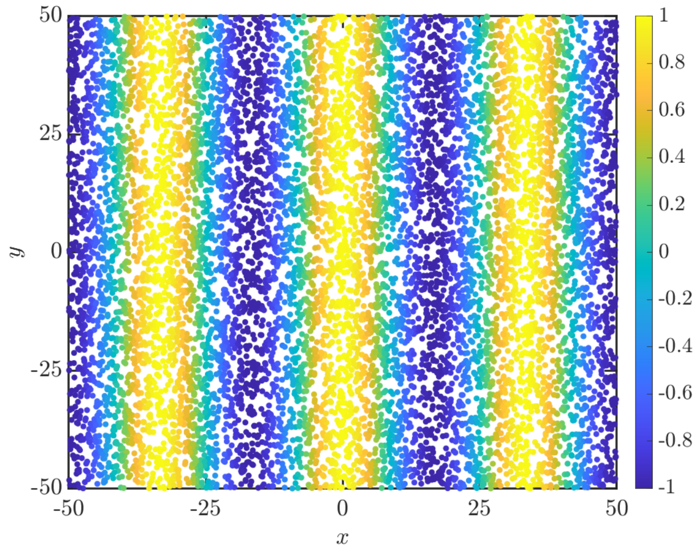
Exact diagonalization



velocities given in colors; disk diameter = range σ; 2D density $n = N\sigma^d/V = 1$, $N = 10^4$ particles, (up to $N = 10^6$) initial wavenumber $q = \frac{2\pi}{L}3$,

spring function $f(r) = \exp\{-(\frac{r}{\sigma})^2/2\}$

The ERM-model

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Field theory

- Response function $G(\boldsymbol{q}, \omega = \sqrt{z})$

$$G(q,z) = \overline{\frac{1}{V}\sum_{i,j=1}^{N} e^{i\boldsymbol{q}\cdot(\boldsymbol{r_i}-\boldsymbol{r_j})}\left[\frac{1}{z-M}\right]_{ij}}$$

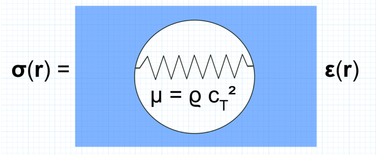
$$= \frac{n}{\underbrace{z-\omega_0^2(q)}_{G_0^{-1}} - n\Sigma(q,z)}$$

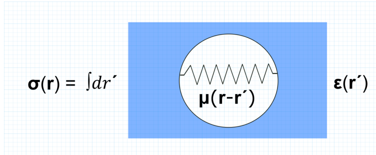
- Self-energy $\Sigma(q,z)$ self-consistent†
- non-planar diagrams‡

† Grigera et al. , Phys. Rev. Lett. 87, 085502 (2001)
‡ Vogel, Fuchs, Phys. Rev. Lett. 130, 236101 (2023)

ERM self-consistent field theory*

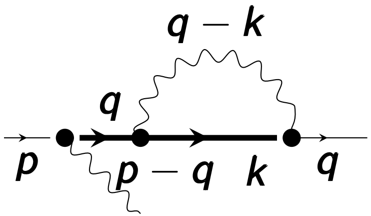
heterogeneous elasticity in non-local stress-strain relation



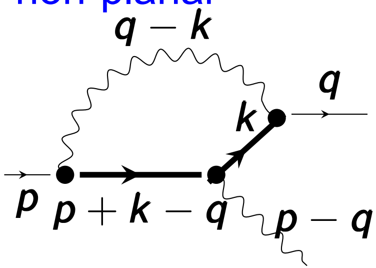


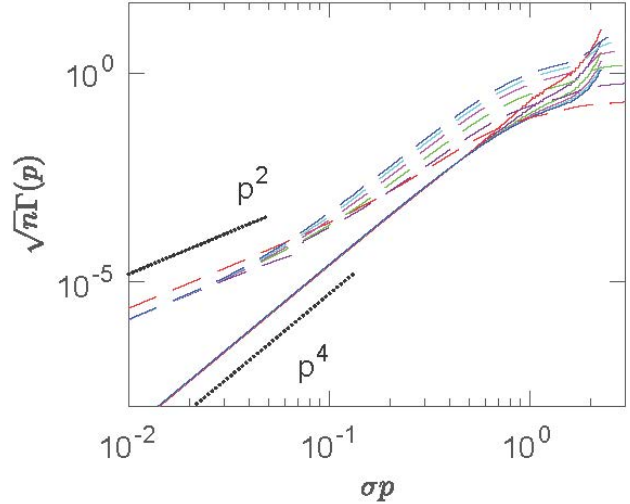
shows up in non-planar diagrams in perturbation expansion

planar



non-planar†





- damping:
  Rayleigh $\Gamma \propto q^4$ (non-planar)
  hydrodynamic $\Gamma \propto q^2$ (planar)
- HET‡ disorder: $\gamma = (n\hat{f}''(0))^2$

∗ Vogel, Fuchs, Phys. Rev. Lett. 130, 236101 (2023)
† Grigera et al. , J. Stat. Mech. P02015 (2011)
‡ Schirmacher et al., J. Phys. A, 52, 464002 (2019)

ERM — stable glass

ERM - exact diagonalization

$$\Phi_i(t) = \sum_k (\mathbf{\Phi}(0) \cdot \mathbf{e}^k) \cos(\omega^k t)\, e_i^k$$

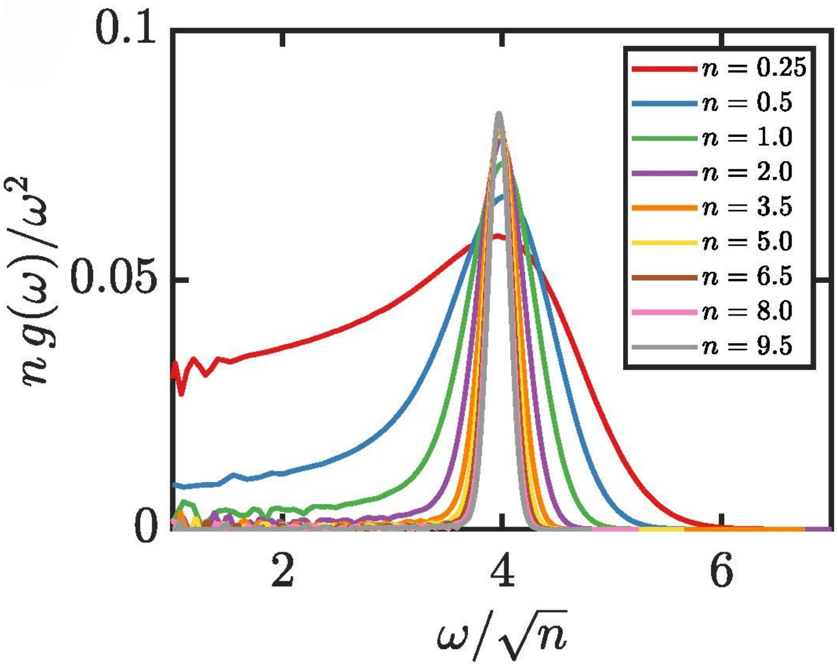
ERM - field theo

$$S(q, \omega) = \frac{-2\omega}{n\pi} \mathrm{Im}\{G(q, z = \omega^2 + i0)\}$$

Results

- Density of states
  $g(\omega) = S(q \to \infty, \omega)$

reduced vDOS



- $g(\omega) \to A_0 \omega^2$ gives Debye $A_0 \propto (1/n c_T^3)$

Baumgärtel, Vogel, Fuchs, Phys. Rev. E 109, 014120 (2024)

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Results

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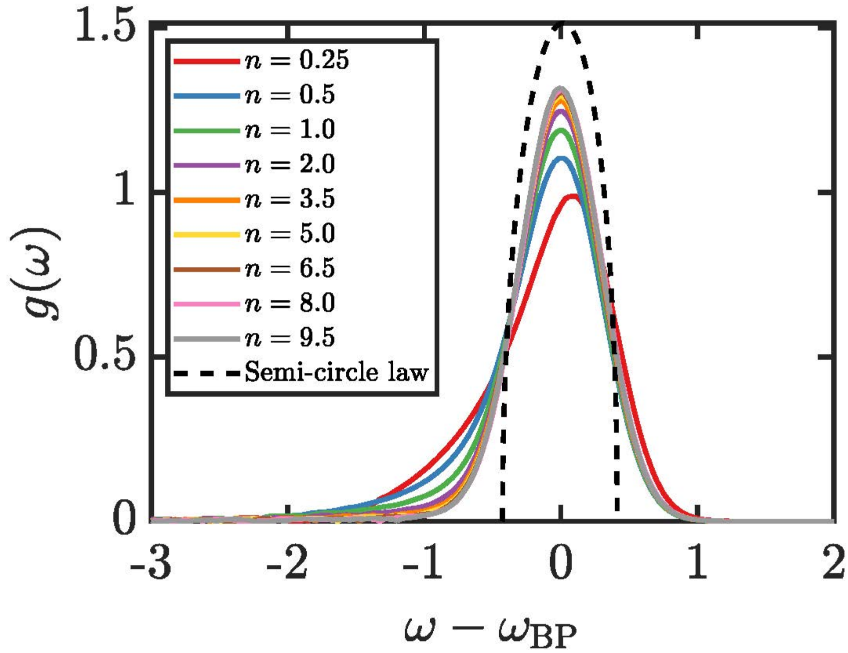
  $g(\omega) = S(q \to \infty, \omega)$

shifted vDOS



- Wigner semi-circle law for boson peak

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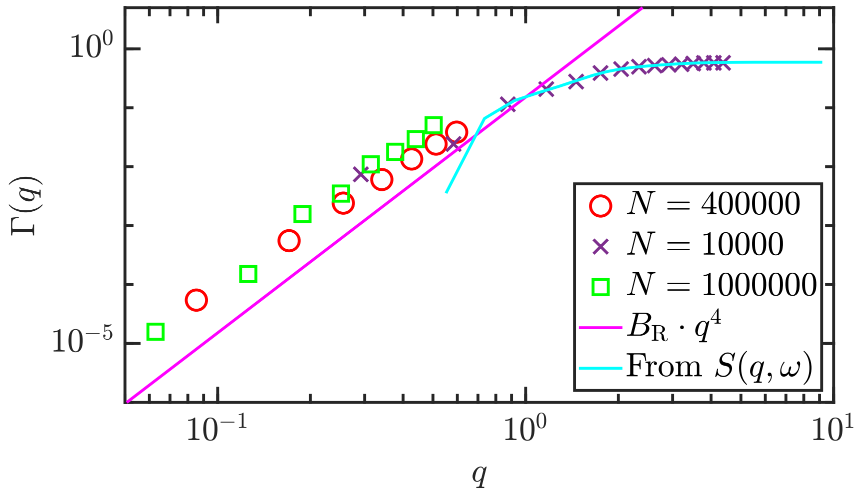
Results

- Density of states
  $g(\omega) = S(q \to \infty, \omega)$
- Rayleigh sound damping

sound damping $(n = 1)$



- self energy $\Sigma(q, z \to 0) \propto q^2 z^{3/2}$

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ERM - exact diagonalization

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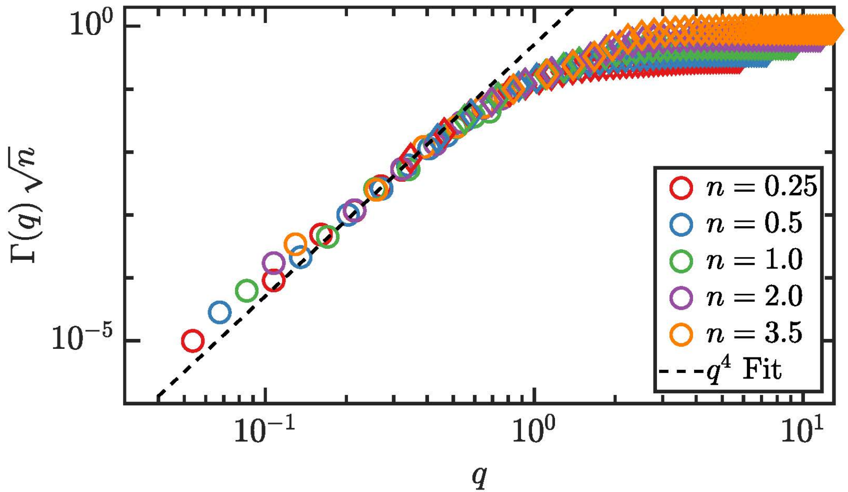


- damping increases w disorder, $\Gamma \propto 1/\sqrt{n}$

ERM — stable glass

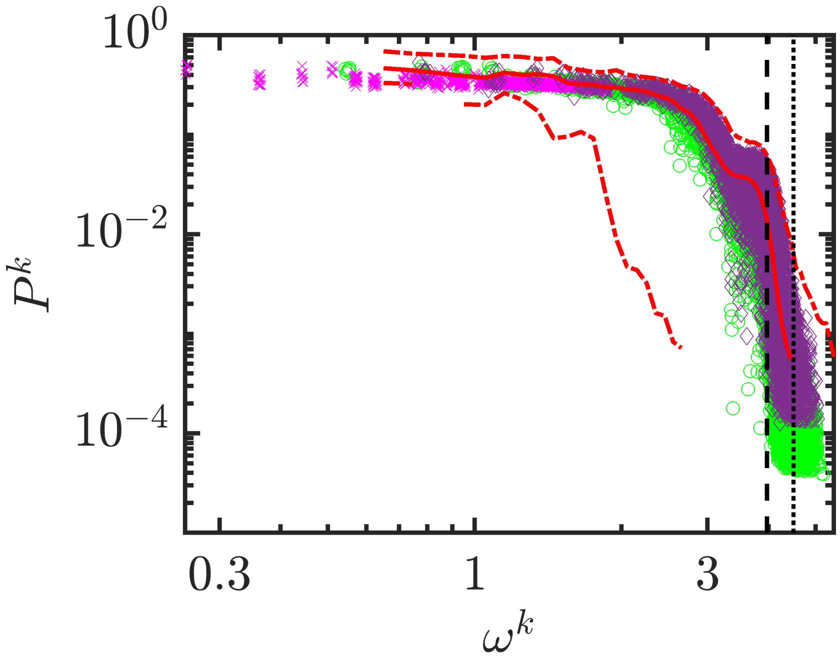
ERM - exact diagonalization

$$\Phi_i(t) = \sum_k (\mathbf{\Phi}(0) \cdot \mathbf{e}^k) \cos(\omega^k t)\, e_i^k$$

Results

- Density of states $g(\omega) = S(q \to \infty, \omega)$
- Rayleigh sound damping
- waves -to- localized modes

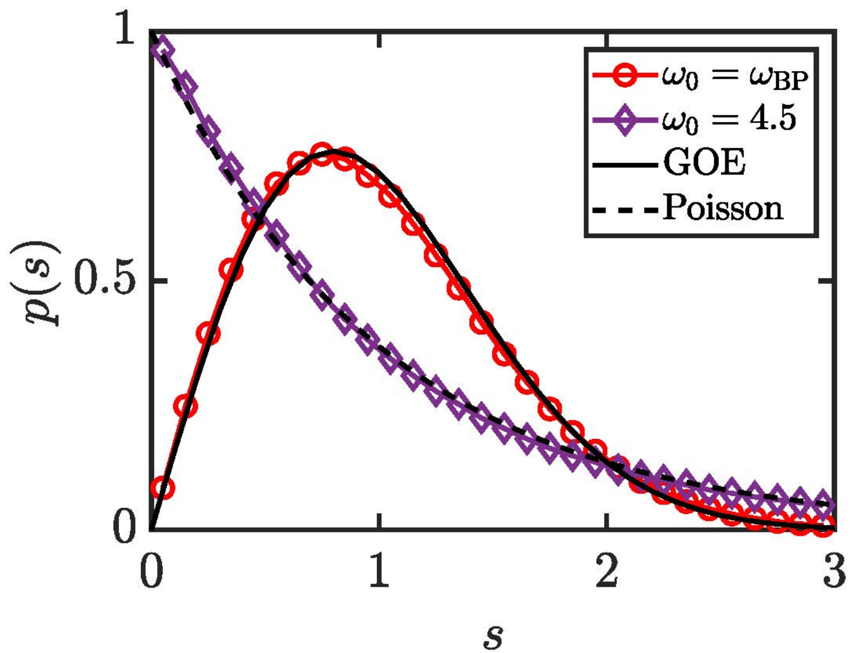
participation ratio $(n = 1)$



- modes localized above boson peak

ERM — stable glass

level spacing $(n = 1)$



ERM - exact diagonalization

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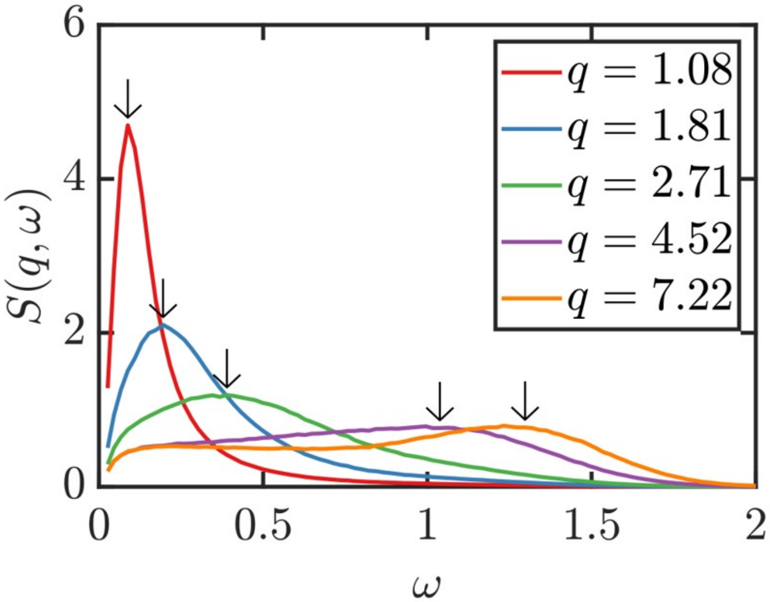
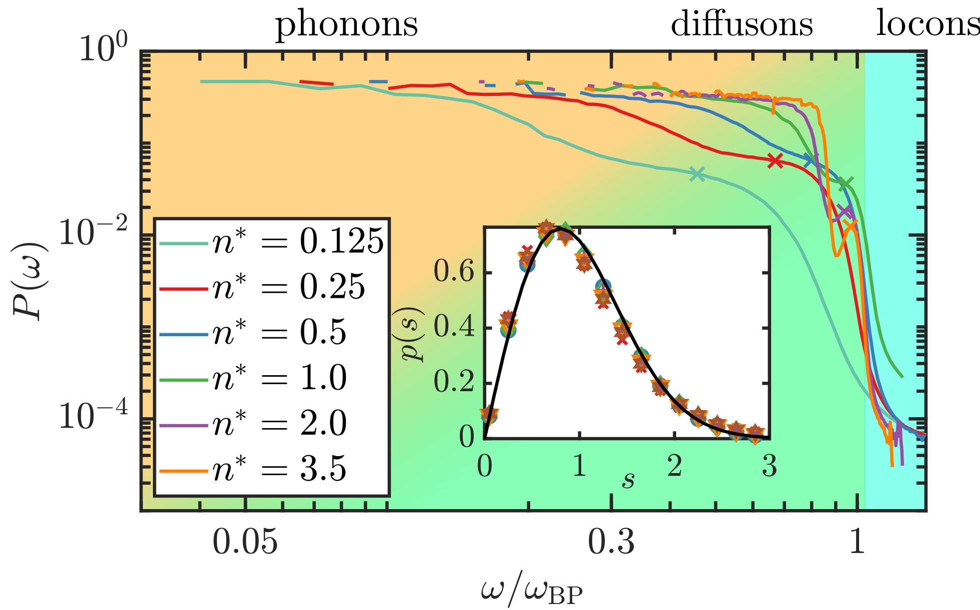
Results

- Density of states $g(\omega) = S(q \to \infty, \omega)$
- Rayleigh sound damping
- waves -to- localized modes

- Wigner's surmise on level spacing at ω_{BP}

Stronger disorder in Gaussian ERM





- dynamic structure factor broadens beyond Ioffe-Regel limit ($n = 1/16$)

- propagons, diffusons, locons
- Wigner level repulsion

ERM-model: finite coordination

Harmonic oscillators

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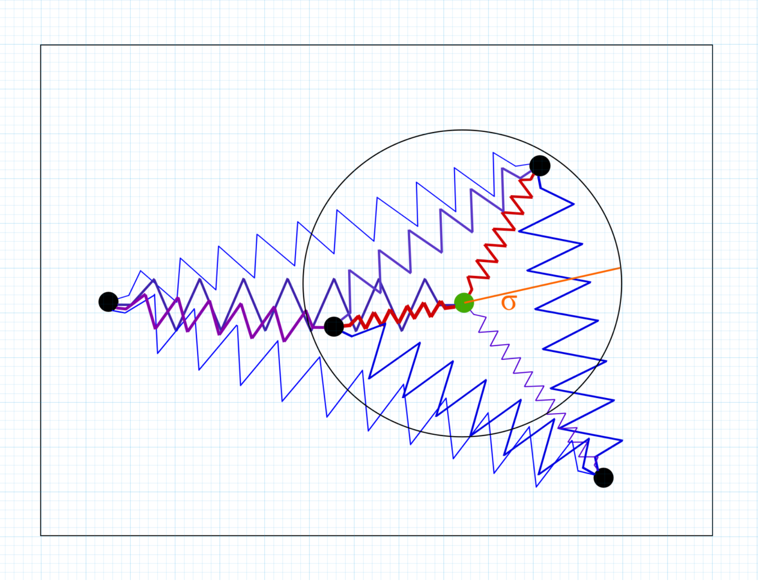
perform disorder average $\overline{\ldots}$

$\Rightarrow$ Euclidean random matrix (ERM) ensemble*

Model



spring function $f(r) = \Theta(\sigma - r)$

∗ Mezard et al., Nucl. Phys. 559B, 689 (1999)

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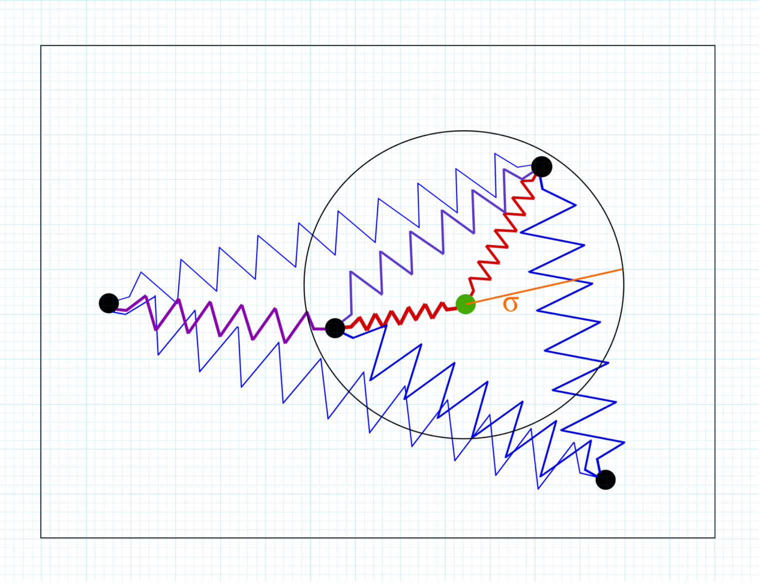

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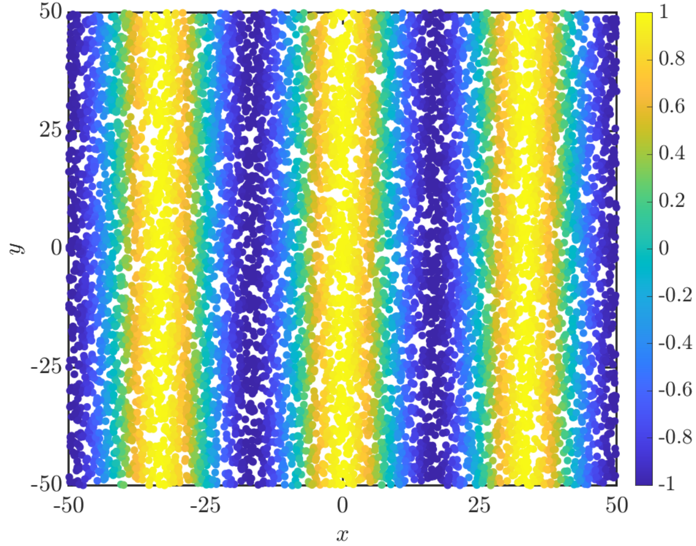

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spring function $f(r) = \Theta(\sigma - r)$

finite coordination number $\bar{z} = 5.2$

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Un-jamming transition

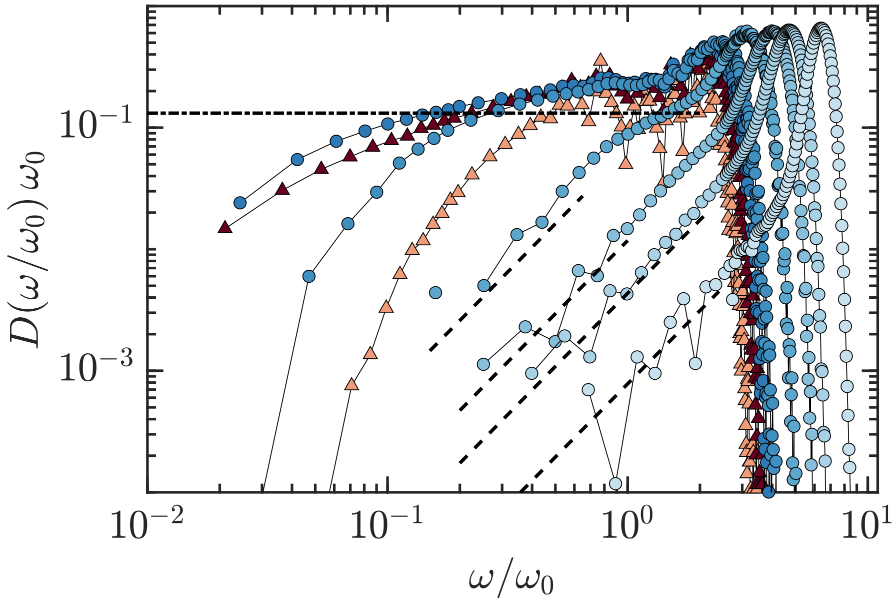
Maxwell's isostatic criterion

- Number of degrees of freedom $=$ number of constraints
- Each bond shared by 2 particles

$$\Rightarrow \quad dN = z_c N/2$$

- critical coordination number* z_c

- finite range $f(r)$ gives: $\bar{z} = \overline{M}/N - 1$
  $\overline{M}$ = average number of entries in M_{ij}
  $\bar{z} = V_d n$, with volume V_d of sphere of radius σ



- non-monotonous low-frequency vDOS
- floppy modes in un-jammed state

$*$ Wyart, Ann. Phys. 30, 1 (2005)

Self-consistent theory of transverse modes

- Transverse modes change character at transition
- Structure is frozen-in ($S_q(t) = S_q$) at $T \ll T_g$

Transverse velocity correlator

Laplace-frequency s

$$K_q^{\perp}(s) = \frac{m}{Nk_BT}\langle v^{\perp}(\mathbf{q})^* \frac{1}{s-\Omega} v^{\perp}(\mathbf{q})\rangle = \frac{1}{s + \frac{q^2}{mn}\mathrm{G}_q^{\perp}(s)}$$

with generalized viscosity

$$\mathrm{G}_q^{\perp}(s) = \frac{1}{Vk_BT}\,\frac{1}{q^2}\langle F^{\perp}(\mathbf{q})^* \overbrace{\mathcal{Q}\frac{1}{s-\mathcal{Q}\Omega\mathcal{Q}}\mathcal{Q}}^{R'(s)}\, F^{\perp}(\mathbf{q})\rangle$$

projector: $\mathcal{Q} = 1 - \mathcal{P} = 1 - \mathbf{v}^{\perp}(\mathbf{q})\rangle \frac{m}{Nk_BT}\langle \mathbf{v}^{\perp}(\mathbf{q})^*$ (Hansen/McDonald)

Search for closure

Zwanzig Mori

Projector: $\mathcal{Q}_F = 1 - \mathcal{P}_F = 1 - \mathbf{F}^{\perp}(\mathbf{q})\rangle \frac{1}{k_B T V q^2 \mathrm{G}_q^{\perp}(0)} \langle \mathbf{F}^{\perp}(\mathbf{q})^*$

$$\mathrm{G}_q^{\perp}(s) = \frac{\mathrm{G}_q^{\perp}(t=0)}{s + \mathrm{W}_q^{\perp}(s)} \qquad \left(\underset{T>T_g}{\approx} G^{\mathrm{gM}}(s) = \frac{G_\infty}{s + \frac{1}{\tau}} \right)$$

Stress-current coupling

$$\dot{\boldsymbol{\sigma}}^{(p)}(\mathbf{q}) = \frac{2}{V} \sum_{\mathbf{k}} \delta\rho(\mathbf{p})(-i\mathbf{k} \cdot \mathbf{v}(\mathbf{k}))\, \Re\{\mathbf{X}(\mathbf{k}, \mathbf{q})\}$$

Fluidity approximation

$$W_q^{\perp}(s) = \frac{1}{(c_q^{\perp})^2 (d-1)} \sum_{\boldsymbol{k}} \mathrm{Tr}\{V_{\boldsymbol{k},\boldsymbol{q}} \cdot \mathcal{V}_{\boldsymbol{k},\boldsymbol{q}}(s)\}$$

renormalized vertex $\mathcal{V}_{\boldsymbol{k},\boldsymbol{q}}(s)$ captures topology of scattering events

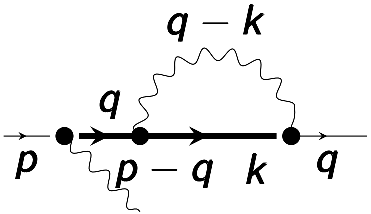
Connection to the ERM-model

Small Fluidity (Small Vertex) Approximation

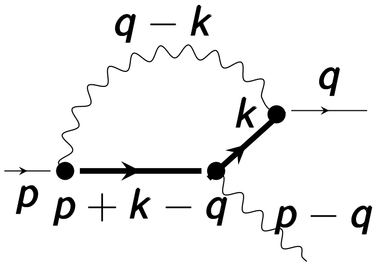
$$\chi_q(s) = -\frac{K_q(s)}{s} = -\frac{1}{s^2 + (qc_q^{\perp})^2 - \underbrace{W_q(s)/s}_{\hat{=} -\Sigma_{ERM}(\boldsymbol{q},s)}}$$

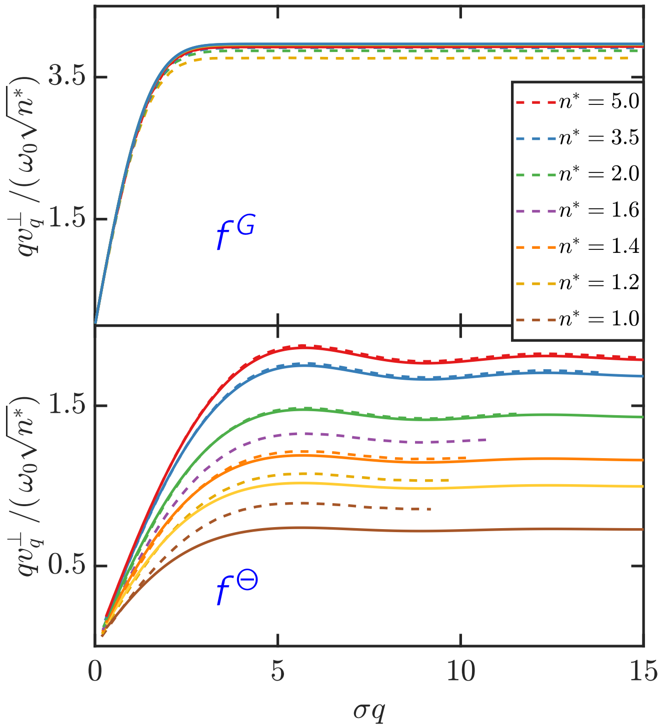
Self-Energy contains renormalized vertex, recovers field theory expansion* for $n \to \infty$

planar



non-planar





dispersion relation softens (jammed)

* see also G. Szamel, arXiv:2407.13039 (2024)

Un-jammed state

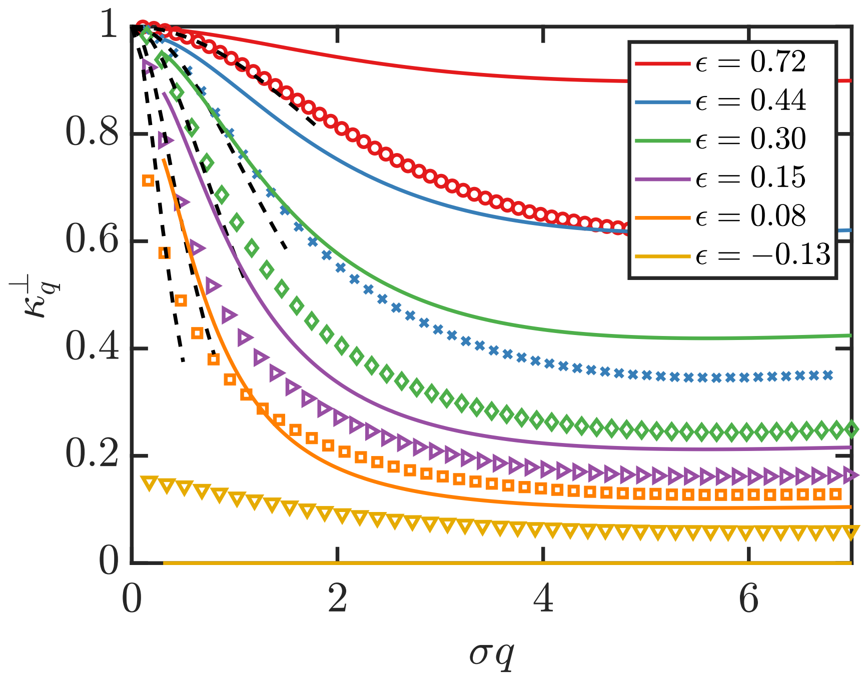
Velocity response

$$\lim_{s\to 0} sK_q^{\perp}(s) = \kappa_q^{\perp}$$

quasi-static motion without restoring forces

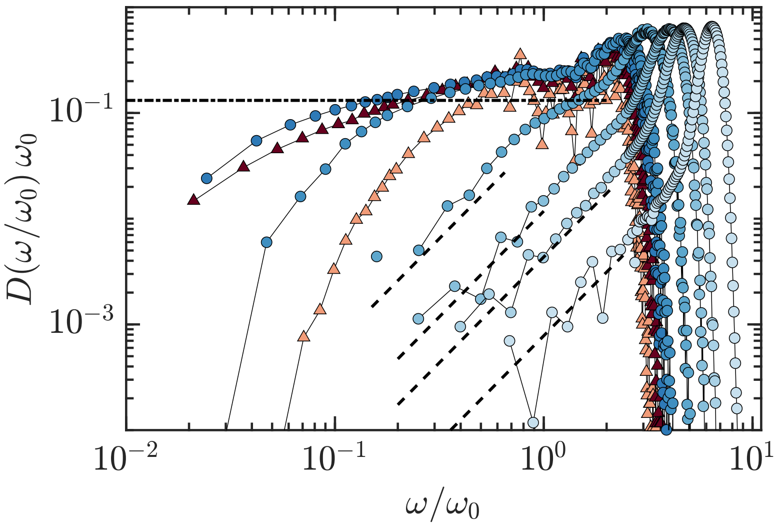
$$\kappa_q^{\perp} \to \frac{1}{1+(q\lambda_{-}^{\perp})^2} \quad \text{for } q \to 0$$

cooperative motion of un-bonded clusters

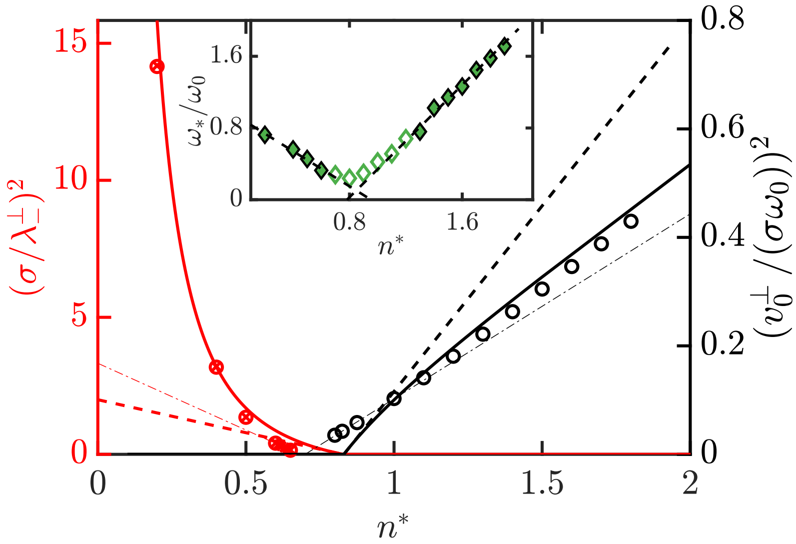


divergent cluster size $\lambda_{-}^{\perp}$ (un-jammed)

Glass-instability in ERM & self-consistent transverse response theory

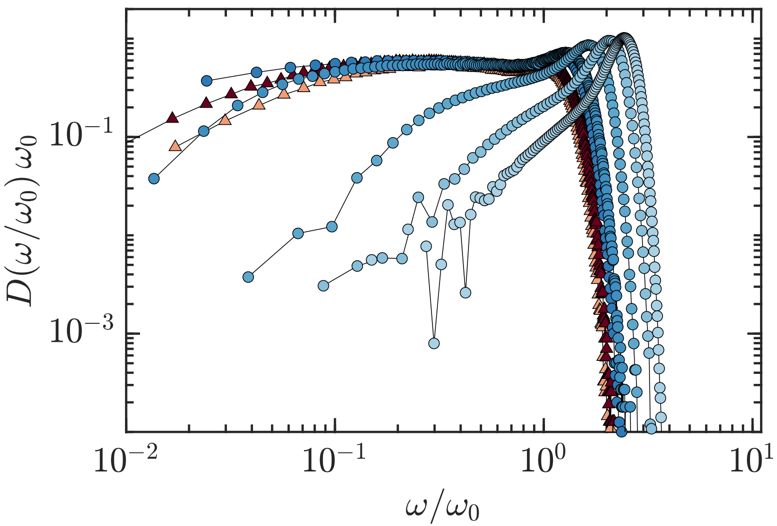


- const vDOS above $\omega_* \propto |z - z_c|$

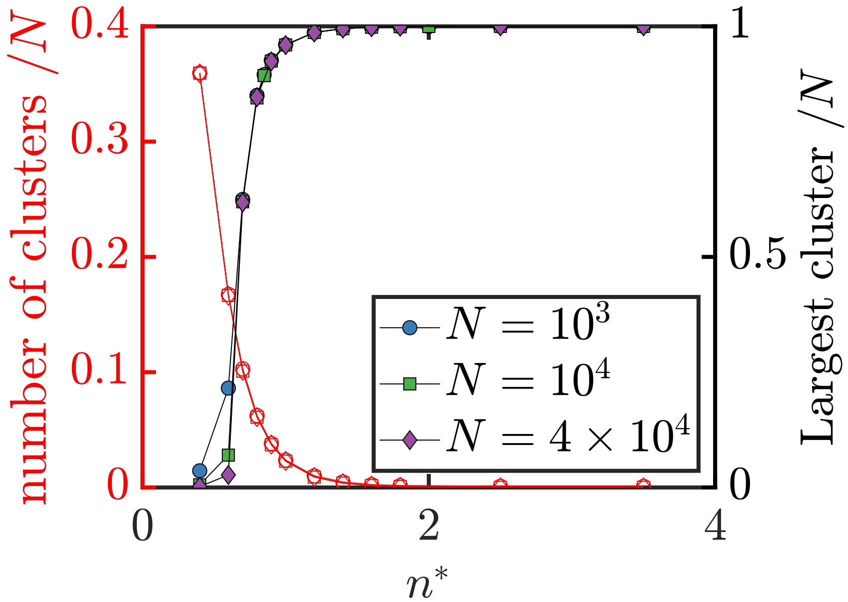


- sound velocity vanishes (jammed)
- cluster size diverges (un-jammed)

Un-jamming in ERM, linear spring function: $f(r) = (1 - \frac{r}{\sigma})\Theta(\sigma - r)$



- const vDOS above $\omega_* \propto |z - z_c|$

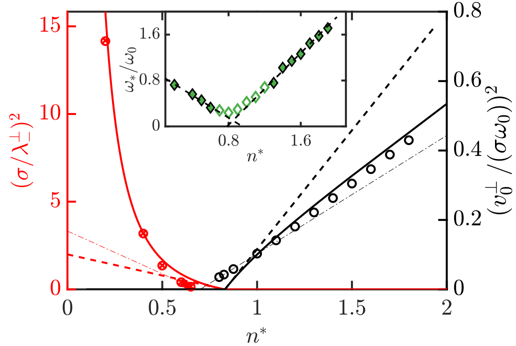


- percolation of bonds, length σ at $n \to n_p \approx 0.838$ ($z_p \approx 3.51$)

Summary

ERM-model for vibrations in glass

- explains stable glass
- exact diagonalization
- self-consistent field theory
- un-jamming
    - microscopic theory



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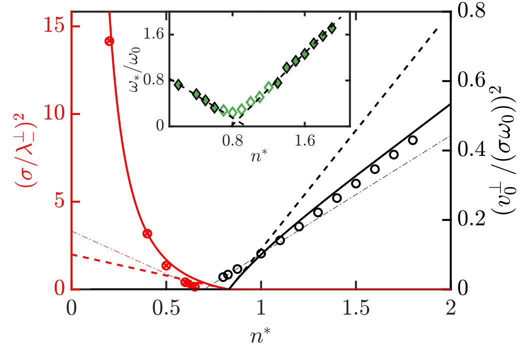

Thank you at UKN

Florian Vogel

Philipp Stengele

group & colleagues

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ERM-model for vibrations in glass

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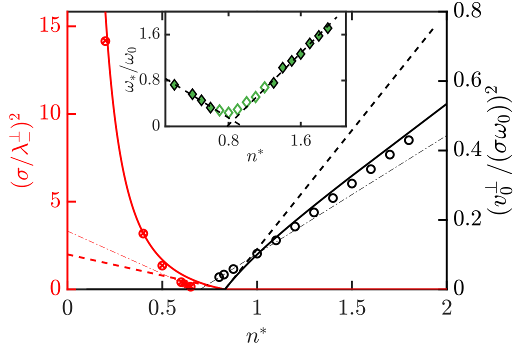
Thank you

for your attention



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