Jamming as the Extreme Limit of a Solid

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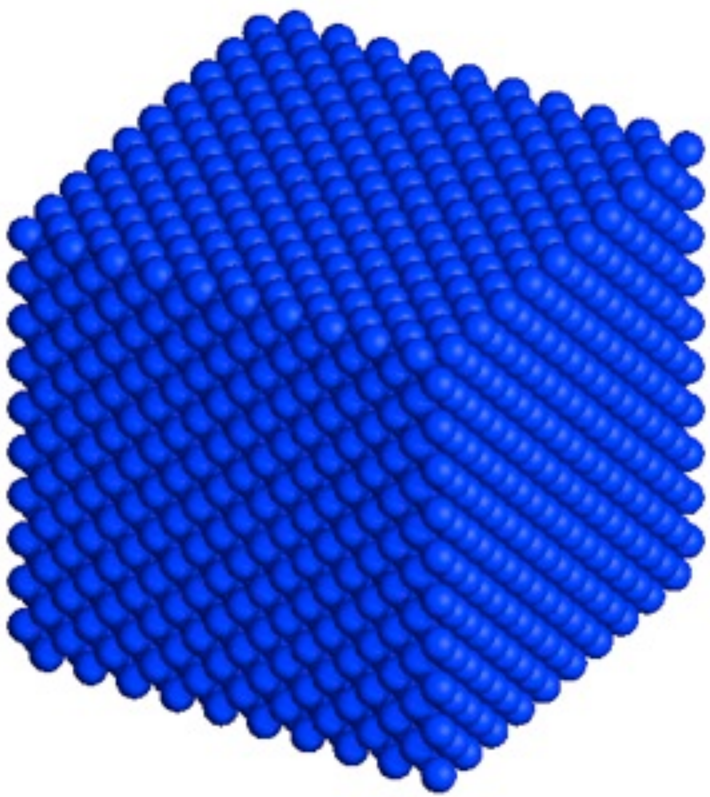
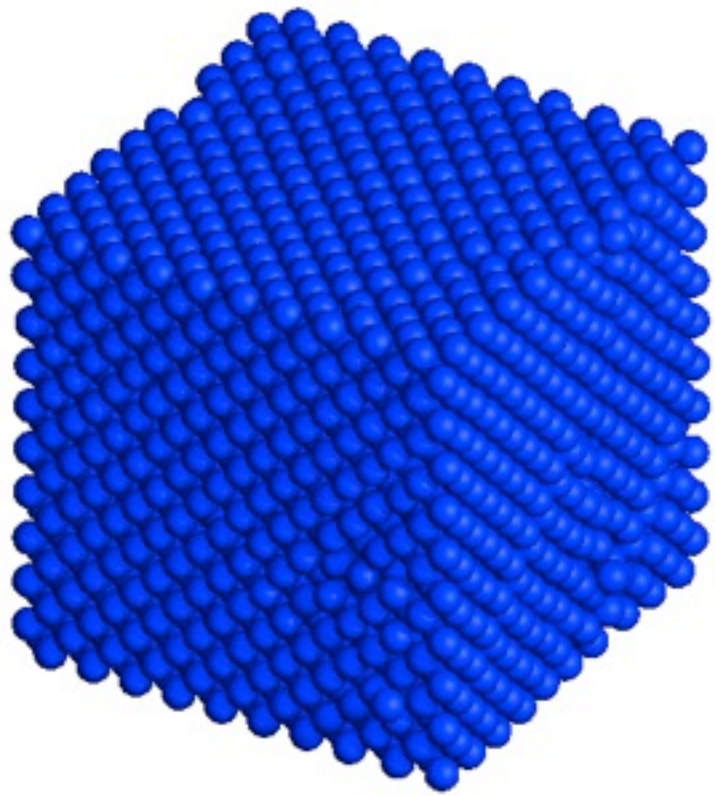
Tim Still	UPenn
Arjun Yodh	UPenn

Physics of Perfect Crystals

- Start with T=0 perfect crystal
  - look at vibrational, electronic, etc. properties
  - add defects as perturbation (chapter 30)

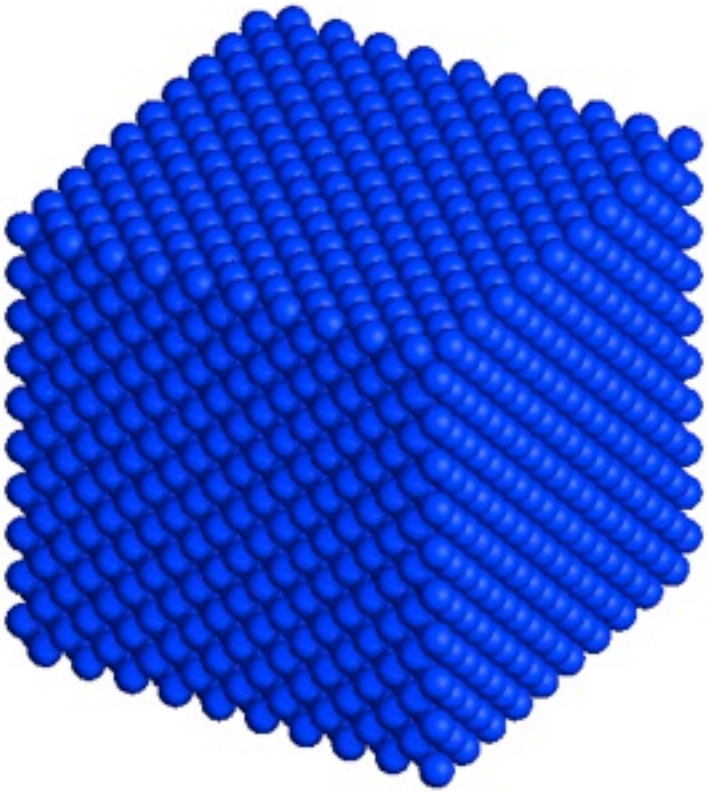
Perturbing away from the crystal

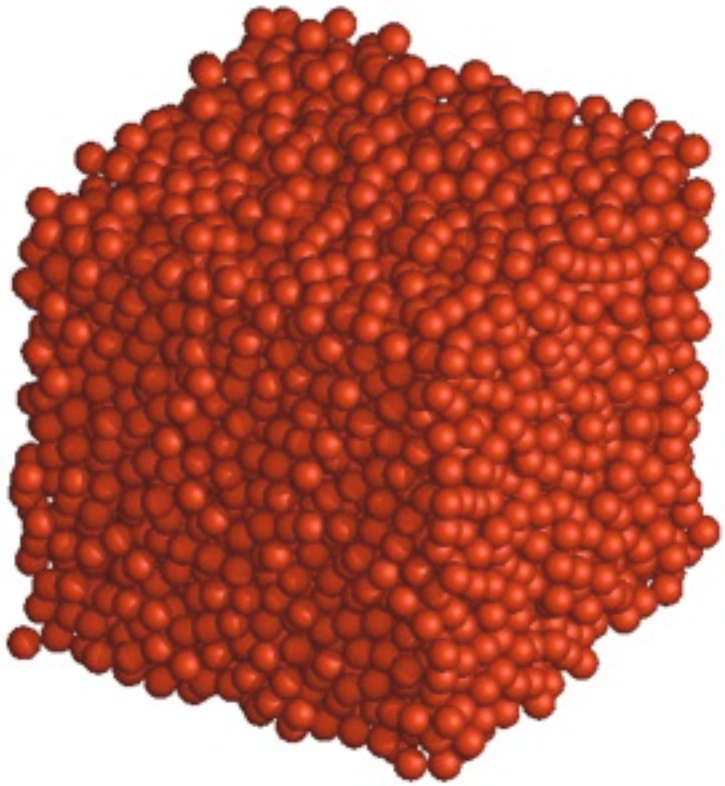




Perturbing away from the crystal

But what about this?





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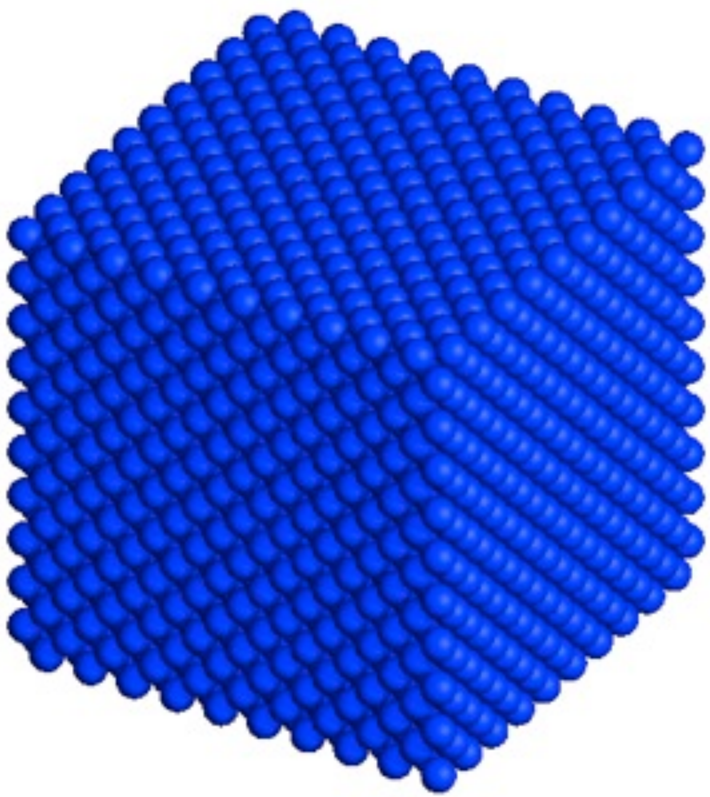
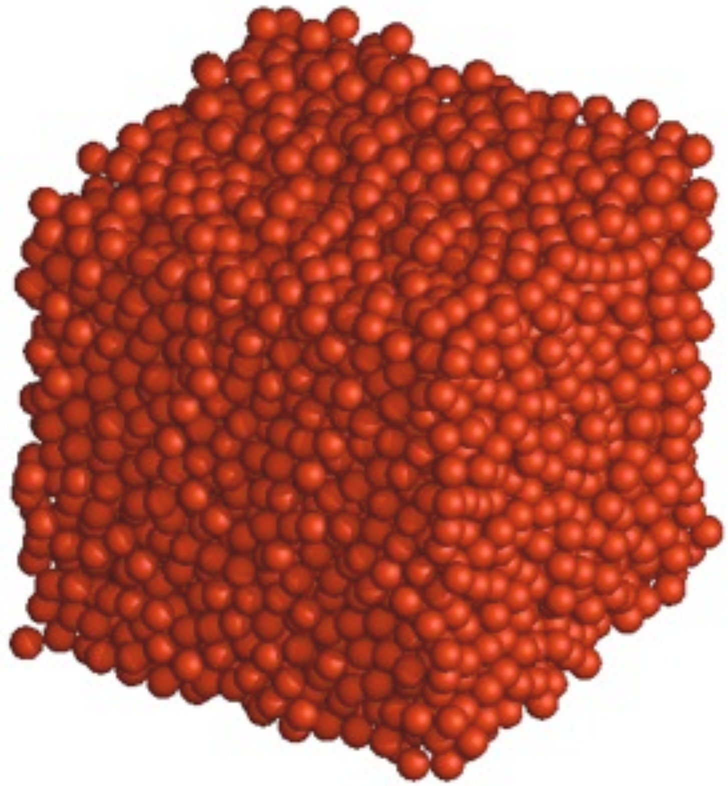




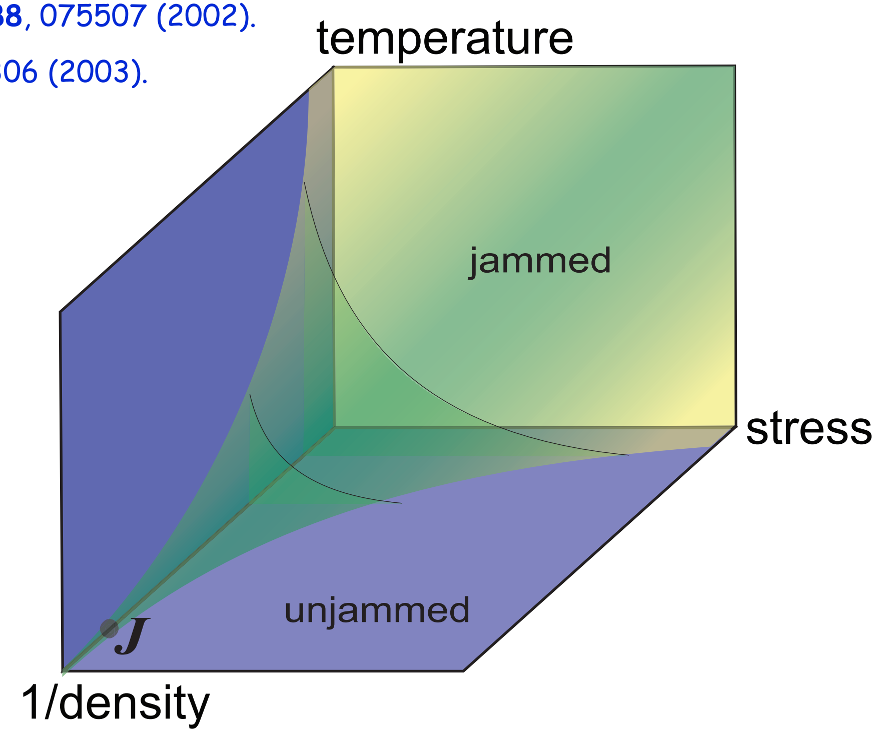
Is there an opposite pole to the perfect crystal, corresponding to rigid solid with complete disorder?

If so, we could describe ordinary solids as somewhere in between

Jamming Transition for "Ideal Spheres"

C. S. O'Hern, S. A. Langer, A. J. Liu and S. R. Nagel, Phys. Rev. Lett. **88**, 075507 (2002).

C. S. O'Hern, L. E. Silbert, A. J. Liu, S. R. Nagel, Phys. Rev. E **68**, 011306 (2003).



- Study models with smooth transitions
  - from G/B=0 (like liquid)
  - to G/B>0 (like crystal)

Bubble model for foams

D. J. Durian, PRL 75, 4780 (1995).

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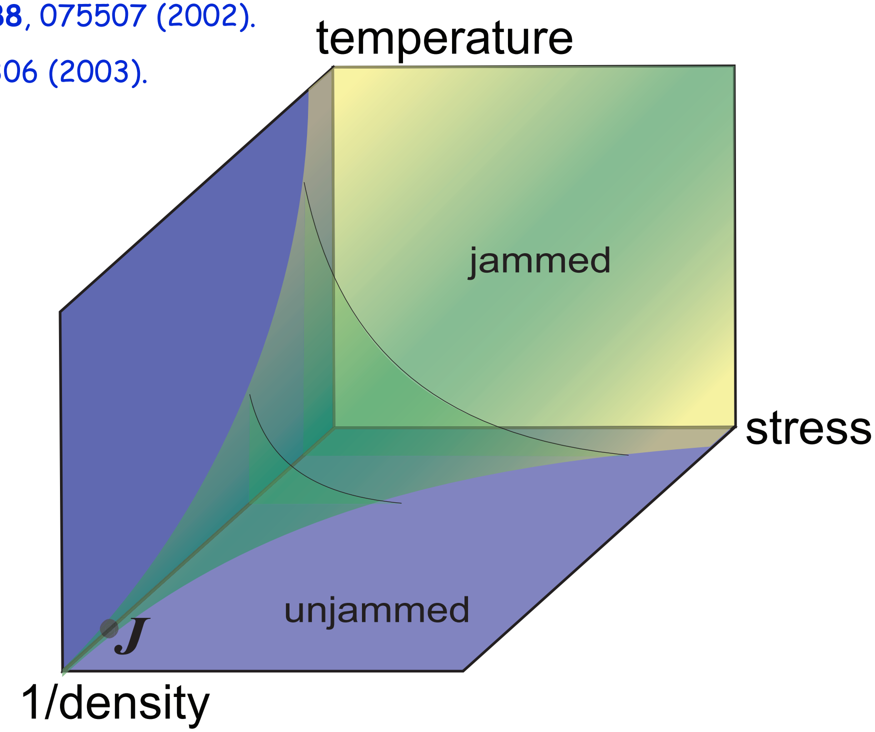
$$V(r) = \begin{cases} \dfrac{\varepsilon}{\alpha}\left(1 - \dfrac{r}{\sigma}\right)^{\alpha} & r \leq \sigma \\ 0 & r > \sigma \end{cases}$$



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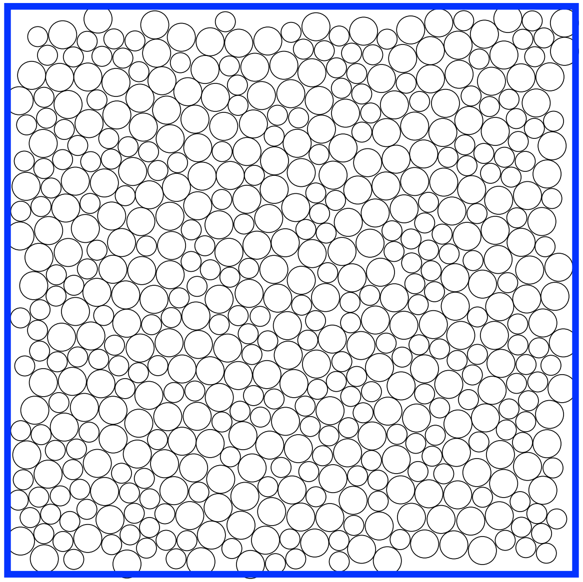
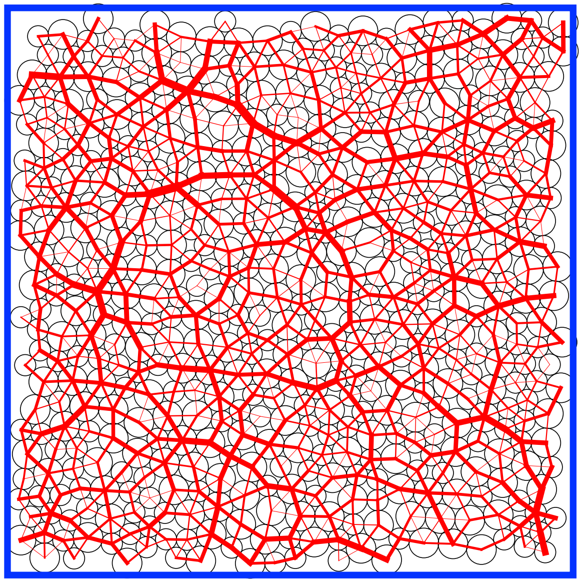
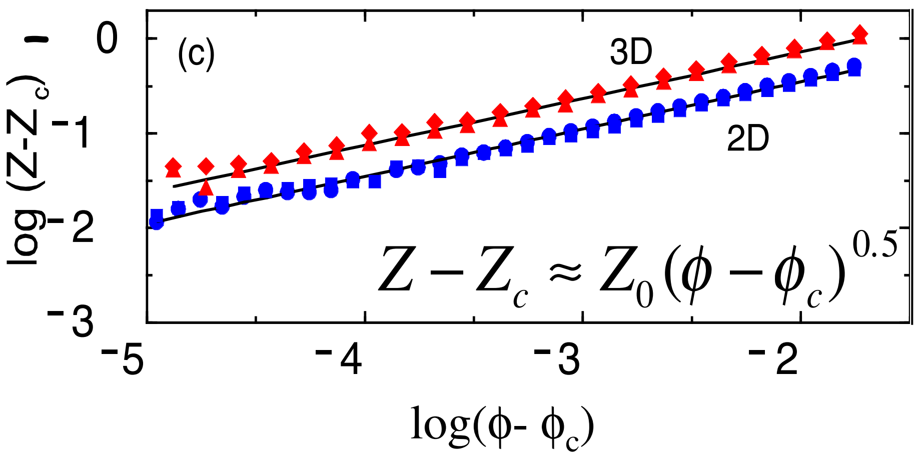
Onset of Jamming in Repulsive Sphere Packings

Just below ϕ_c, no particles overlap





Just above ϕ_c there are Z_c overlapping neighbors per particle



$$Z_c = 3.99 \pm 0.01 \quad \text{(2D)}$$

$$Z_c = 5.97 \pm 0.03 \quad \text{(3D)}$$

Verified experimentally:
G. Katgert and M. van Hecke, EPL **92**, 34002 (2010).

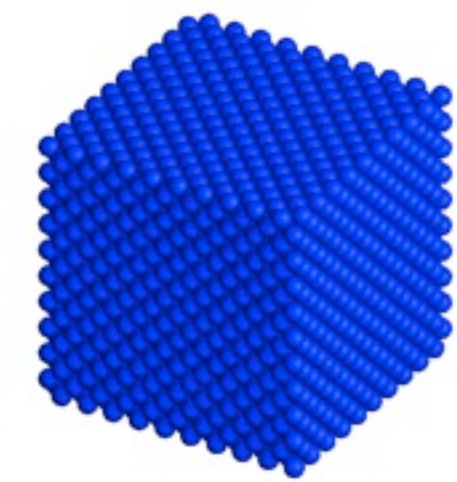
Durian, PRL **75**, 4780 (1995).
O'Hern, Langer, Liu, Nagel, PRL **88**, 075507 (2002).

Isostaticity

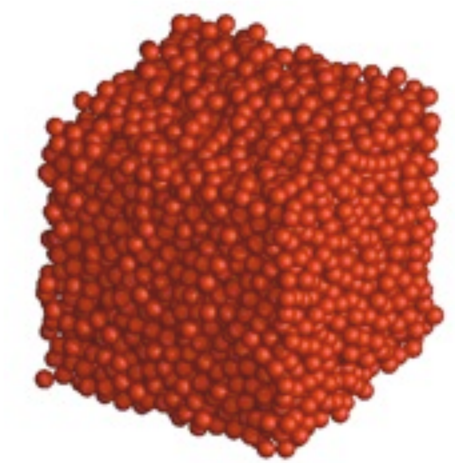
- What is the minimum number of interparticle contacts needed for mechanical equilibrium?
- No friction, N repulsive spheres, d dimensions
- Match
  - number of constraints (number of interparticle normal forces)=NZ/2
  - number of degrees of freedom =Nd-d
- For large N, $Z \geq 2d$

James Clerk Maxwell

Contact Number of Crystal vs. Marginally Jammed Solid

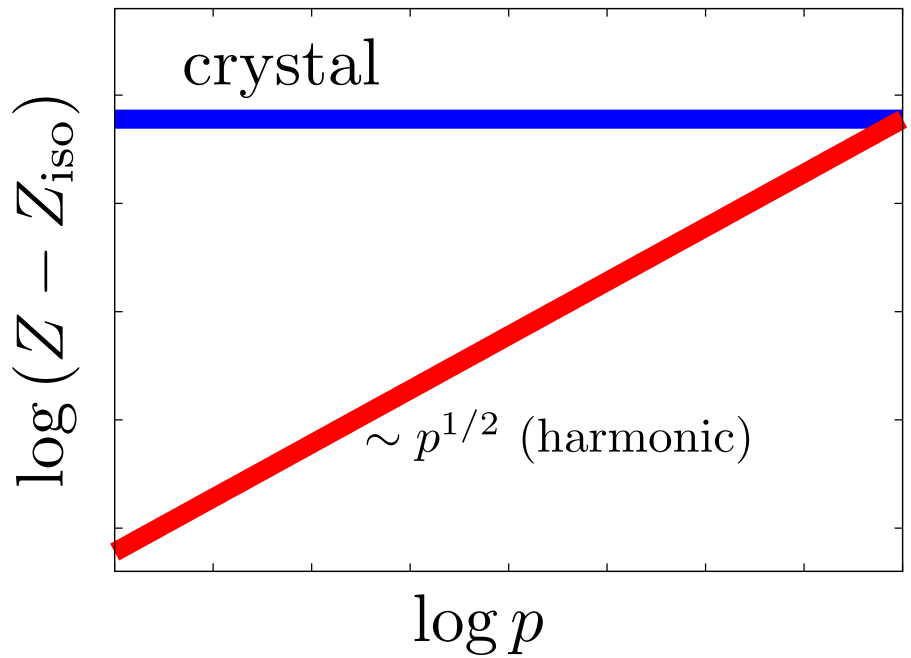


vs



perfect crystal

marginally jammed solid



crystal: Z=12

marginally jammed solid: $Z = Z_{iso} = 6$

Constraint Counting and G/B

- At onset of overlap, ϕ_c, can constrain
  - all soft modes
  - compression of the whole system
- So B>0 but G=0 so G/B=0

Durian, PRL **75**, 4780 (1995).
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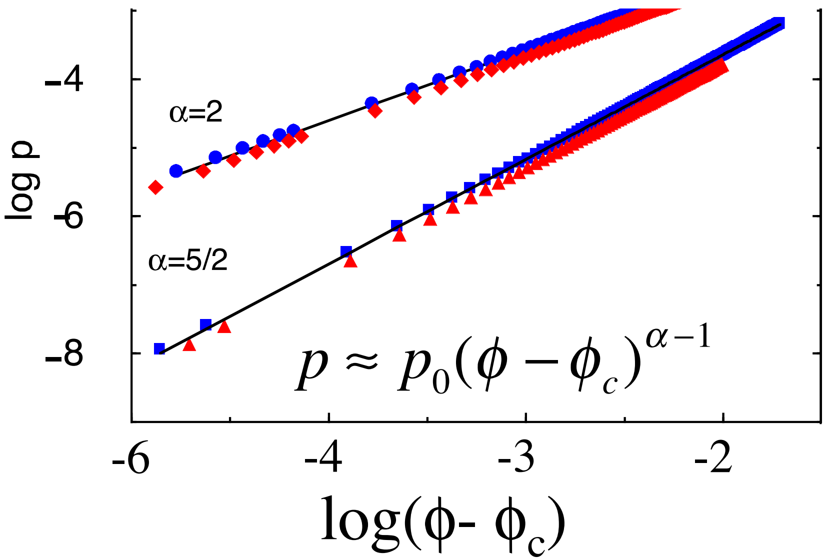

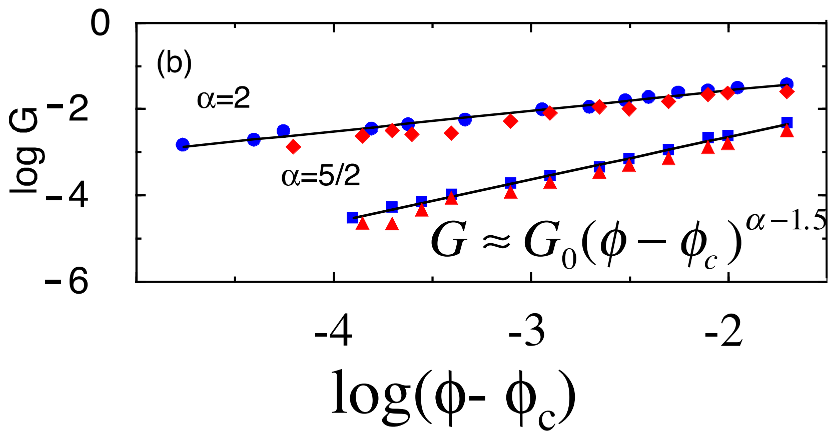

- Above ϕ_c, G/B >0 so ϕ_c also marks onset of jamming

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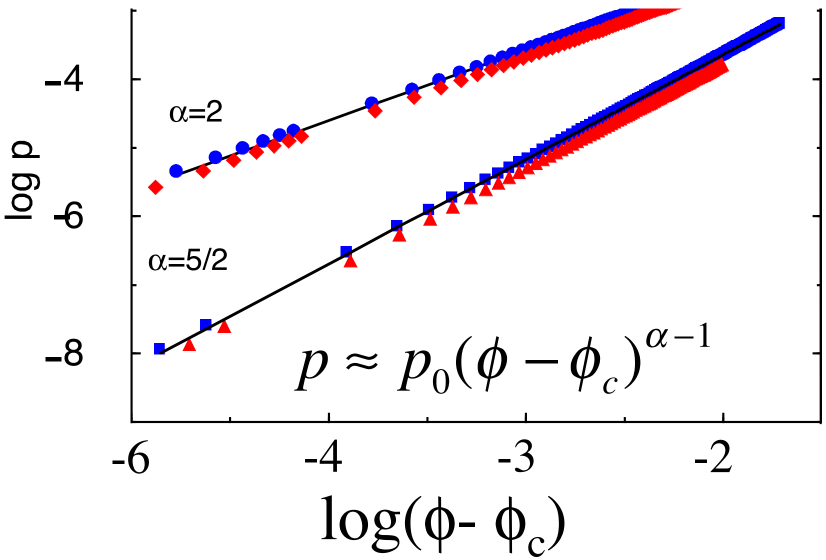
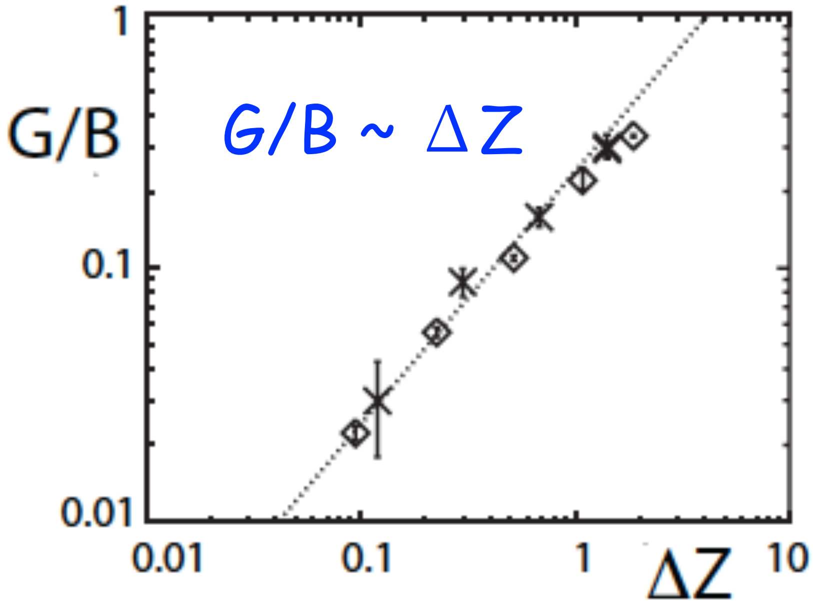


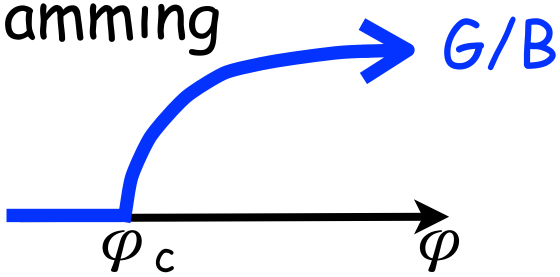
Ellenbroek, Somfai, van Hecke, van Saarloos, PRL 97, 257801 (2006).



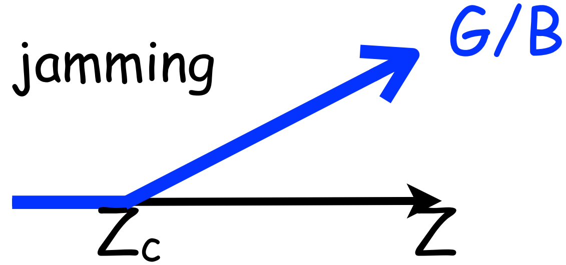
- Above ϕ_c, G/B >0 so ϕ_c also marks onset of jamming

G/B -> 0 with $(\varphi - \varphi_c)^{1/2}$ or Z-Z_c appears unique to jamming

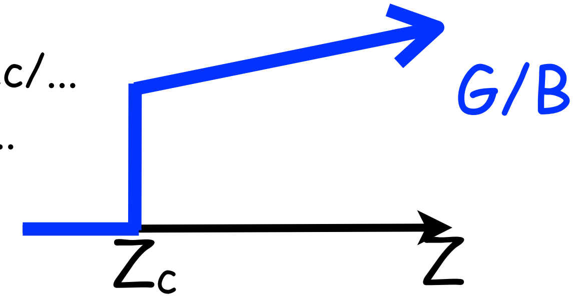
jamming



jamming



randomly diluted hexagonal/fcc/...
randomly decorated kagome/....



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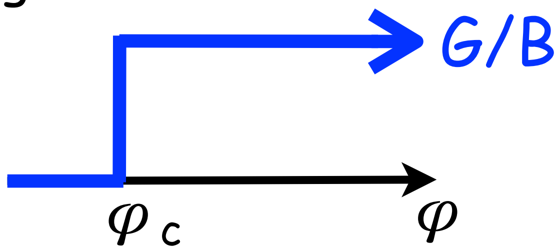
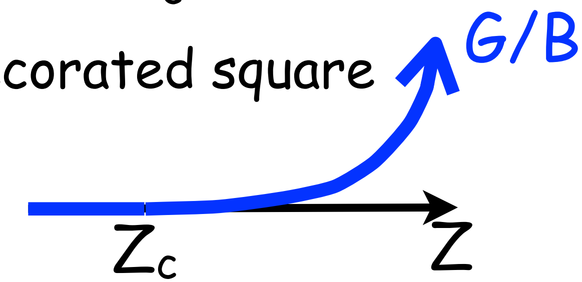
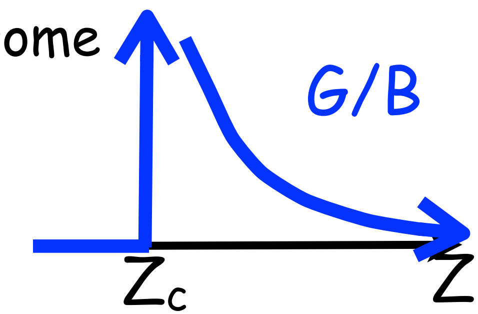


randomly decorated square

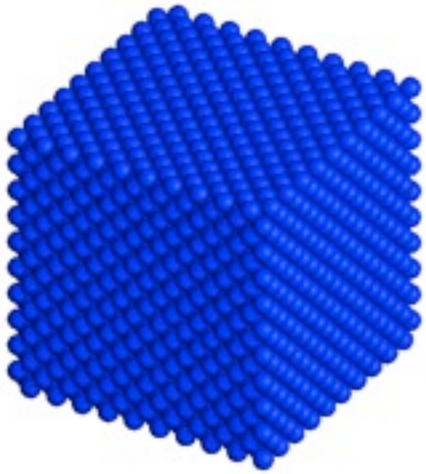


twisted kagome



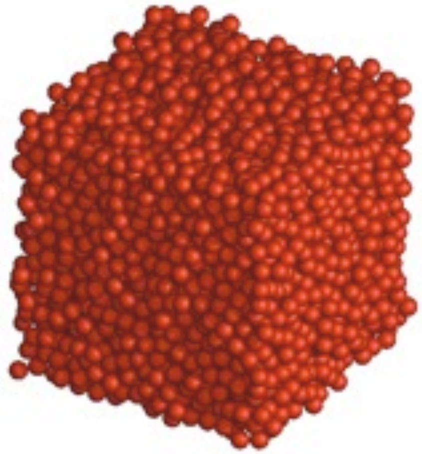
X. Mao, A. Souslov, T. C. Lubensky

Mechanics of crystal vs. marginally jammed solid

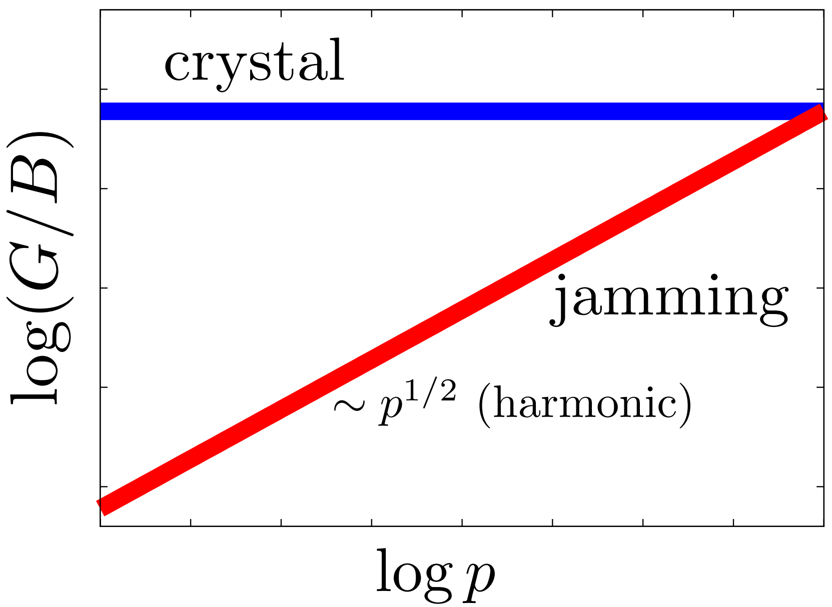


perfect crystal

vs



marginally jammed solid

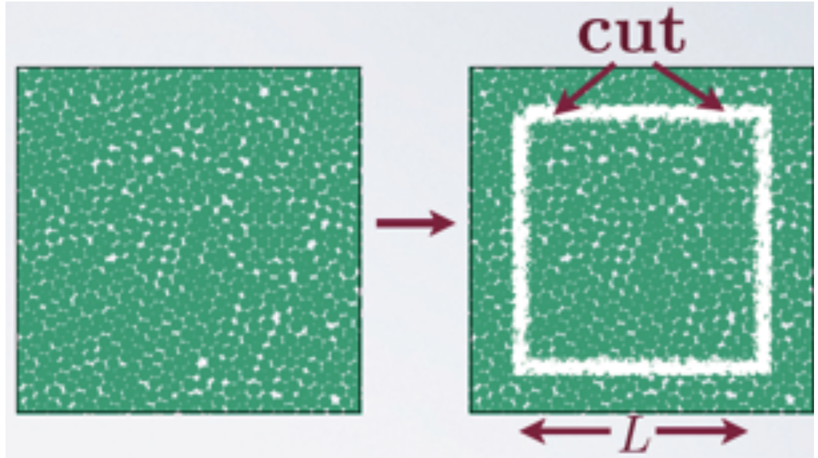


crystal: G/B ~ 1

marginally jammed solid: G/B -> 0

Consequence: Diverging Length Scale

M. Wyart, S.R. Nagel, T.A. Witten, EPL **72**, 486 (05)



- For system at ϕ_c, Z=2d
- Removal of one bond makes entire system unstable by adding a soft mode
- This implies diverging length as ϕ-> ϕ_c

For ϕ> ϕ_c, cut bonds at boundary of size L

Count number of soft modes within cluster

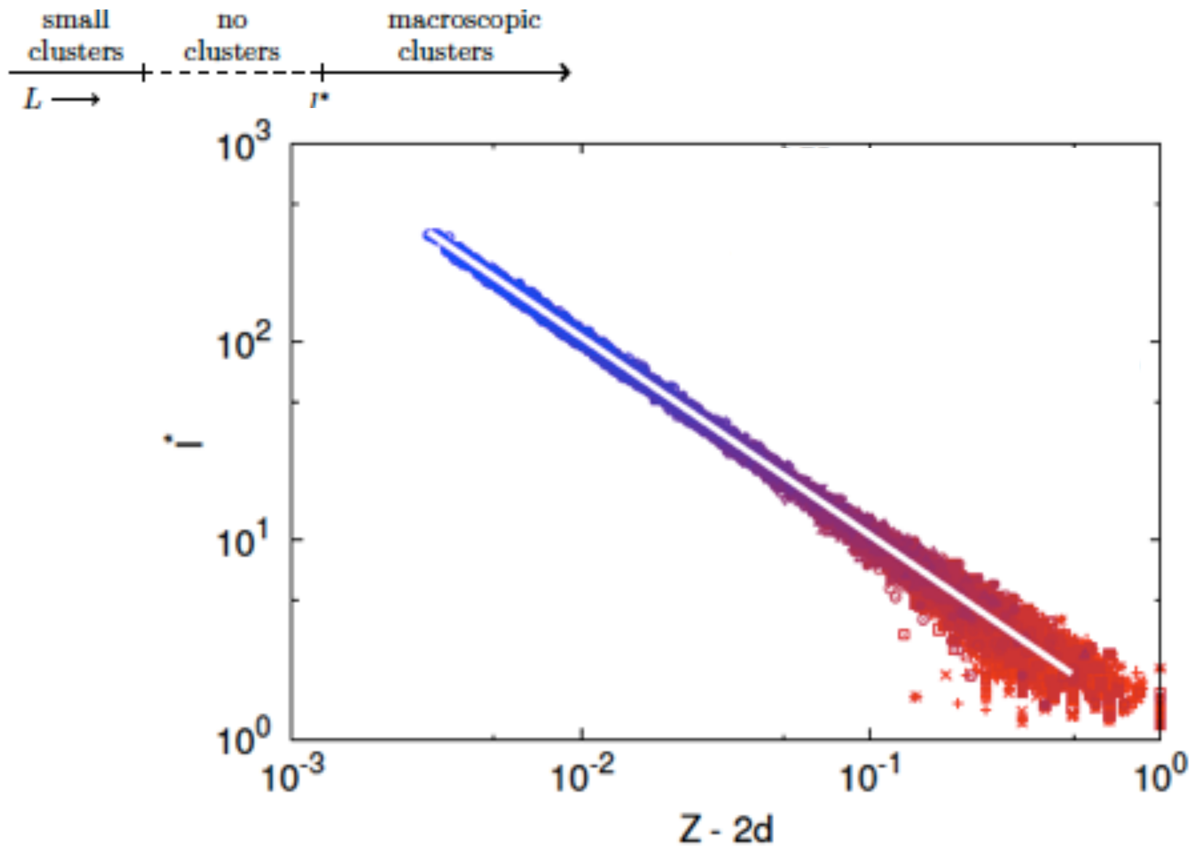
$$N_s \approx L^{d-1} - (Z - Z_c)L^d$$

Define length scale at which soft modes just appear

$$\ell_L \sim \frac{1}{Z - Z_c} \equiv \frac{1}{\Delta z} \sim (\phi - \phi_c)^{-0.5}$$

More precisely

Define ℓ^* as size of smallest macroscopic rigid cluster for system with a free boundary of any shape or size



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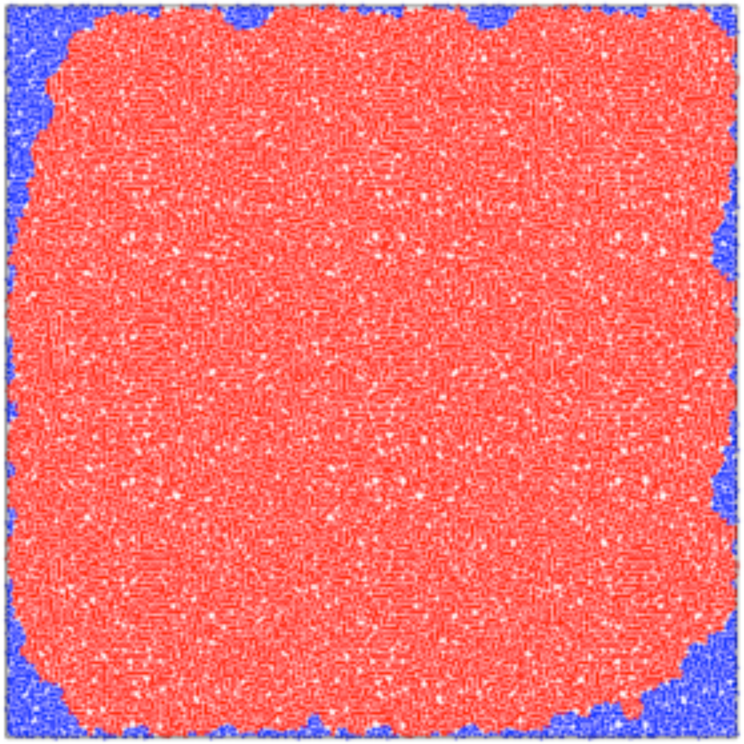

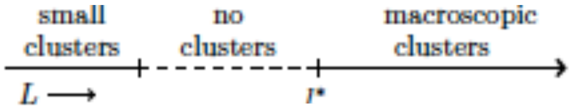

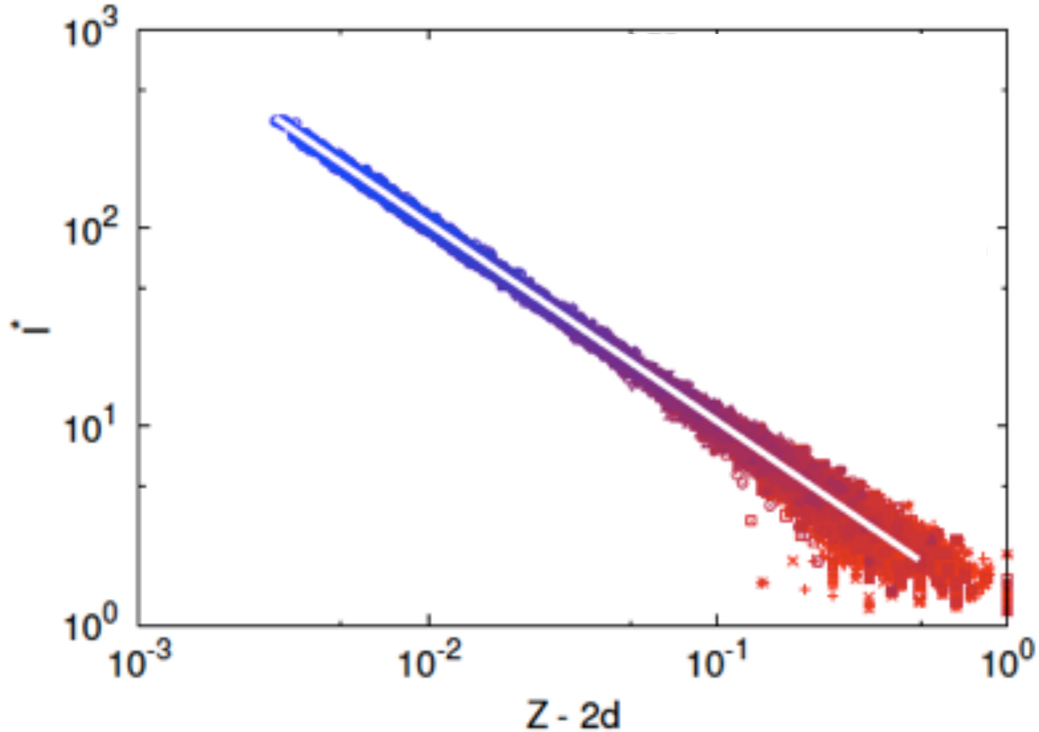

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Vibrations in Disordered Sphere Packings

- Crystals are all alike at low T or low ω
  - density of vibrational states $D(\omega) \sim \omega^{d-1}$ in d dimensions
  - heat capacity $C(T) \sim T^d$
- Why?

Low-frequency excitations are sound modes. At long length scales all solids look elastic

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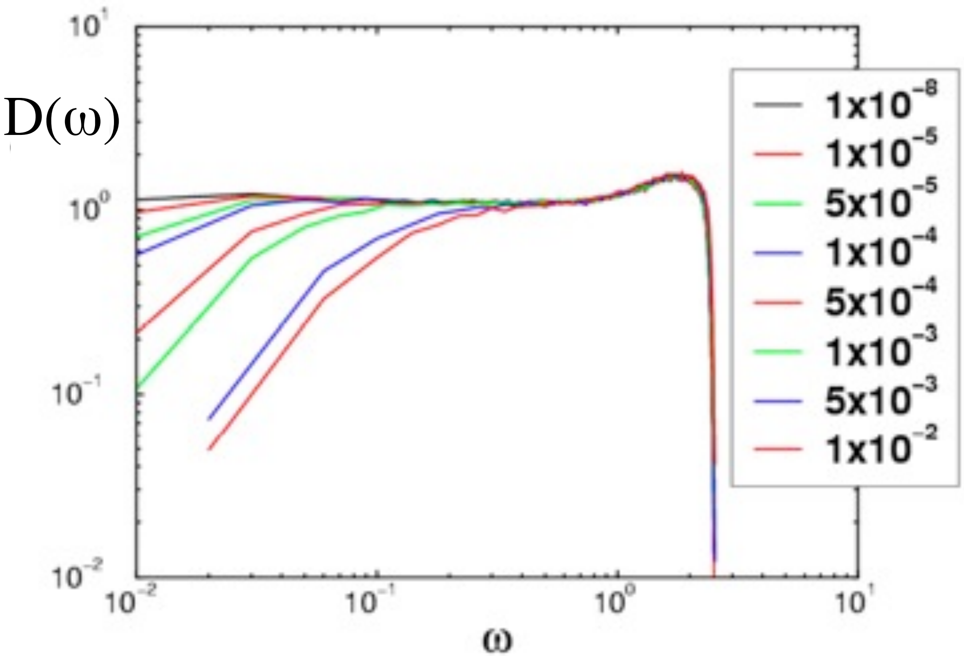
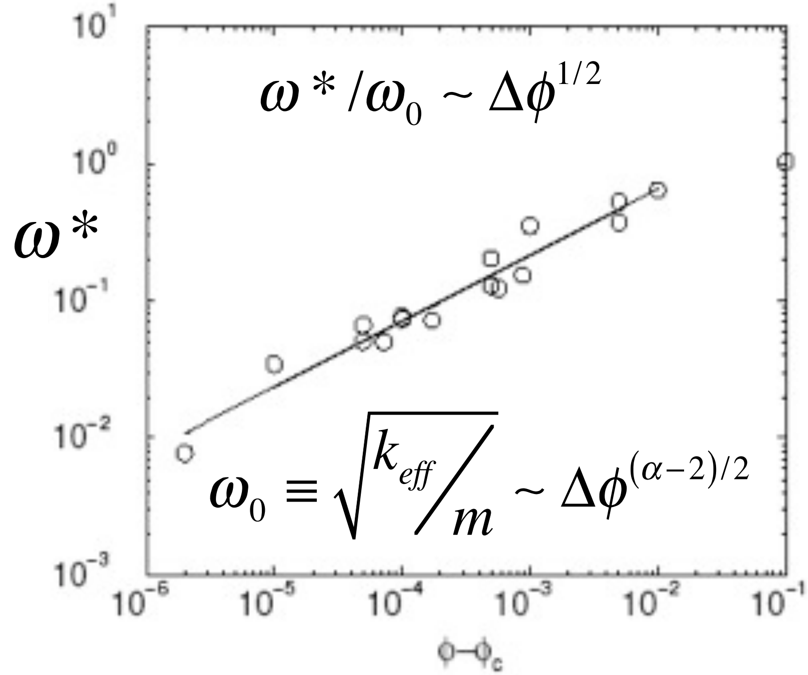
BUT near at Point J, there is a diverging length scale ℓ_L

So what happens?

Vibrations in Sphere Packings

L. E. Silbert, A. J. Liu, S. R. Nagel, PRL **95**, 098301 ('05)





- New class of excitations originates from soft modes at Point J M. Wyart, S.R. Nagel, T.A. Witten, EPL **72**, 486 (05)

- Generic consequence of diverging length scale: $\ell_L \simeq c_L/\omega^*$
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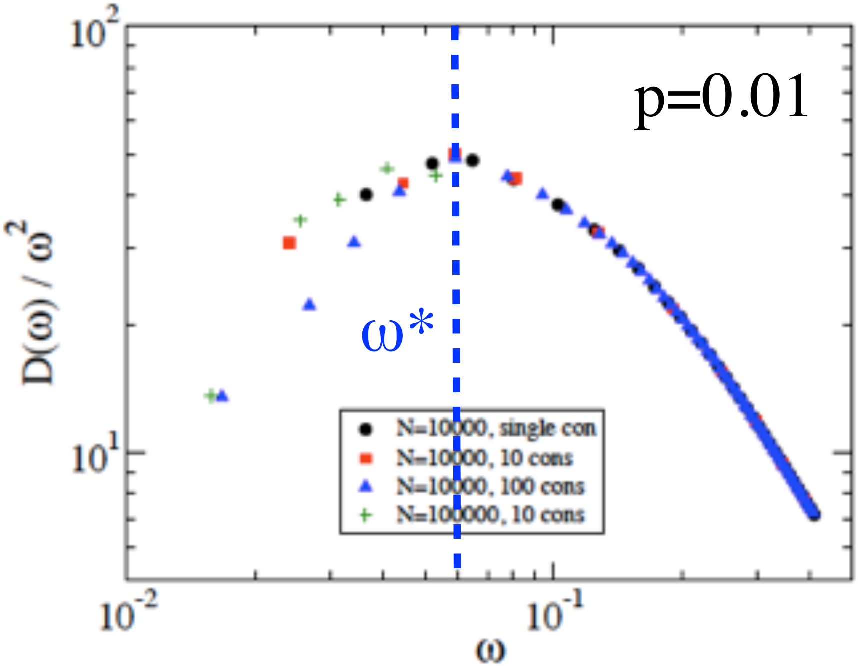

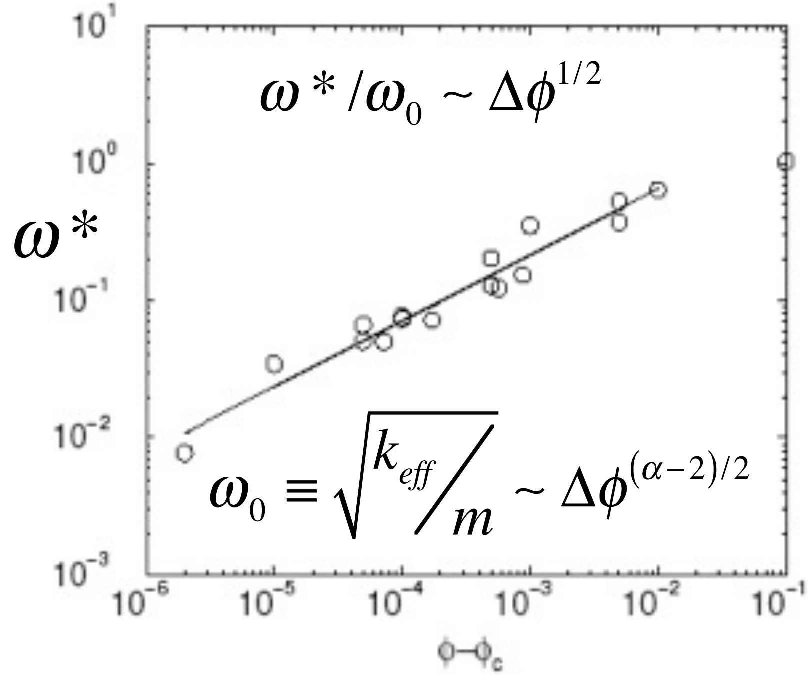

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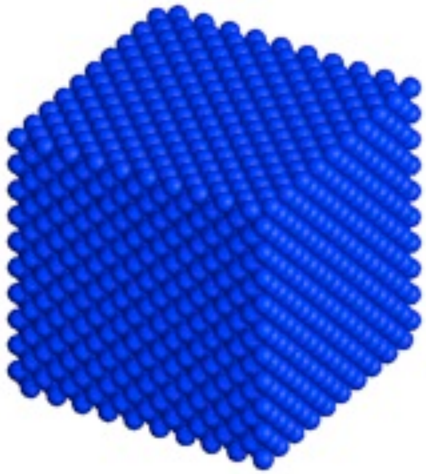
Vibrations of crystal vs. marginally jammed solid



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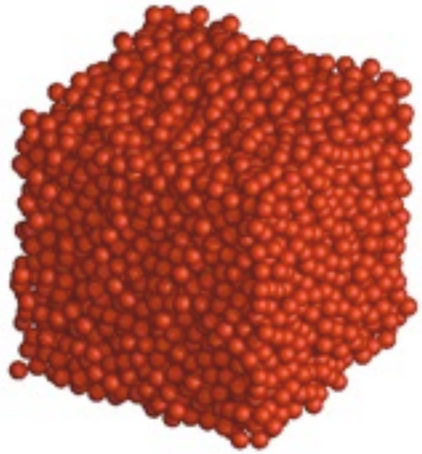
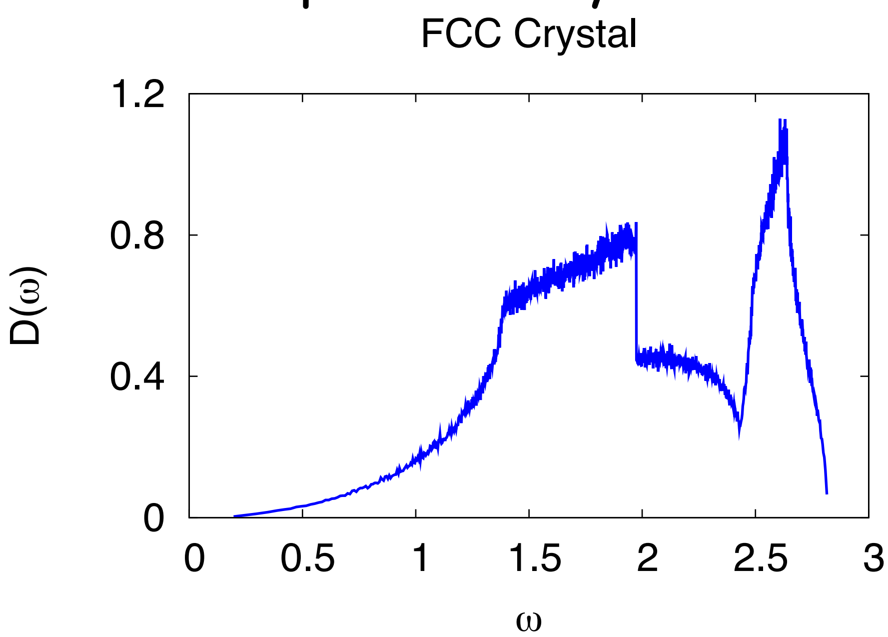
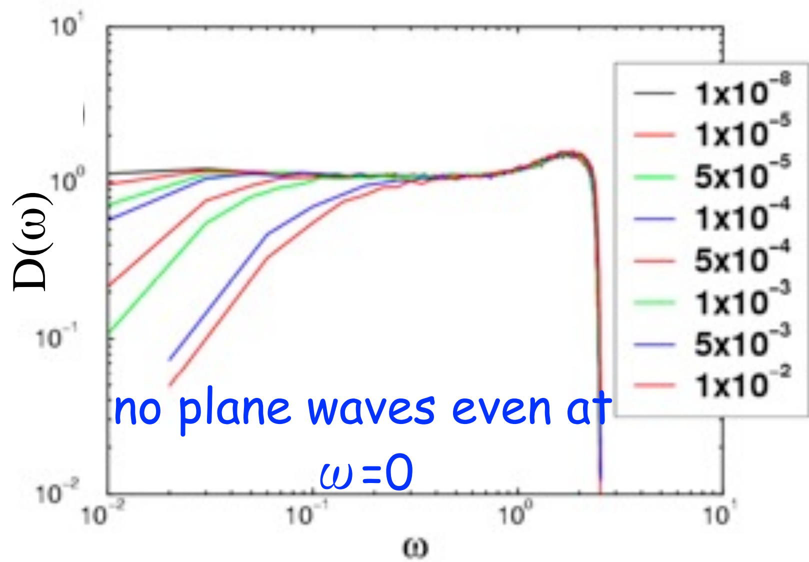


perfect crystal

marginally jammed solid





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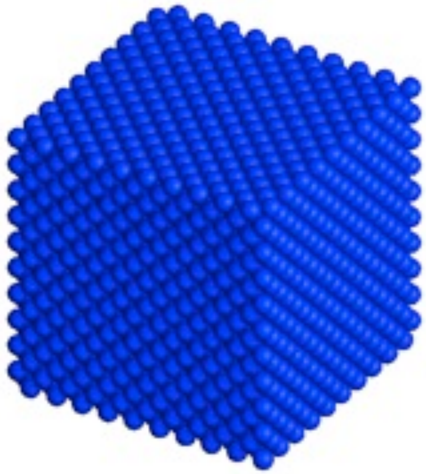

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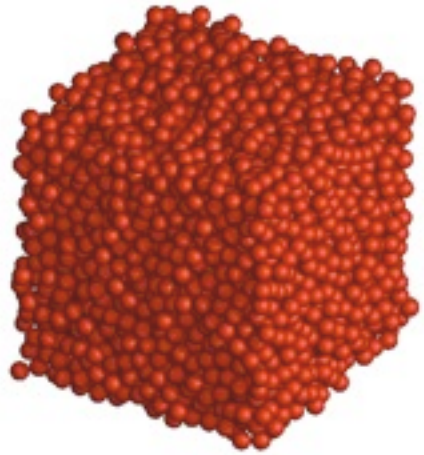

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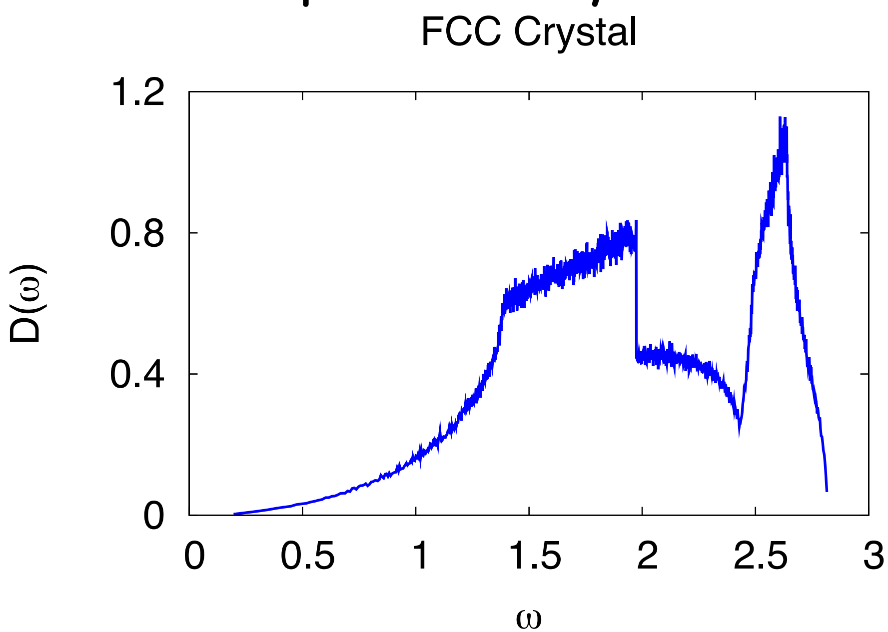

D(ω)

no plane waves even at $\omega=0$

Back to extreme limits

How do we connect physics of jamming and physics of crystals? What happens in between?

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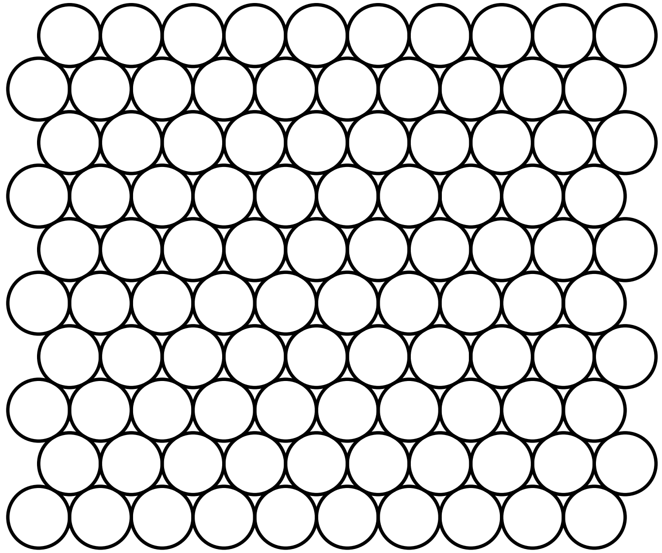

$2d$ illustration

1. start with a perfect FCC crystal

Back to extreme limits

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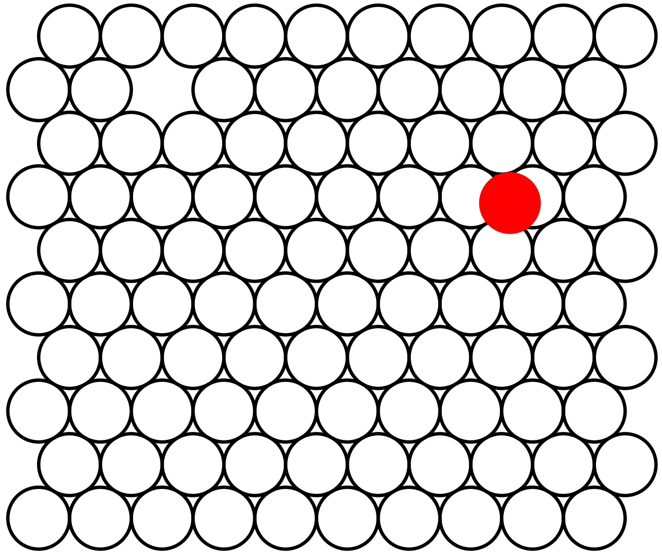

$2d$ illustration

1. start with a perfect FCC crystal

2. introduce 1 vacancy-interstitial pair

Back to extreme limits

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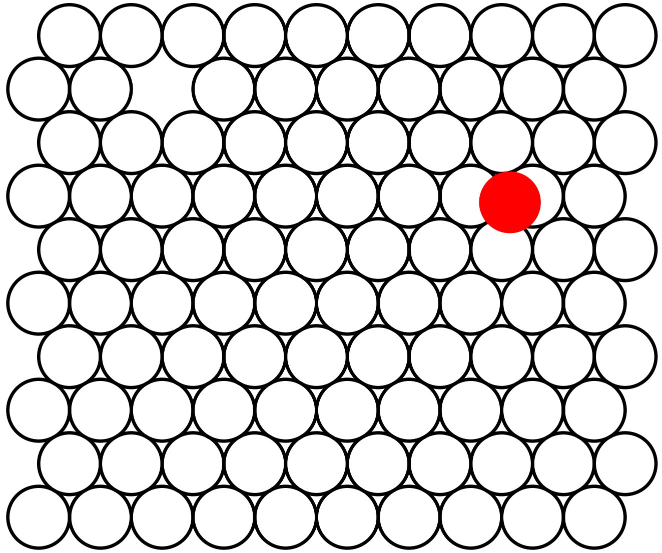

$2d$ illustration

1. start with a perfect FCC crystal

2. introduce 1 vacancy-interstitial pair

3. minimize the energy

Back to extreme limits

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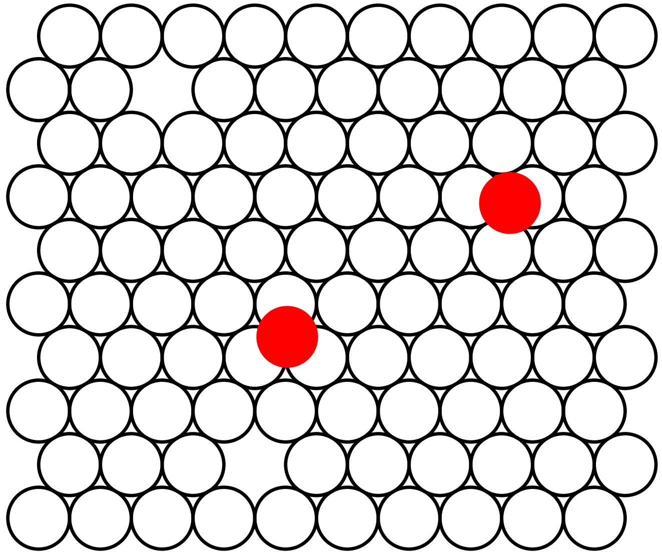


$2d$ illustration

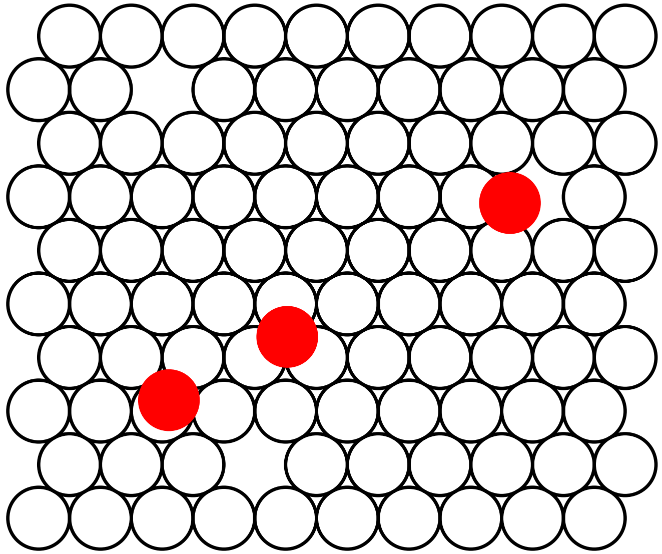
1. start with a perfect FCC crystal

2. introduce 2 vacancy-interstitial pairs

3. minimize the energy

Back to extreme limits

How do we connect physics of jamming and physics of crystals? What happens in between?

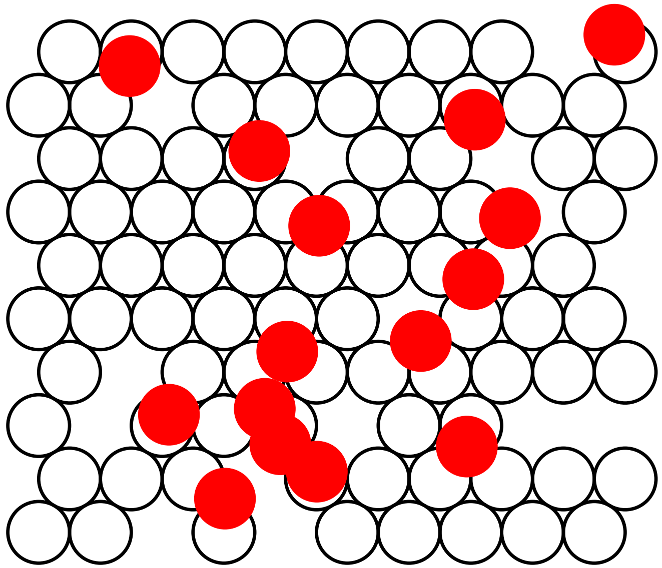


$2d$ illustration

1. start with a perfect FCC crystal
2. introduce 3 vacancy-interstitial pairs
3. minimize the energy

Back to extreme limits

How do we connect physics of jamming and physics of crystals? What happens in between?



$2d$ illustration

1. start with a perfect FCC crystal
2. introduce M vacancy-interstitial pairs
3. minimize the energy

Back to extreme limits

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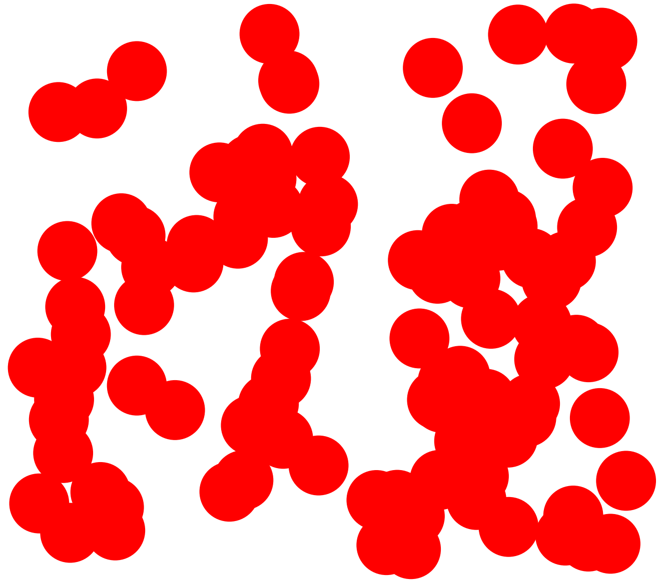


$2d$ illustration

1. start with a perfect FCC crystal
2. introduce N vacancy-interstitial pairs
3. minimize the energy

Order Parameter

Bond-orientational order

$$q_{lm}(i) \equiv \sum_j Y_{lm}(\hat{\mathbf{r}}_{ij})$$

$$S_l(i,j) \equiv \sum_m q_{lm}(i) \cdot q^*_{lm}(j)$$

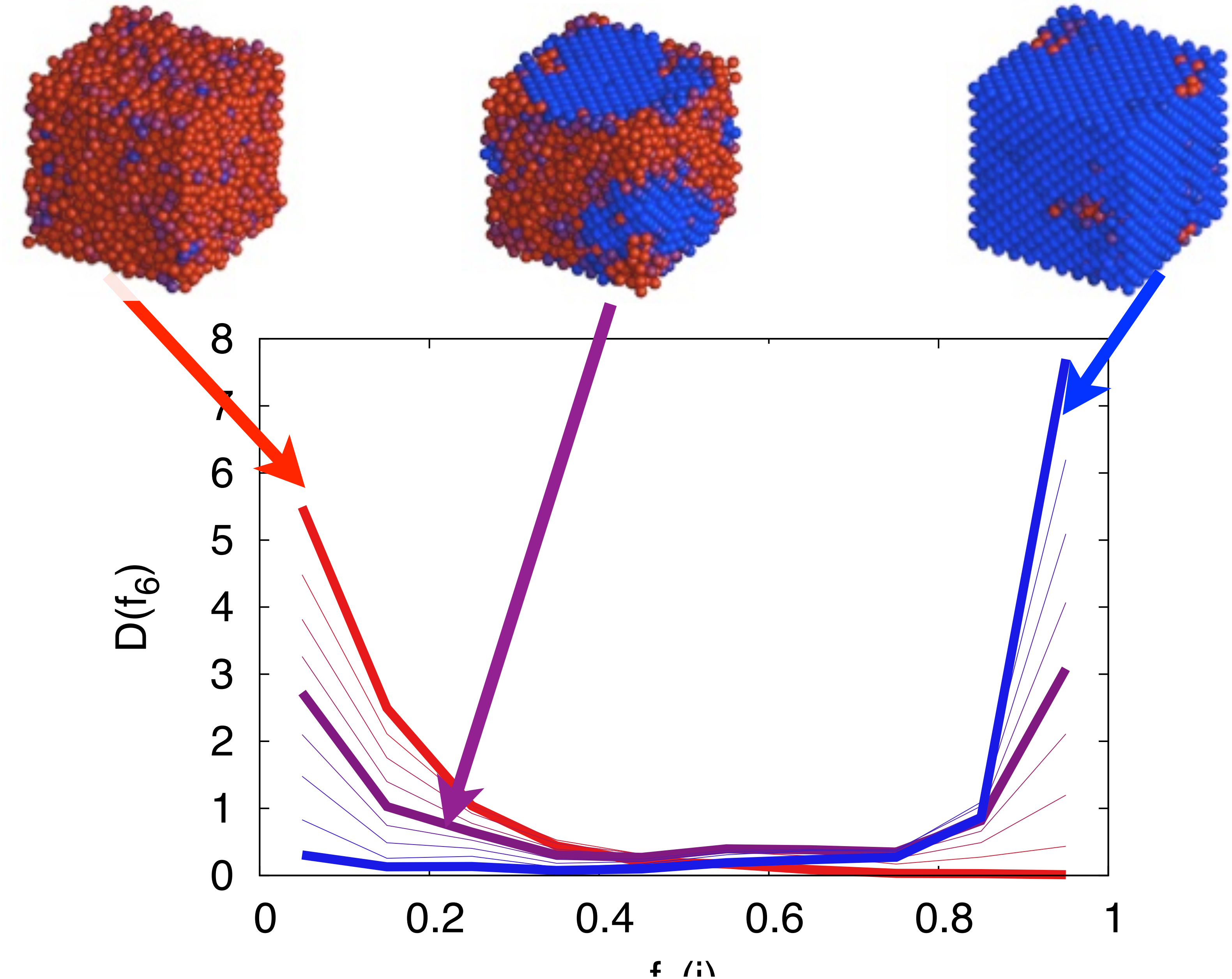
$\boxed{f_6(i) = \text{fraction of highly correlated neighbors (large } S_6)}$

Auer and Frenkel. J. Chem. Phys., 120(6):3015, 2004
Russo and Tanaka. arXiv, cond-mat.soft, 2012.

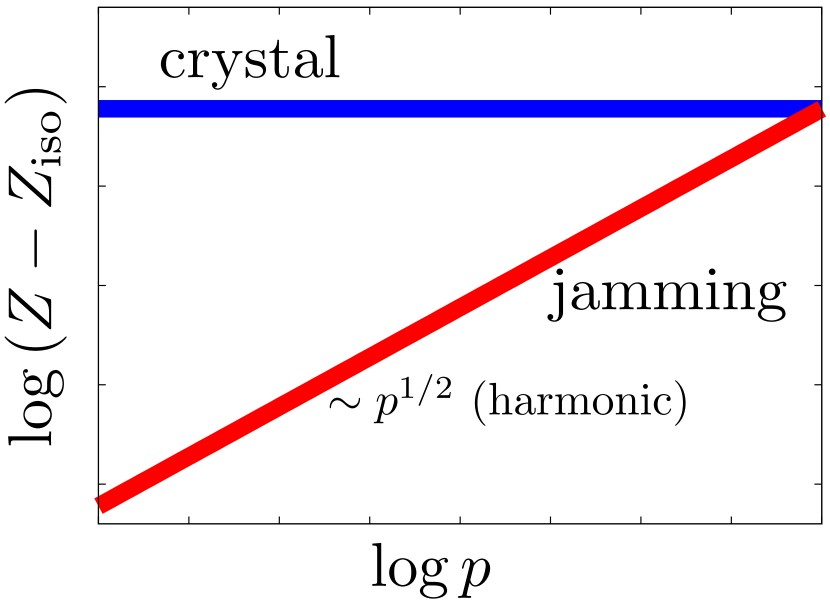
$$f_6 = 1 \;\rightarrow\; \text{crystal}$$

$$f_6 = 0 \;\rightarrow\; \text{disordered}$$

"Coexistence" of ordered and disordered regions

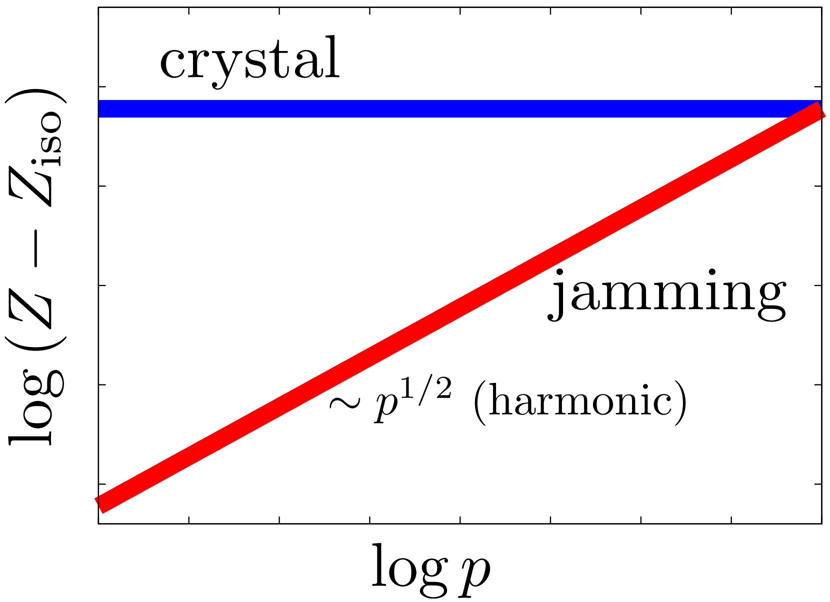


Connecting jamming and crystal physics

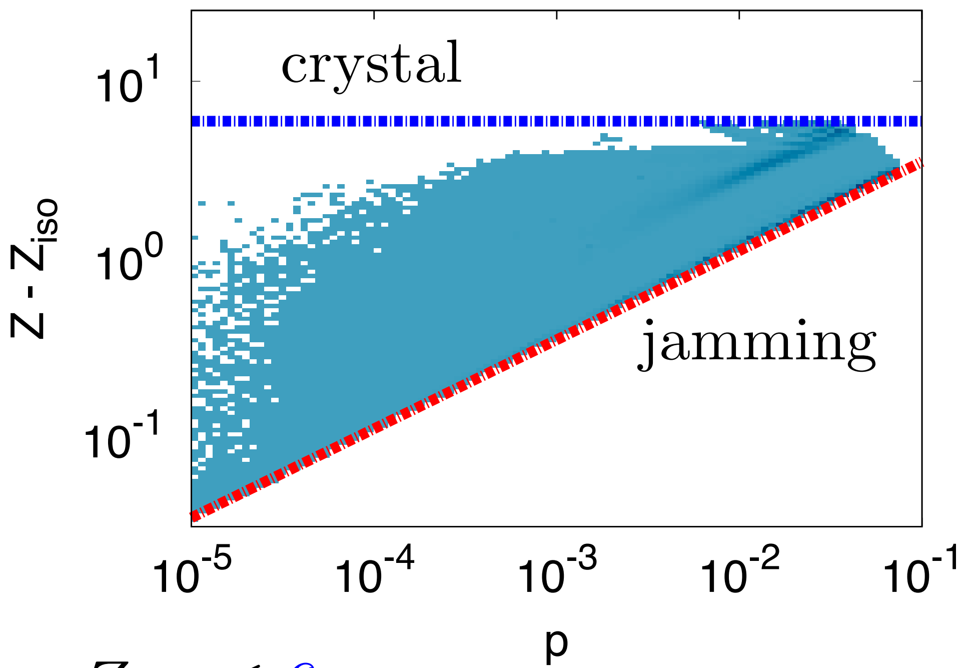


Observed states

Connecting jamming and crystal physics



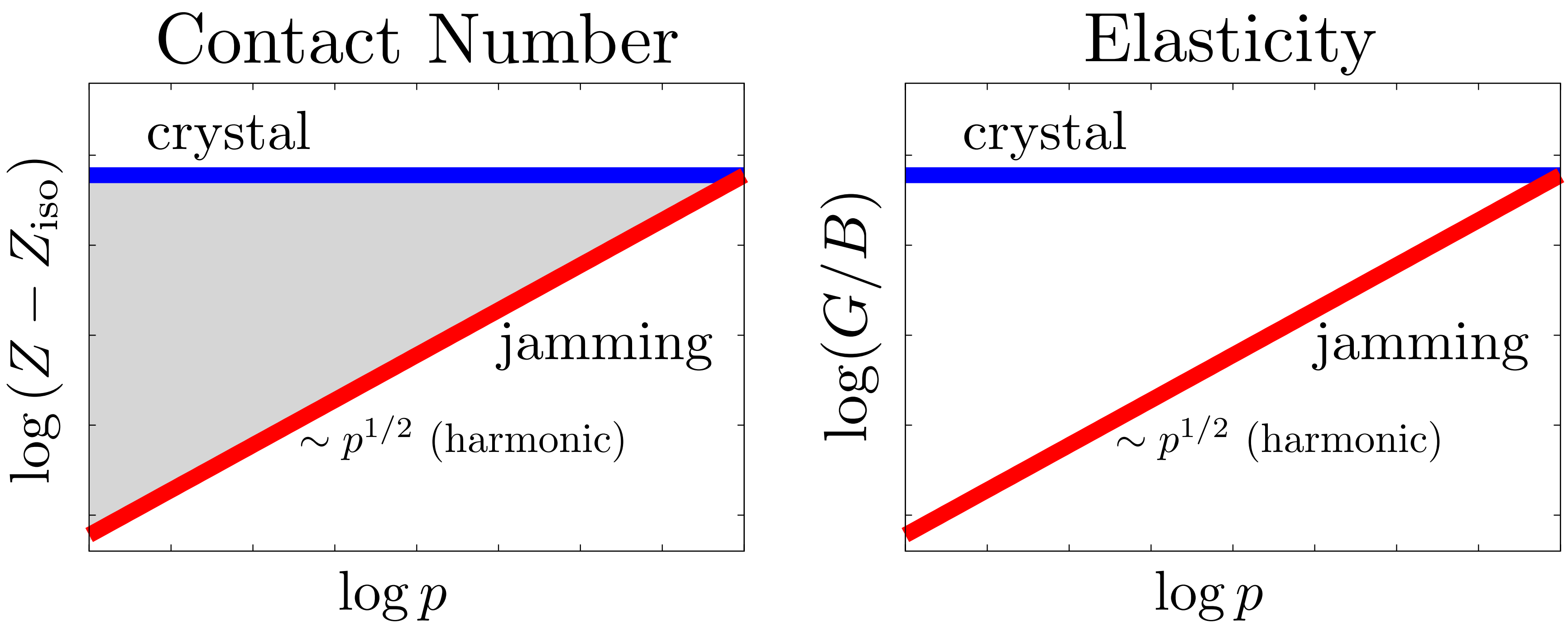
Observed states



$$c_0 p^{1/2} \leq Z - Z_{\mathrm{iso}} \leq 6$$

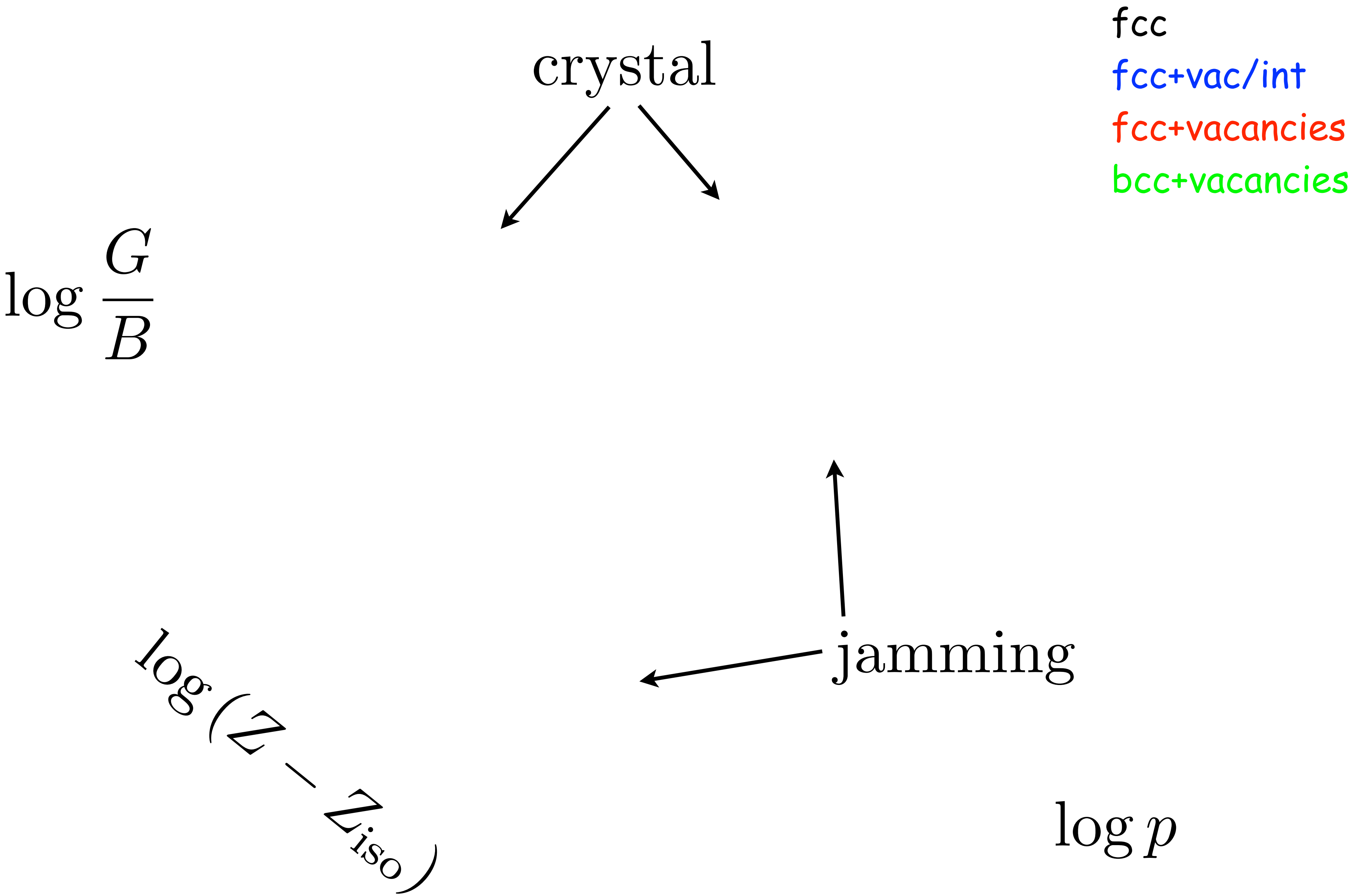
Wyart, *et al*. PRE **72** 051306 (2005)

Elasticity

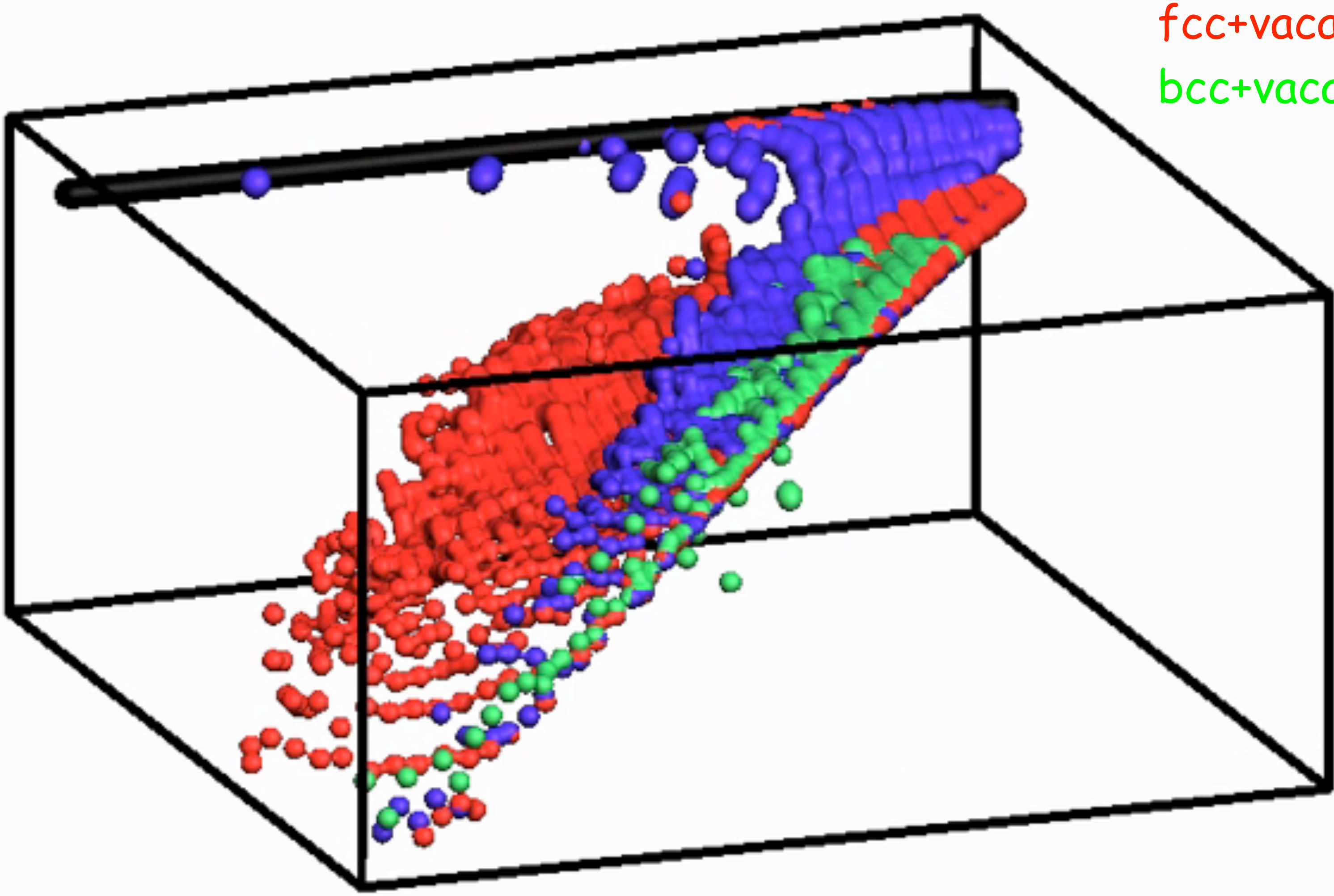


What about systems with intermediate order?

Elasticity

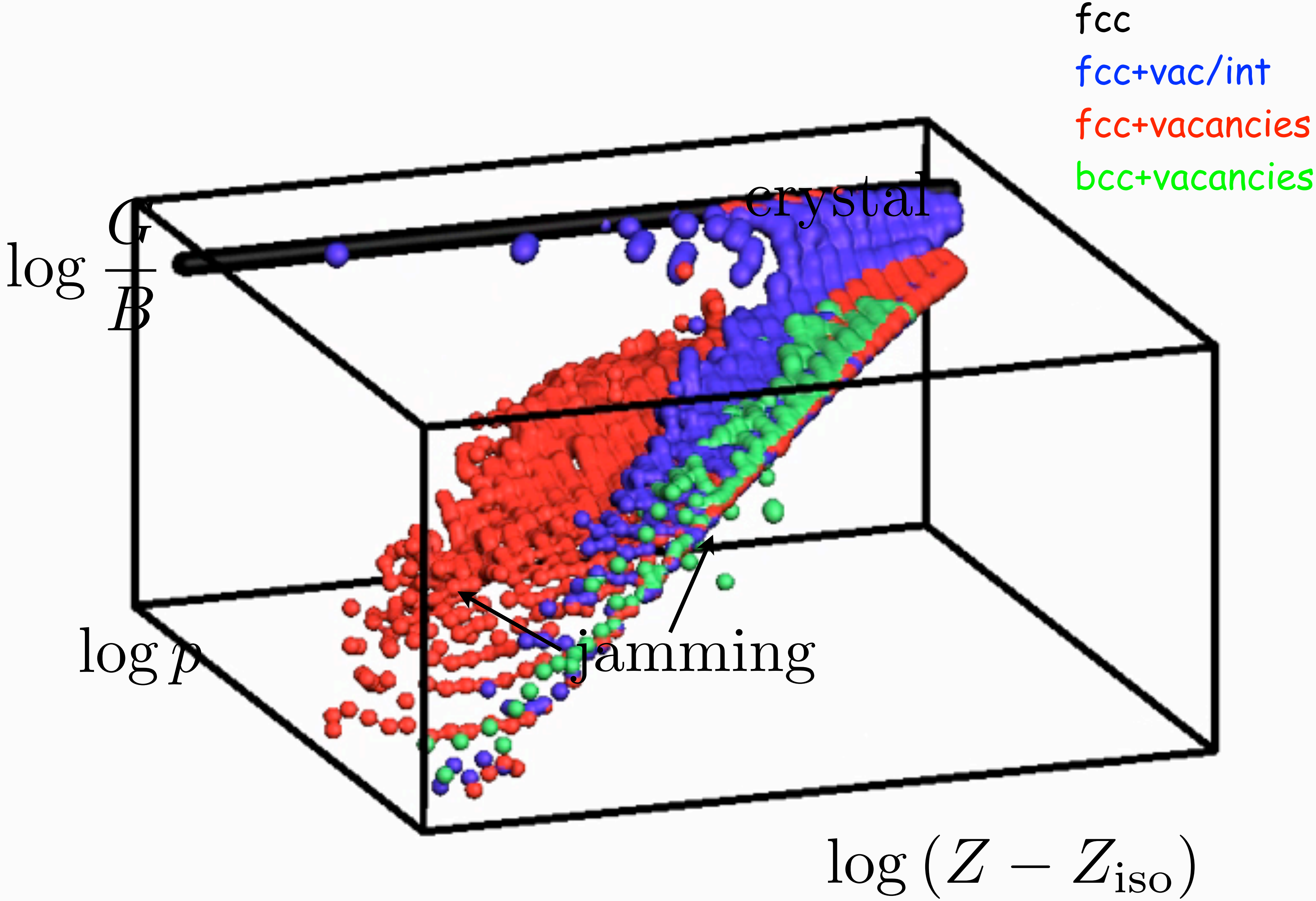

fcc
fcc+vac/int
fcc+vacancies
bcc+vacancies
crystal
$\log \frac{G}{B}$
jamming
$\log (Z - Z_{\mathrm{iso}})$
$\log p$

Elasticity



fcc
fcc+vac/int
fcc+vacancies
bcc+vacancies

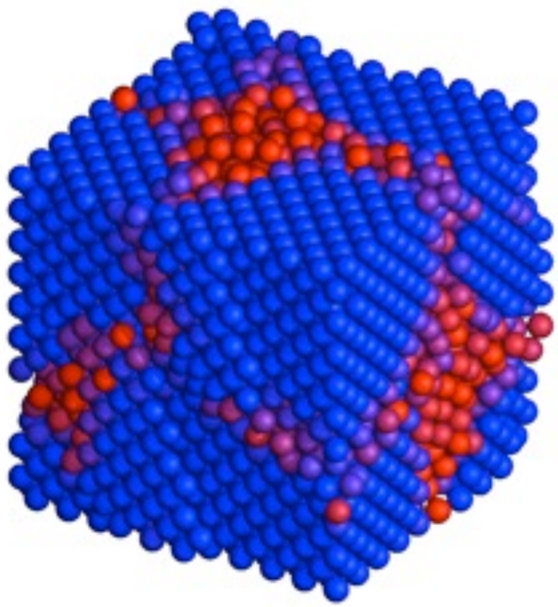
Elasticity



fcc
fcc+vac/int
fcc+vacancies
bcc+vacancies
crystal
$\log \frac{G}{B}$
jamming
$\log p$
$\log\left(Z - Z_{\rm iso}\right)$

Exclude crystalline states

- Include only states where disordered “phase” percolates in all 3 directions



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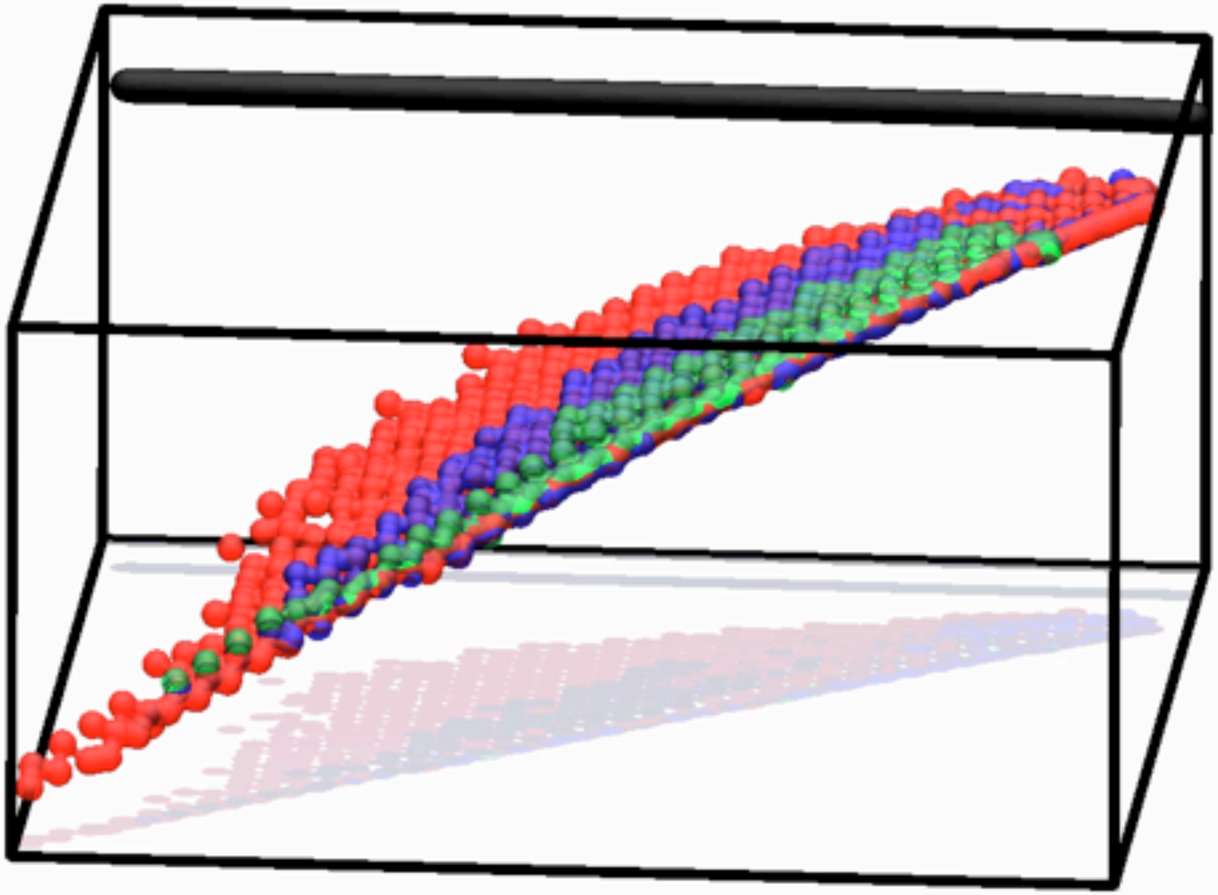

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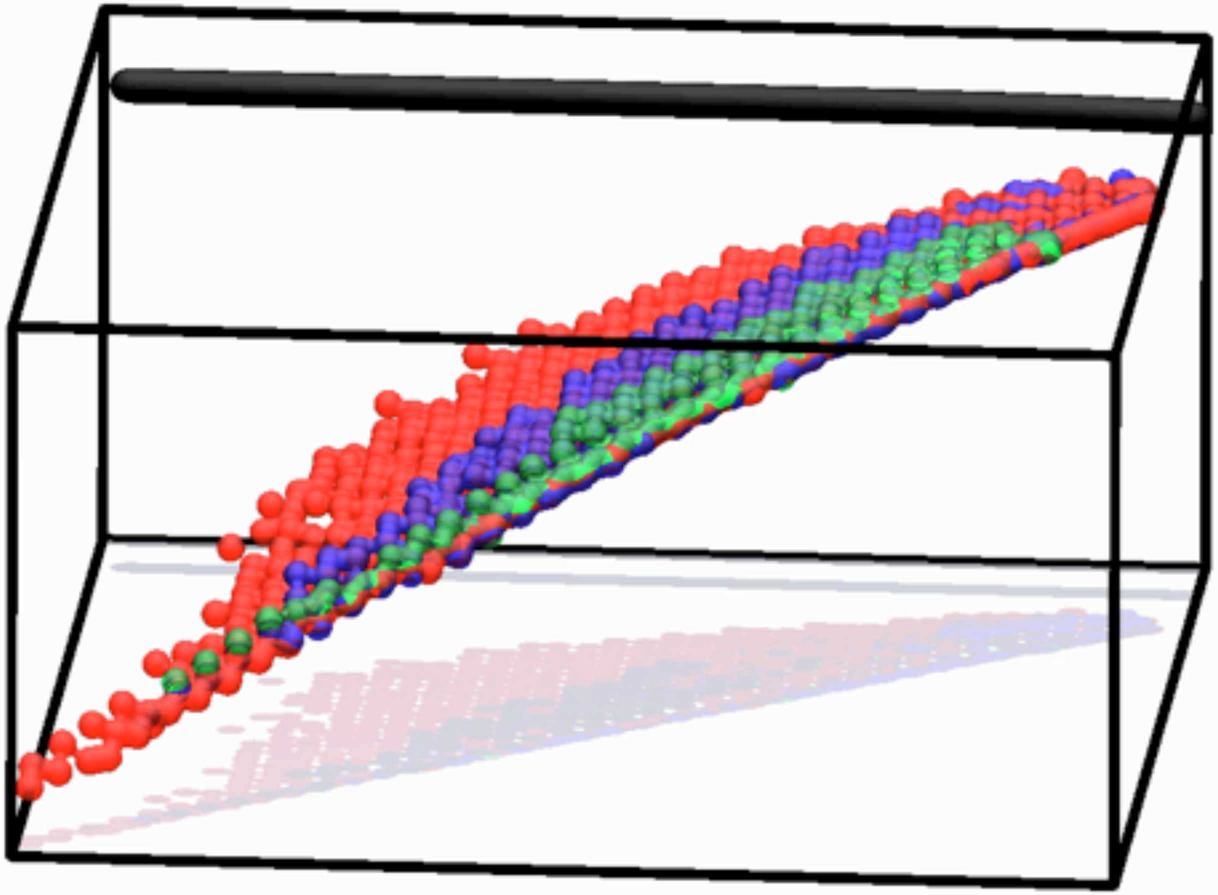


States with intermediate to low order fall on “jamming surface”

Jammed state is not only extreme limit but also very robust

How much does jamming scenario apply to real world?

- What have we left out? ALMOST EVERYTHING
  - friction

K. Shundyak, et al. PRE 75 010301 (2007); E. Somfai, et al. PRE 75 020301 (2007); S. Henkes, et al. EPL 90 14003 (2010).

  - long-ranged interactions/attractions

N. Xu, et al. PRL 98 175502 (2007).

  - non-spherical particle shape

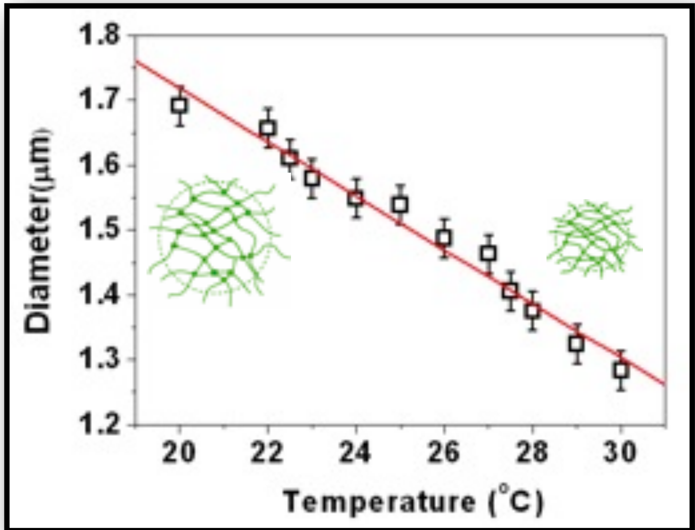
Z. Zeravcic, et al, EPL, **87**, 26001 (2009); M. Mailman, et al, **PRL** 102, 255501 (2009)

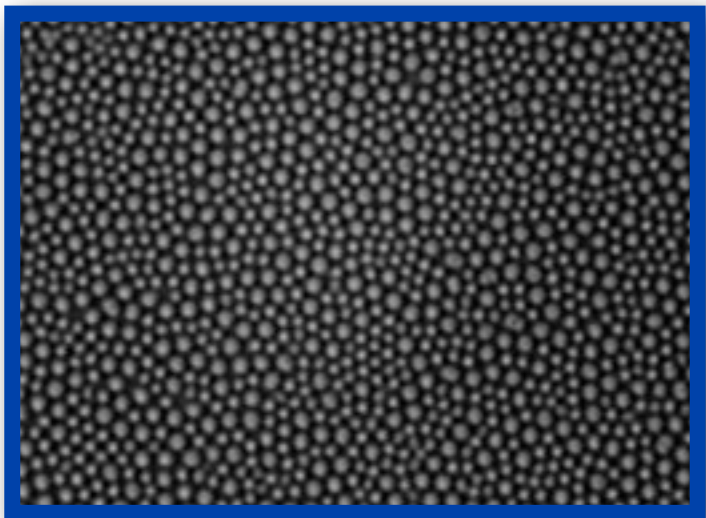
  - temperature

C. Schreck, et al. PRL 107, 078301 (2011); A. Ikeda, et al. J. Chem. Phys. **138**, 12A507 (2013); L. Wang and N. Xu, Soft Matt. **9**, 2475 (2013); T. Bertrand, et al. arXiv:1307.0440.

Real, Thermal Colloidal Glasses

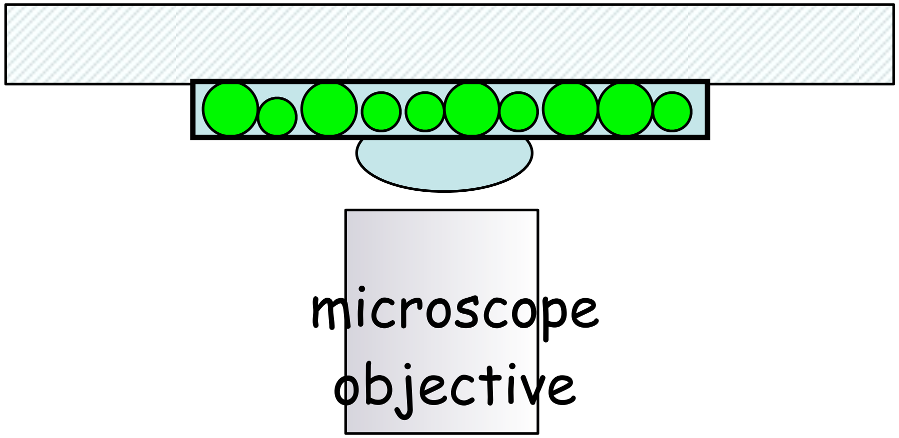
Ke Chen, Wouter Ellenbroek, Arjun Yodh





Video microscopy of 2D jammed packing of colloids

- NIPA microgel particles ⇒ tune packing fraction
- Track particles over ~30000 frames ⇒ $\mathbf{r}_i(t)$



Extract instantaneous displacements from average position

$$\mathbf{u}_i(t) = \mathbf{r}_i(t) - \langle \mathbf{r}_i(t) \rangle_t$$

and the displacement correlation matrix

$$C_{ij} = \langle \mathbf{u}_i(t) \mathbf{u}_j(t) \rangle_t$$

Chen et al., PRL **105**, 025501 (2010)
Ghosh et al., Soft Mat **6**, 3082 (2010)

Colloids are damped, atoms/molecules are not

- BUT displacement correlation is an equilibrium property, independent of dynamics

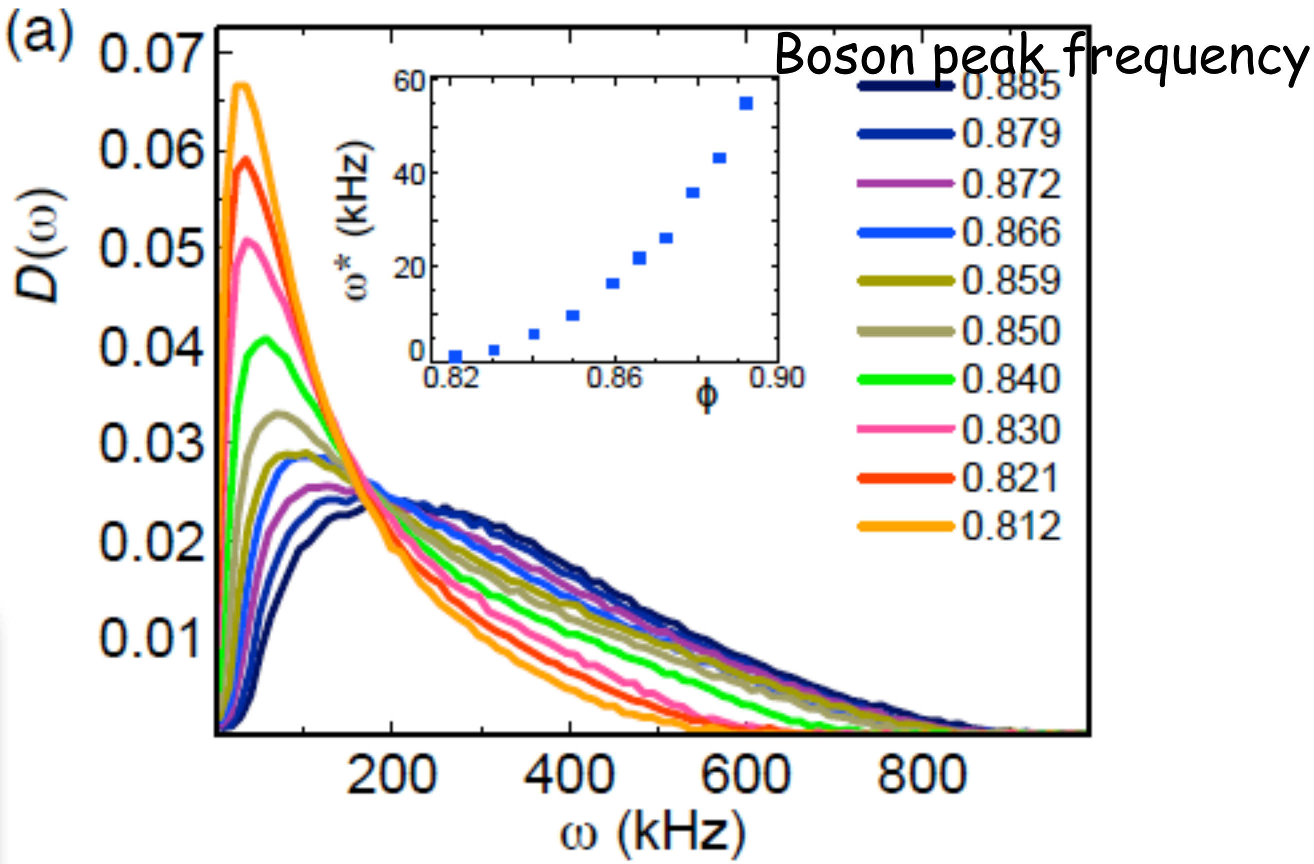
$$C_{ij} = \langle \mathbf{u}_i(t)\mathbf{u}_j(t)\rangle_t$$

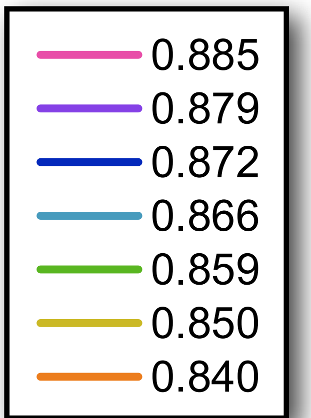
- Can use it to obtain vibrational modes of shadow system with same configuration & interactions but without damping
- In harmonic approximation $V = \frac{1}{2}u^T K u$
- Partition function $Z = \int du \exp(-\beta V)$
- Correlation matrix is inverse of stiffness matrix K

$$C = \langle uu \rangle = K^{-1}$$

Ghosh, Chikkadi, Schall, Kurchan, Bonn, Soft Mat **6**, 3082 (2010)

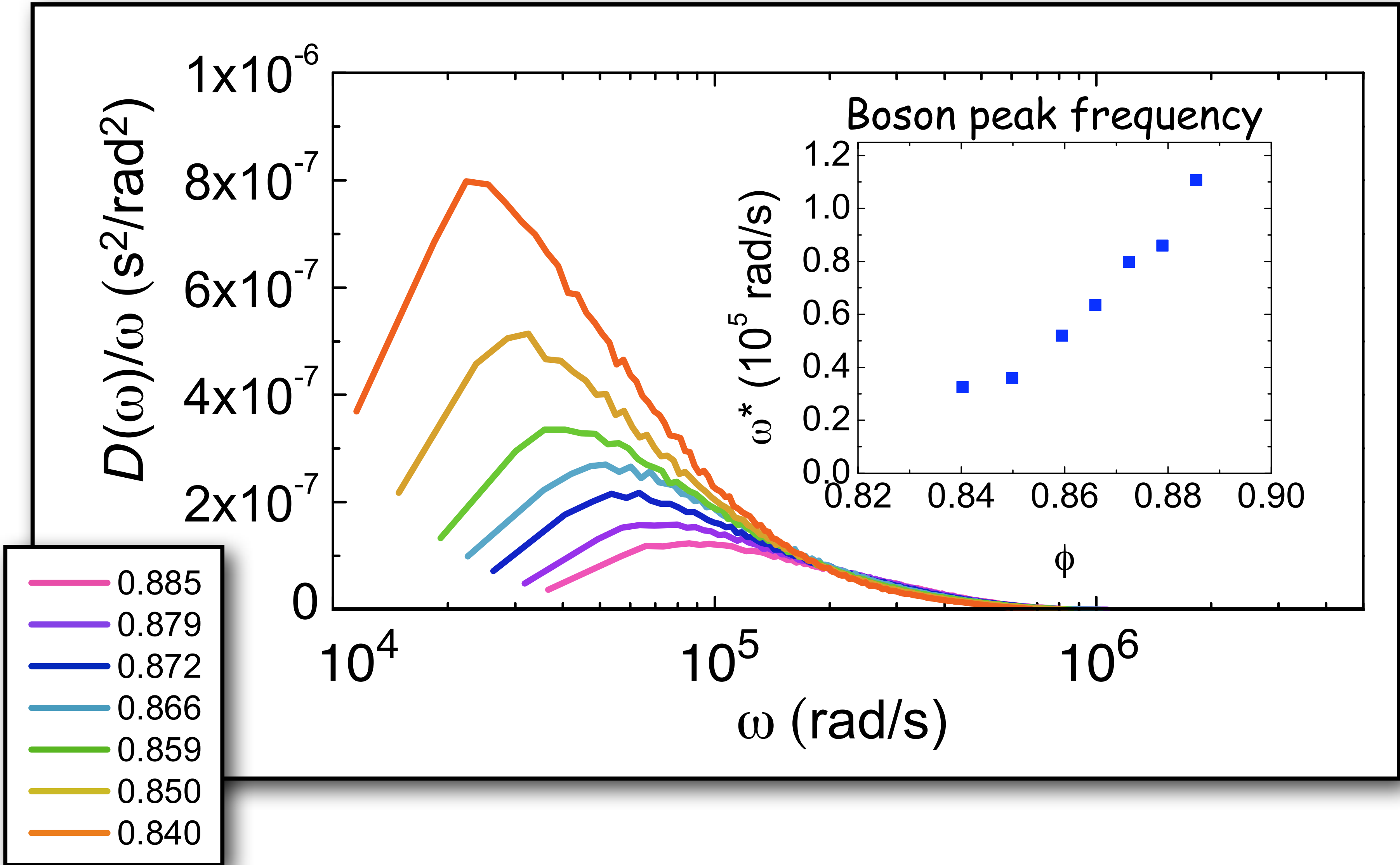
Boson Peak





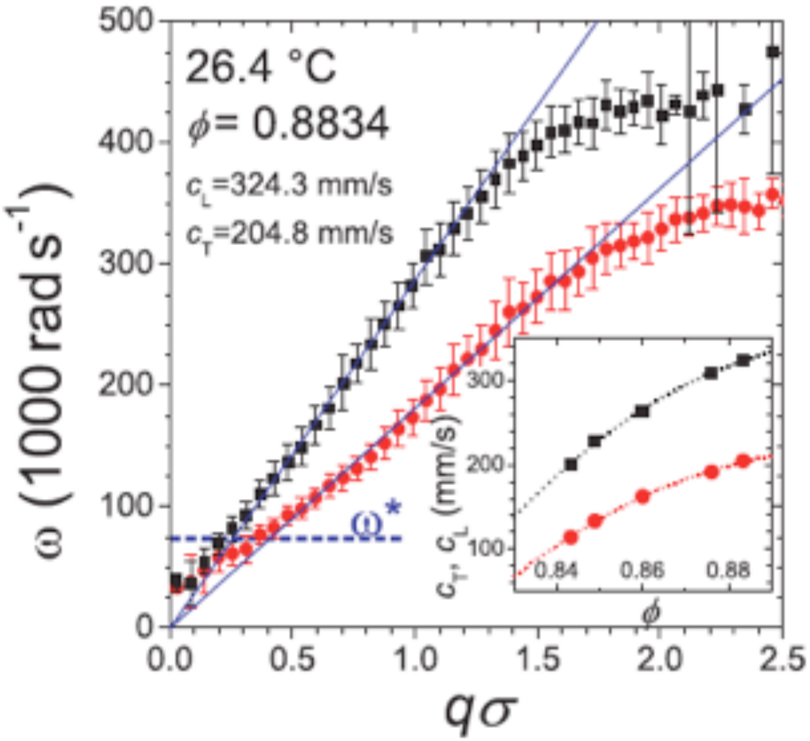
Chen et al., PRL **105**, 025501 (2010)

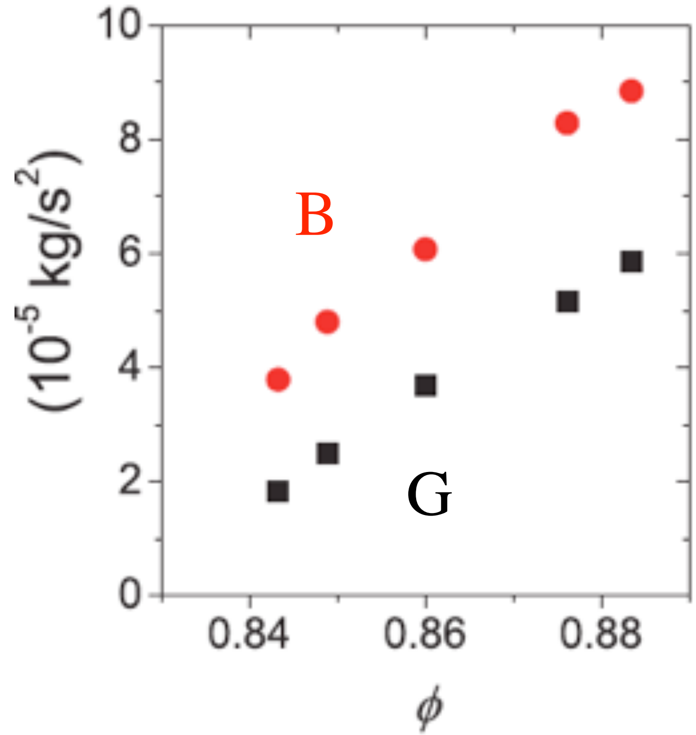
Boson Peak



Chen et al., PRL **105**, 025501 (2010)

Dispersion relation and elastic constants





- From dispersion relation extract sound velocities
- From sound velocities extract elastic constants

G/B behavior

- Recall that G/B does not depend on potential
- For frictionless particles,

$$G/B \approx 0.23\Delta z(1 - 0.14\Delta z)$$

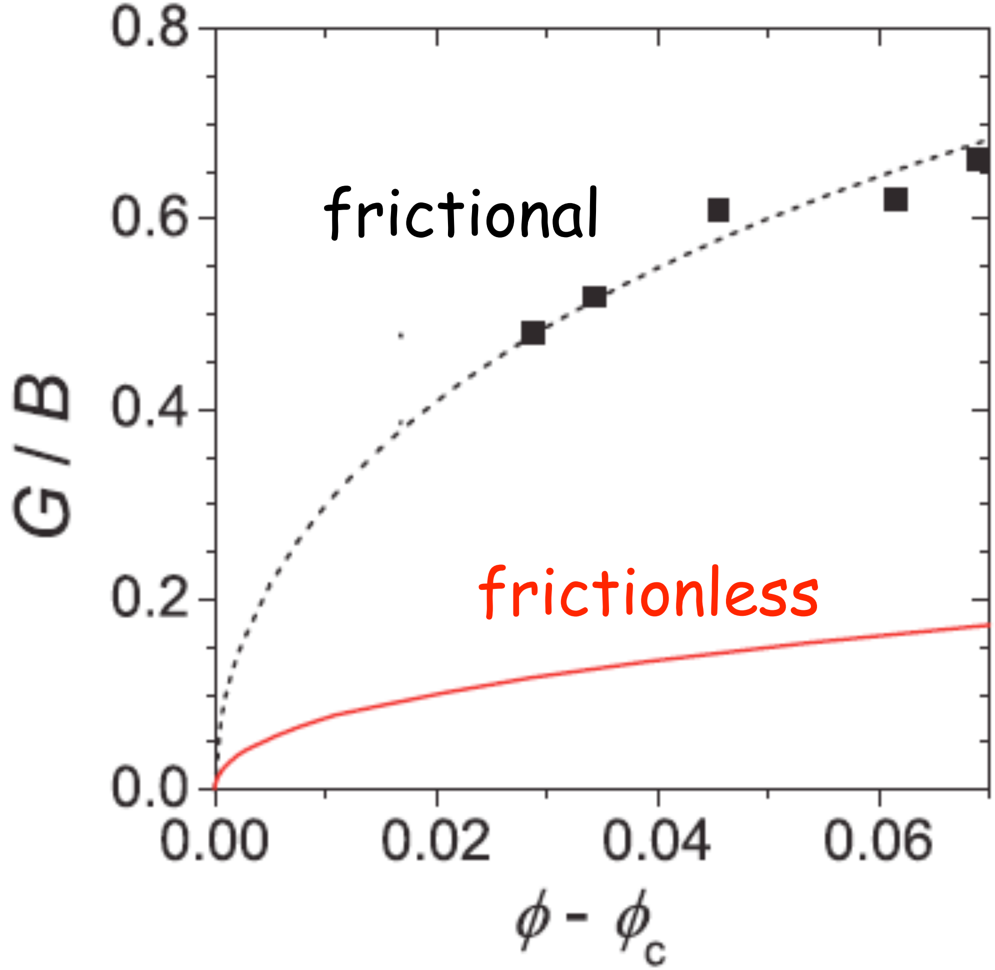
where $\Delta z \equiv z - z_c^0 = 3.3(\phi - \phi_c^0)$

- For frictional particles, E. Somfai, et al. PRE 75, 020301 (2007).

$$G/B \approx 0.98\Delta z(1 - 0.23\Delta z)$$

where $\Delta z \equiv z - z_c^\infty = 3.3(\phi - \phi_c^\infty)$

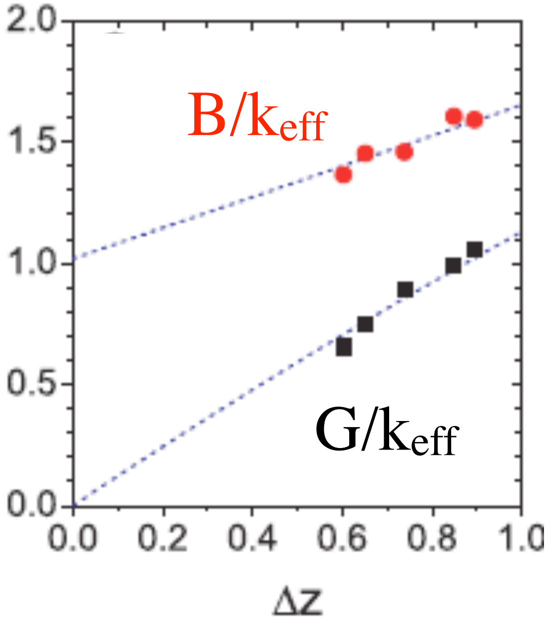
PNIPAM particles are frictional



- one adjustable parameter ϕ_c^∞

G, B

- Interaction most consistent with Hertzian (K. Nordstrom, et al. PRL **105**, 175701 (2010))



$$k_{\rm eff} = \frac{\sqrt{3}\epsilon}{2\sigma^2}\left(\phi - \phi_c^\mu\right)^{1/2}$$

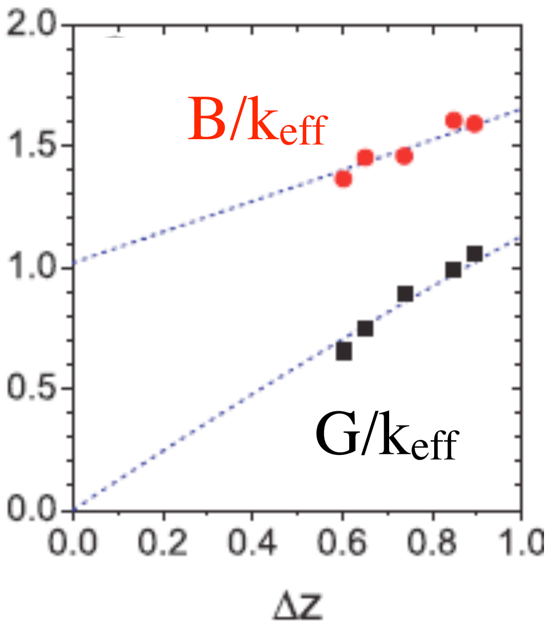
$$k_B T/\epsilon = 3\times 10^{-6}$$

$$\mu \approx 0.6$$

K. Shundyak, et al. PRE 75, 010301 (2007).

G, B

- Interaction most consistent with Hertzian (K. Nordstrom, et al. PRL **105**, 175701 (2010))



$$k_{\text{eff}} = \frac{\sqrt{3}\boxed{\epsilon}}{2\sigma^2}(\phi - \boxed{\phi_c^{\mu}})^{1/2}$$

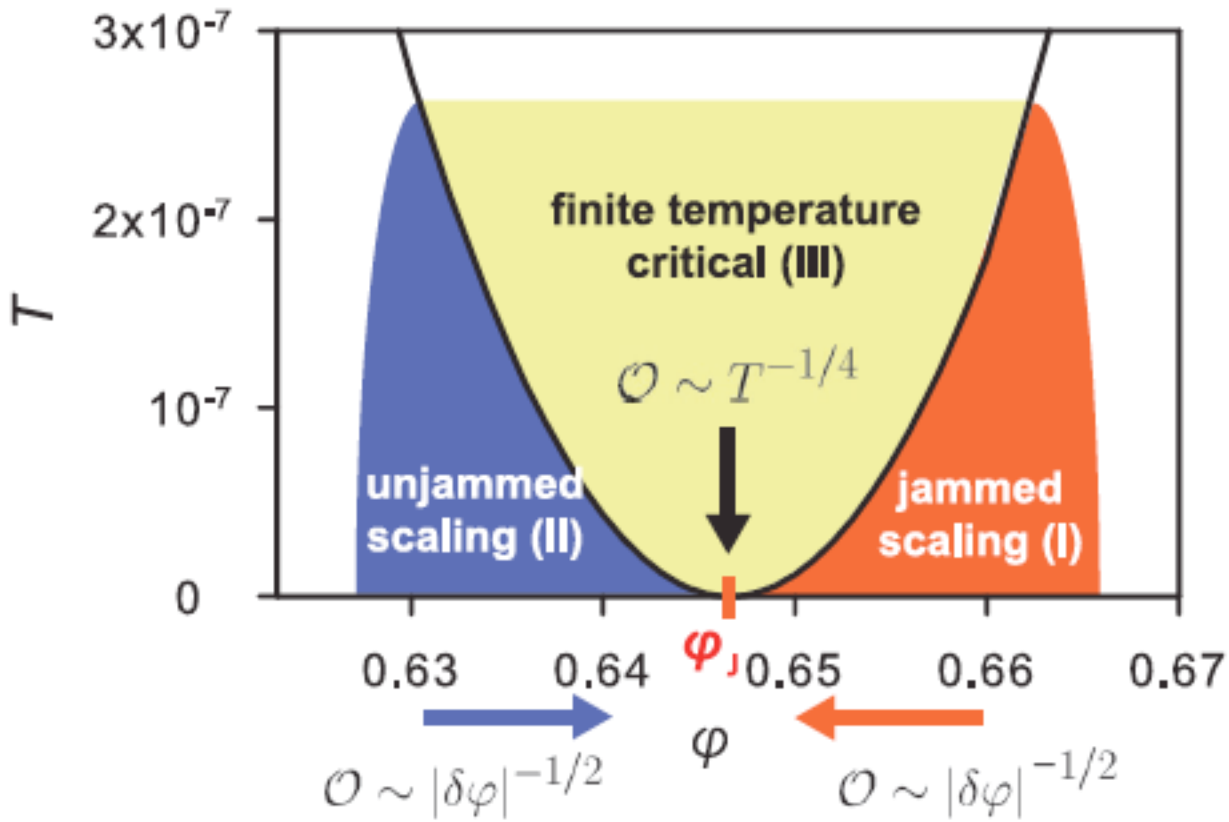
two adjustable parameters

$$k_B T/\epsilon = 3 \times 10^{-6}$$

$$\mu \approx 0.6$$

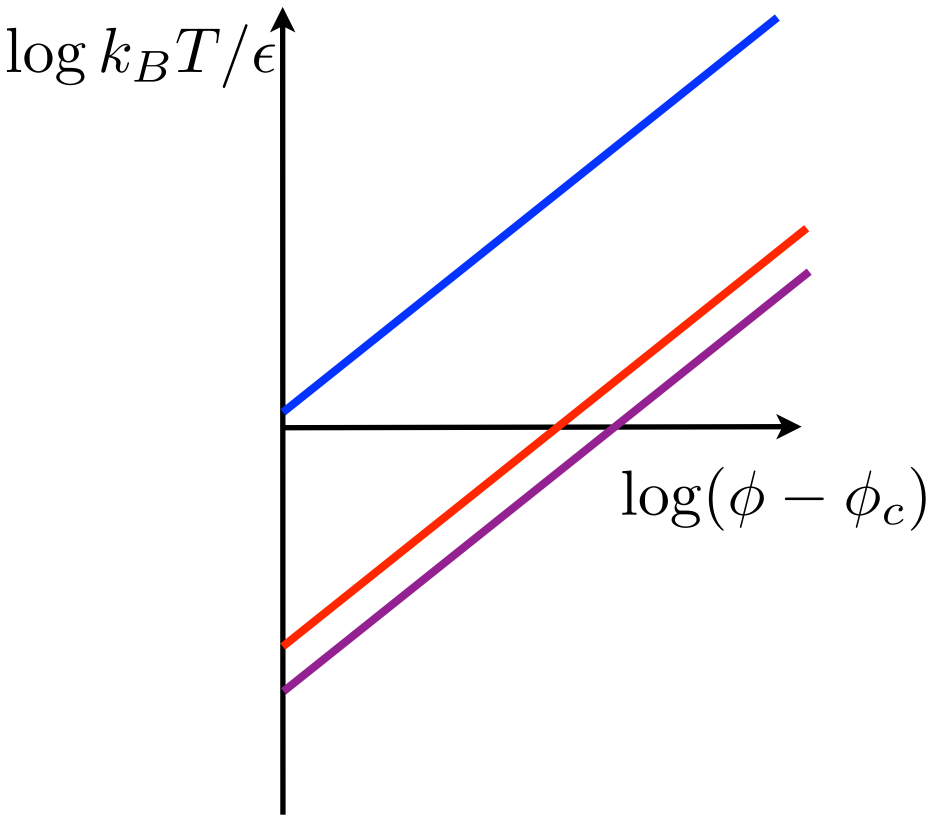
K. Shundyak, et al. PRE 75, 010301 (2007).

Jamming and temperature



A. Ikeda, L. Berthier and G. Biroli, J. Chem. Phys. **138**, 12A507 (2013)

Effect of Temperature



$k_B T^*$ is temperature at which T=0 description breaks down

Bertrand, et al.

$$k_B T^*/\epsilon \approx C(N)(\phi - \phi_c)^{5/2}$$

where $C(N) \to 0$ as $N \to \infty$

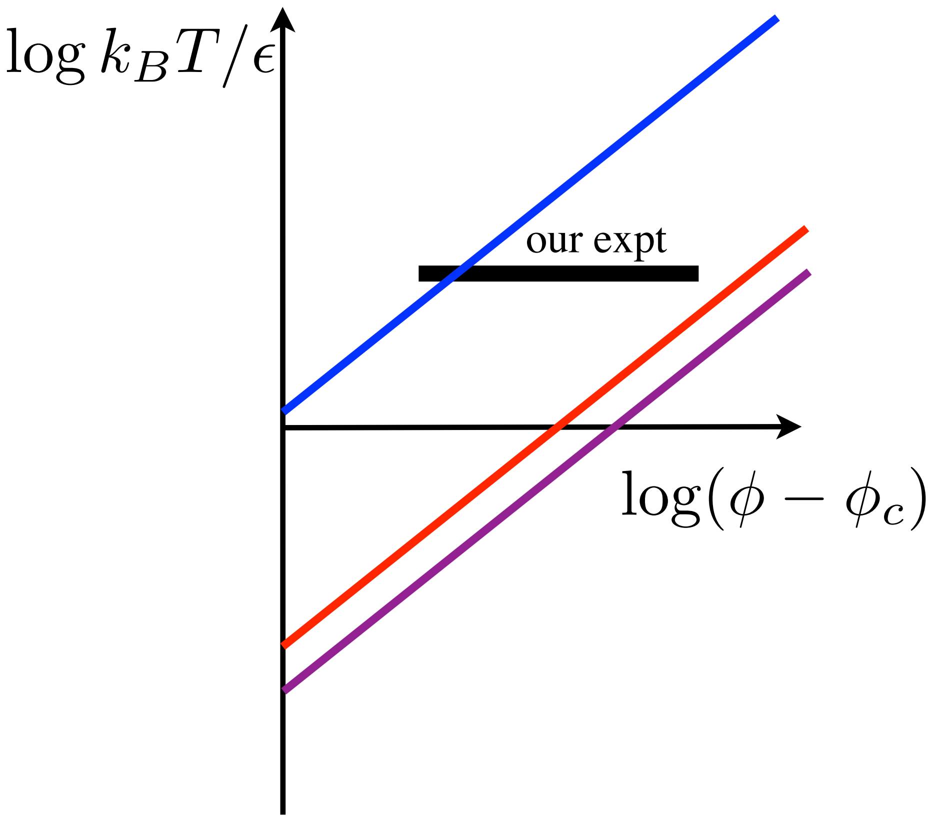
Ikeda, et al.

$$k_B T^*/\epsilon \approx 10^{-3}(\phi - \phi_c)^{5/2}$$

Wang and Xu

$$k_B T^*/\epsilon \approx 0.2(\phi - \phi_c)^{5/2}$$

Effect of Temperature



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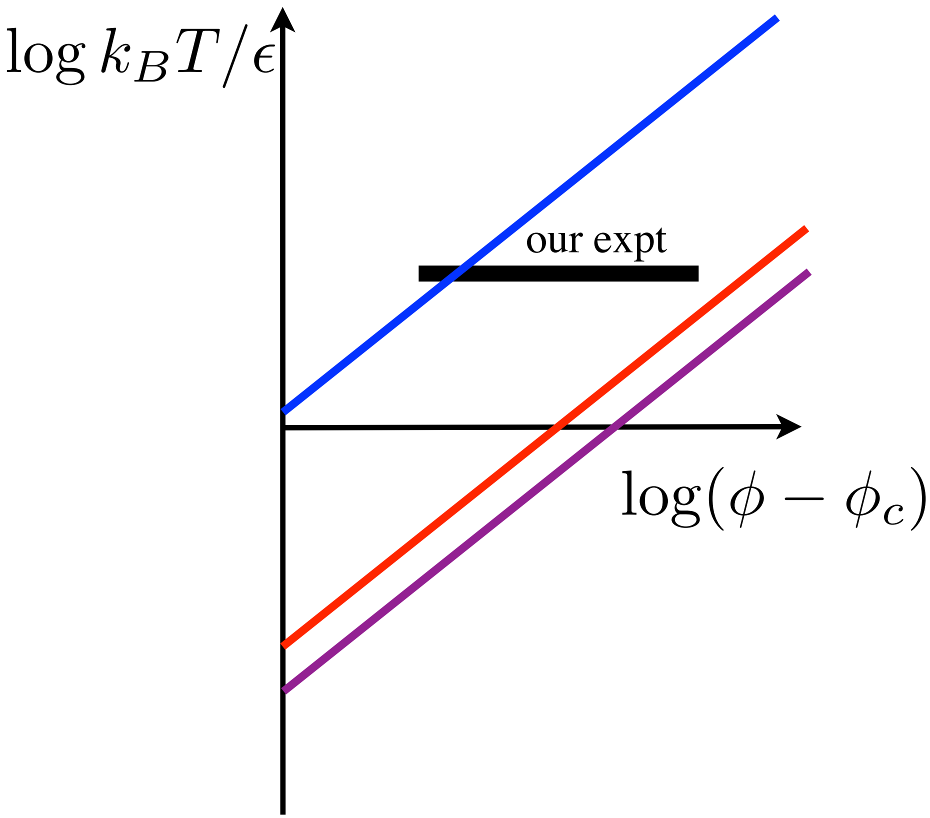

Breaks down for what?

$k_B T^*$ is temperature at which T=0 description breaks down

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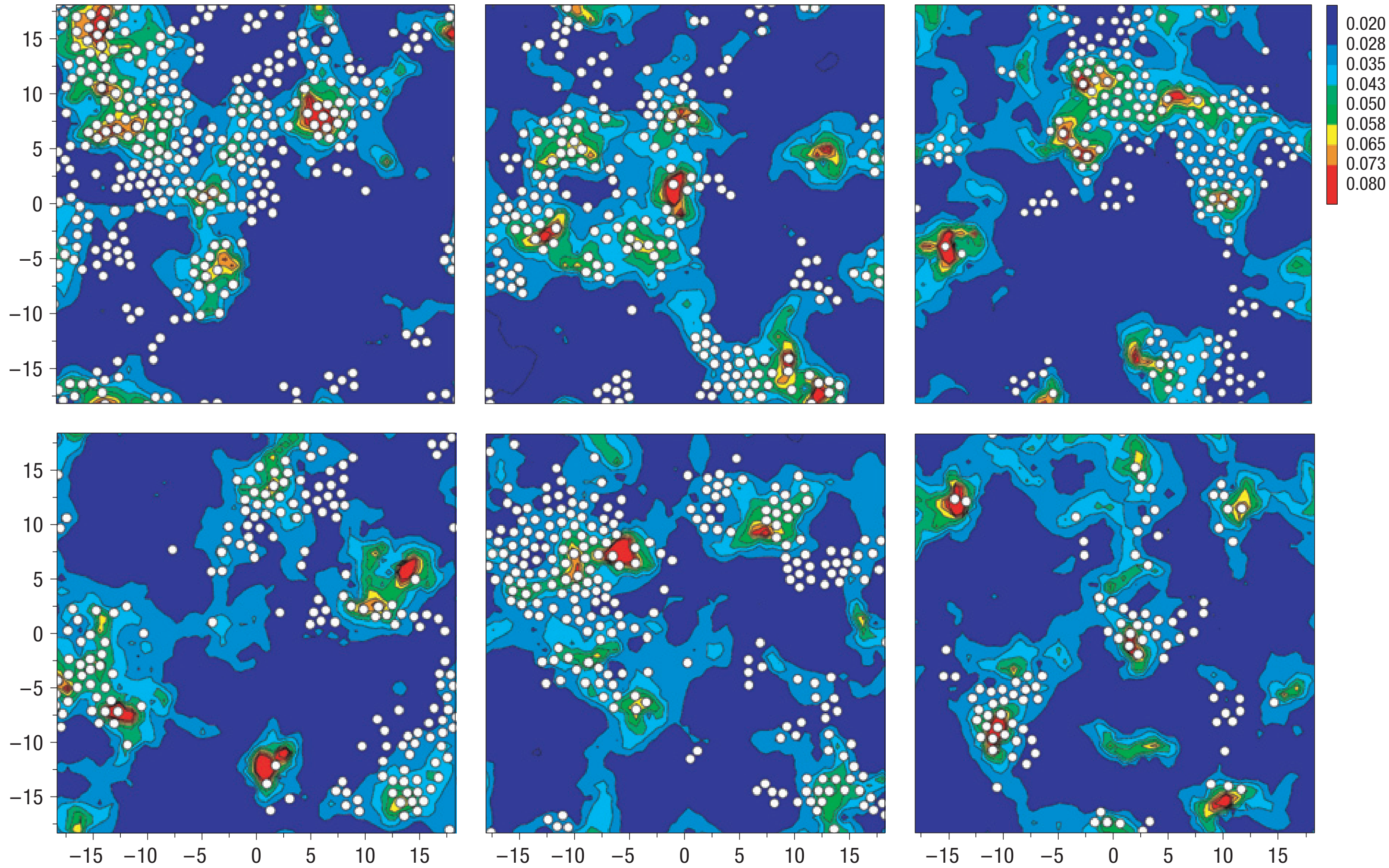
Quasilocalized modes predict rearrangements above T_g

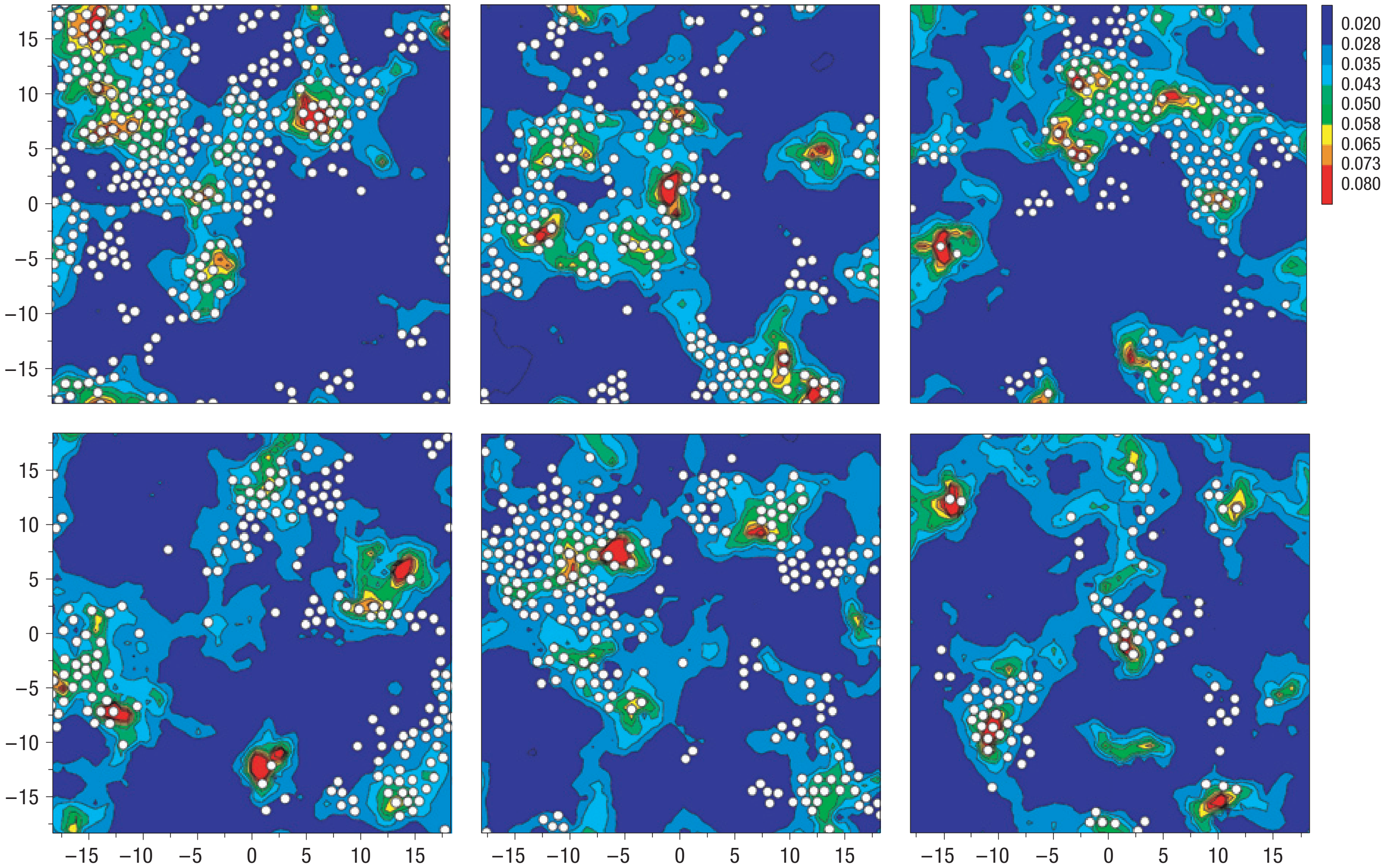
Widmer-Cooper, Perry, Harrowell, Reichman, Nat. Phys. 4,711 (2008)



- Color contours: Sum (polarization vector magnitudes)^2 for each particle over lowest 30 vibrational modes
- white circles: particles that rearranged in relaxation time interval

Quasilocalized modes predict rearrangements above T_g

Widmer-Cooper, Perry, Harrowell, Reichman, Nat. Phys. 4,711 (2008)



- Color contours: Sum (polarization vector magnitudes)^2 for each particle over lowest 30 vibrational modes   Why 30? ω^*
- white circles: particles that rearranged in relaxation time interval

Summary

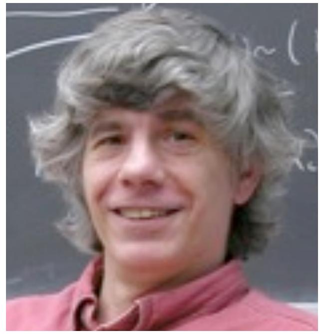
- The marginally jammed state represents extreme limit at the opposite pole from the perfect crystal

- The behavior of systems over a wide range of order/disorder follows jamming scaling
- So the marginally jammed is a robust extreme limit--more robust than the perfect crystal

- Jamming scenario provides conceptual basis for commonality of low temperature/frequency properties of disordered solids
- relevance to glass transition is still an open question

Thanks to

Carl Goodrich



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