Jamming as the Extreme Limit of a Solid

Andrea J. Liu
Department of Physics & Astronomy
University of Pennsylvania

Carl Goodrich
UPenn

Sidney Nagel
U Chicago

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?
Perturbing away from the crystal

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

Tuesday, July 16, 13
Jamming Transition for “Ideal Spheres”

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


Bubble model for foams
Jamming Transition for "Ideal Spheres"


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

- Study models with smooth transitions
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Bubble model for foams
Onset of Jamming in Repulsive Sphere Packings

Just below \( \phi_c \), no particles overlap.

Just above \( \phi_c \) there are \( Z_c \) overlapping neighbors per particle.

\[
Z - Z_c \approx Z_0 (\phi - \phi_c)^{0.5}
\]

\( Z_c = 3.99 \pm 0.01 \) \hspace{1cm} (2D)

\( Z_c = 5.97 \pm 0.03 \) \hspace{1cm} (3D)

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


Tuesday, July 16, 13
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

perfect crystal

vs

marginally jammed solid

crystal: $Z=12$
marginally jammed solid: $Z=Z_{\text{iso}}=6$

$log (Z - Z_{\text{iso}})$

$log p$

$\sim p^{1/2}$ (harmonic)
Constraint Counting and $G/B$

- At onset of overlap, $\phi_c$, can constrain
  - all soft modes
  - compression of the whole system

- So $B>0$ but $G=0$ so $G/B=0$

Above $\phi_c$, $G/B >0$ so $\phi_c$ also marks onset of jamming
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$p \approx p_0 (\phi - \phi_c)^{\alpha - 1}$

$G/B \sim \Delta Z$

$log \phi - \phi_c$ vs $log p$

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

X. Mao, A. Souslov, T. C. Lubensky
Mechanics of crystal vs. marginally jammed solid

Perfect crystal

Marginal jammed solid

crystal: $G/B \sim 1$
marginal jammed solid: $G/B \to 0$

$log(p)$

$log(G/B)$

$\sim p^{1/2}$ (harmonic)
Consequence: Diverging Length Scale

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

• For system at $\phi_c$, $Z=2d$

• Removal of one bond makes entire system unstable by adding a soft mode

• This implies diverging length as $\phi \rightarrow \phi_c$.

For $\phi > \phi_c$, 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

$$\ell_L \sim \frac{1}{Z - Z_c} \equiv \frac{1}{\Delta Z} \sim (\phi - \phi_c)^{-0.5}$$
Define $\ell^*$ as size of smallest macroscopic rigid cluster for system with a free boundary of any shape or size.

- $\ell^*$ diverges at Point J as expected from scaling argument.
More precisely

Define $\ell^*$ as size of smallest macroscopic rigid cluster for system with a free boundary of any shape or size.

- $\ell^*$ diverges at Point J as expected from scaling argument.

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Vibrations in Disordered Sphere Packings

- Crystals are all alike at low T or low $\omega$
  - 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 $\ell L$

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: \( \ell \propto c_L/\omega^* \)
  \( \ell_t \propto c_T/\omega^* \)

\[
\omega^*/\omega_0 \sim \Delta \phi^{1/2}
\]

\[
\omega_0 \equiv \sqrt{\frac{k_{eff}}{m}} \sim \Delta \phi^{(\alpha-2)/2}
\]
• 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: \( l_L = c_L / \omega^* \)
\( l_T = c_T / \omega^* \)
Vibrations of crystal vs. marginally jammed solid

perfect crystal

marginally jammed solid

D(\omega)

no plane waves even at \omega = 0
Vibrations of crystal vs. marginally jammed solid

perfect crystal

FCC Crystal

vs

marginally jammed solid

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?
Back to extreme limits

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1. start with a perfect FCC crystal

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2d illustration
How do we connect physics of jamming and physics of crystals? What happens in between?

1. start with a perfect FCC crystal
2. introduce 1 vacancy-interstitial pair
Back to extreme limits

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

1. start with a perfect FCC crystal

2. introduce 1 vacancy-interstitial pair

3. minimize the energy
How do we connect physics of jamming and physics of crystals? What happens in between?

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?

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

Tuesday, July 16, 13
How do we connect physics of jamming and physics of crystals? What happens in between?

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

2d illustration
Back to extreme limits

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

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

$2d$ illustration
**Order Parameter**

**Bond-orientational order**

\[
q_{lm}(i) \equiv \sum_{j} Y_{lm}(\hat{r}_{ij})
\]

\[
S_l(i, j) \equiv \sum_{m} q_{lm}(i) \cdot q_{lm}^{*}(j)
\]

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

\[
f_6 = 1 \rightarrow \text{crystal}
\]

\[
f_6 = 0 \rightarrow \text{disordered}
\]

"Coexistence" of ordered and disordered regions
Connecting jamming and crystal physics

Observed states

\[ \log (Z - Z_{\text{iso}}) \sim p^{1/2} \text{ (harmonic)} \]
Connecting jamming and crystal physics

\[ \log (Z - Z_{iso}) \]

\[ \log p \]

\[ \sim p^{1/2} \text{ (harmonic)} \]

\[ c_0 p^{1/2} \leq Z - Z_{iso} \leq 6 \]

Observed states

Wyart, et al. PRE 72 051306 (2005)
What about systems with intermediate order?

Contact Number

\[ \log (Z - Z_{iso}) \]

\[ \sim p^{1/2} \text{ (harmonic)} \]

Elasticity

\[ \log (G/B) \]

\[ \sim p^{1/2} \text{ (harmonic)} \]
Elasticity

\[ \log \frac{G}{B} \]

\[ \log (Z - Z_{\text{iso}}) \]

jamming

\[ \log p \]

fcc

fcc+vac/int

fcc+vacancies

bcc+vacancies

crystal
Elasticity

- fcc
- fcc+vac/int
- fcc+vacancies
- bcc+vacancies
Elasticity

\[ \log \left( \frac{G}{B} \right) \]

\[ \log \rho \]

\[ \log \left( Z - Z_{iso} \right) \]

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

Crystal

Jamming
Exclude crystalline states

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

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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
  
  - long-ranged interactions/attractions
  
  - non-spherical particle shape
  
  - temperature
Real, Thermal Colloidal Glasses

Ke Chen, Wouter Ellenbroek, Arjun Yodh

Video microscopy of 2D jammed packing of colloids
- NIPA microgel particles $\Rightarrow$ tune packing fraction
- Track particles over $\sim$30000 frames $\Rightarrow r_i(t)$

Extract instantaneous displacements from average position
$$u_i(t) = r_i(t) - \langle r_i(t) \rangle_t$$
and the displacement correlation matrix
$$C_{ij} = \langle u_i(t) u_j(t) \rangle_t$$

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

\[ C_{ij} = \langle u_i(t)u_j(t) \rangle_t \]

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

  \[ G/B \approx 0.98\Delta z(1 - 0.23\Delta z) \]
  where $\Delta z \equiv z - z_c^\infty = 3.3(\phi - \phi_c^\infty)$
PNIPAM particles are frictional

- one adjustable parameter $\phi_c$
• Interaction most consistent with Hertzian (K. Nordstrom, et al. PRL 105, 175701 (2010))

\[ k_{\text{eff}} = \frac{\sqrt{3}\epsilon}{2\sigma^2} \left( \phi - \phi_{\mu} \right)^{1/2} \]

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

\[ \mu \approx 0.6 \]


\[ k_{\text{eff}} = \frac{\sqrt{3} \epsilon}{2\sigma^2} (\phi - \phi_{\mu, c})^{1/2} \]

two adjustable parameters

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

\[ \mu \approx 0.6 \]

Jamming and temperature

**Effect of Temperature**

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

Bertrand, et al.

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

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

Ikeda, et al.

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

Wang and Xu

$$\frac{k_B T^*}{\epsilon} \approx 0.2(\phi - \phi_c)^{5/2}$$
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Quasilocalized modes predict rearrangements above $T_g$

- **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 $T_g$

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

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

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Bread for Jam:
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