Jamming and the Glass Transition

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Focus on foams/emulsions or frictionless granular material
- soft, repulsive, finite-range spherically-symmetric potentials

Such systems have T=0 1st/2nd-order phase transition

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- soft, repulsive, finite-range spherically-symmetric potentials

Such systems have T=0 1st/2nd-order phase transition
How we study Point $J$

- **Generate configurations near $J$**
  - Start with some initial config
  
  \[
  V(r) = \begin{cases} 
  \frac{\varepsilon}{\alpha} \left(1 - \frac{r}{\sigma}\right)^\alpha & r \leq \sigma \\
  0 & r > \sigma 
  \end{cases}
  \]

  - Conjugate gradient energy minimization (inherent structures, Stillinger & Weber)

- **Classify resulting configurations**

  - Non-overlapped
    
    \(V=0\)  
    \(p=0\)
    
    \(T_f=0\)
    
  - Overlapped
    
    \(V>0\)  
    \(p>0\)
    
    \(T_f=0\)
Onset of Overlap is Onset of Jamming

- Pressures for different states collapse on a single curve
- Shear & bulk moduli, $G$ & $B$, vanish at same $\phi_c$
- $G/B \sim (\phi - \phi_c)^{\gamma \approx 1/2}$

D. J. Durian, PRL 75, 4780 (1995);
Onset of Overlap has 1st-Order Character

Just below $\phi_c$, no particles overlap

Just above $\phi_c$, there are $Z_c$ overlapping neighbors per particle

$Z_c = 3.99 \pm 0.01$ (2D)

$Z_c = 5.97 \pm 0.03$ (3D)

Verified experimentally:

Isostaticity

• What is the minimum number of interparticle contacts needed for mechanical equilibrium?

• No friction, spherical particles, D dimensions
  - Match
    unknowns (number of interparticle normal forces)
    equations (force balance for mechanical stability)
  - Number of unknowns per particle = Z/2
  - Number of equations per particle = D

James Clerk Maxwell

Phillips, Thorpe, Boolchand, Edwards, Ball, Blumenfield
Isostaticity and 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 one soft mode

• This implies diverging length as $\phi \to \phi_c^+$

For $\phi > \phi_c$, cut bonds at boundary of circle of size $L$

Count number of soft modes within circle

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

Define length scale at which soft modes just appear

$$\ell \approx \frac{1}{Z - Z_c} \approx (\phi - \phi_c)^{-0.5}$$
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Consequences of Diverging Length Scale

• Solids are all alike at low T or $\omega$:
  
  - density of vibrational states $D(\omega) \sim \omega^2$ in d=3
  
  - vibrational heat capacity $C(T) \sim T^3$
  
  - thermal conductivity $\kappa(T) \sim C_v \ell \sim T^3$

• Why?

  Low-frequency excitations are sound modes. At long length scales all solids look elastic
Consequences of Diverging Length Scale

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

  **BUT** at Point J, there is a diverging length scale $\ell^*$

  So what happens?
• More and more modes in excess of Debye prediction as $\phi \to \phi_c$ (boson peak)

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

• Robust for systems near isostaticity  
  Souslov, Liu, Lubensky, PRL 103, 205503 (2009); Mao, Xu, Lubensky arXiv: 09092616
Vibrational Modes Predict Soft Spots

• Adams-Gibbs Cooperatively-Rearranging Regions?
• Shear Transformation Zones?

M. Lisa Manning’s talk next week
Summary of Point J

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

- Mixed first-order/second-order transition (RFOT)
- Number of overlapping neighbors per particle

\[ Z = \begin{cases} 0 & \phi < \phi_c \\ Z_c + z_0 (\phi - \phi_c)^{\beta \approx 1/2} & \phi \geq \phi_c \end{cases} \]

- Static shear modulus/bulk modulus

\[ \frac{G}{B} \sim (\phi - \phi_c)^{\gamma \approx 1/2} \]

- Two diverging length scales

\[ \ell^* \sim (\phi - \phi_c)^{-\nu \approx -1/2} \]
\[ \ell^\dagger \sim (\phi - \phi_c)^{-\nu^\dagger \approx -1/4} \]
Similarity to Other Models

- This behavior has only been found in a few models, all in mean-field limit
  - 1-RSB p-spin interaction spin glass Kirkpatrick, Thirumalai, Wolynes
  - compressible frustrated Ising antiferromagnet Yin, Chakraborty
  - kinetically-constrained Ising models Sellitto, Toninelli, Biroli, Fisher
  - k-core percolation and variants Schwarz, Liu, Chayes, Toninelli, Biroli, Fisher, Harris, Jeng
  - Mode-coupling approximation of glasses Biroli, Bouchaud
  - 1-RSB solution of hard spheres Zamponi, Parisi

- These other models all exhibit glassy dynamics!!

First hint of quantitative connection between sphere packings and glass transition
• How do ideal spheres behave at nonzero temperature?
Dramatic Increase of Relaxation Time

Colloidal glass transition

\[ \tau = \tau_0 \exp \left( \frac{A}{(\phi - \phi_0)^x} \right) \]

Brambilla, et al., arXiv/0809.3401

Glass transition

\[ \tau = \tau_0 \exp \left( \frac{A}{(T - T_0)^x} \right) \]


Similar fitting functions.

WHY??
Very Different Underlying Pictures

Colloidal glass transition
- free volume

Glass transition
- complex energy landscape

Pressure is most important
- It governs amount of free volume

Temperature is most important
- It allows system to overcome energy barriers
Very Different Underlying Pictures

Colloidal glass transition
  free volume

Glass transition
  complex energy landscape

Pressure is most important
It governs amount of free volume

Temperature is most important
It allows system to overcome energy barriers

There are systems for which these two transitions are the same phenomenon
Relaxation Time

- Look at relaxation time along different trajectories
  - Fix $p$, lower $T$
  - Fix $T$, raise $p$
• Look at relaxation time along different trajectories
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Relaxation Time

- Look at relaxation time along different trajectories
  - Fix $p$, lower $T$
  - Fix $T$, raise $p$
Data Collapse!

Data for different (p, T) collapse on to single scaling curve!
Dimensional Analysis

- Recall interaction potential
  \[ V(r) = \begin{cases} \frac{\varepsilon}{2} \left(1 - \frac{r}{\sigma}\right)^2 & r \leq \sigma \\ 0 & r > \sigma \end{cases} \]

- We have 3 dimensional parameters in model: \( \varepsilon, m, \sigma \)

Relaxation time
\[ \tau \sqrt{\frac{\varepsilon}{m\sigma^2}} = h \left( \frac{T}{\varepsilon}, \frac{p\sigma^3}{\varepsilon} \right) \]

or equivalently
\[ \tau \sqrt{\frac{p\sigma}{m}} = g \left( \frac{T}{p\sigma^3}, \frac{p\sigma^3}{\varepsilon} \right) \]
Dimensional Analysis

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or equivalently

\[ \tau \sqrt{\frac{p \sigma}{m}} = g \left( \frac{T}{p \sigma^3}, \frac{p \sigma^3}{\varepsilon} \right)^0 \]
In low p limit, the relaxation time depends only on T/p.

Data collapse for different trajectories

Dimensional Analysis

\[
\lim_{p\sigma^3/\varepsilon \to 0} \tau \sqrt{\frac{p\sigma}{m}} = \lim_{p\sigma^3/\varepsilon \to 0} g\left(\frac{T}{p\sigma^3}, \frac{p\sigma^3}{\varepsilon}\right) = f\left(\frac{T}{p\sigma^3}\right)
\]

- T, p equally important!
- In low p limit, the relaxation time depends only on T/p
- Data collapse for different trajectories
Data Collapse for Different Potentials

- $p\sigma^3/\varepsilon \to 0$ corresponds to low $p$ limit for soft spheres AND to the hard sphere limit
- Should see collapse for any $\alpha \geq 0$ including $\alpha = 0$ (hard spheres)

$$V(r) = \begin{cases} \frac{\varepsilon}{\alpha} \left(1 - \frac{r}{\sigma}\right)^\alpha & r \leq \sigma \\ 0 & r > \sigma \end{cases}$$
Data Collapse for Different Potentials

- \( p\sigma^3/\varepsilon \rightarrow 0 \) corresponds to low \( p \) limit for soft spheres AND to the hard sphere limit
- Should see collapse for any \( \alpha \geq 0 \) including \( \alpha = 0 \) (hard spheres)

Glass transition equivalent to colloidal glass transition as \( p\sigma^3/\varepsilon \rightarrow 0 \)

\[
\lim_{\tau/\varepsilon \rightarrow 0} \tau \sqrt{\frac{p\sigma}{m}} = f\left(\frac{T}{p\sigma^3}\right)
\]

\[\Delta V \sim T/p\]

T does work against pressure to open up free volume

YES!
As spheres soften, relaxation time decreases (Weitz/Reichman).

New mechanism of relaxation controlled by $p\sigma^3/\varepsilon$ emerges.
Soft spheres have smaller equivalent hard sphere diameter

Soft spheres with diameter $\sigma$

Hard spheres with reduced diameter $\sigma_{\text{eff}} < \sigma$

smaller effective volume fraction
more free volume
faster relaxation

How to choose $\sigma_{\text{eff}}$?
Rowlinson, Barker-Henderson, Andersen-Weeks-Chandler

- Taylor expand free energy around hard-sphere potential
- Choose $\sigma_{\text{eff}}$ so that first-order functional derivative of free energy with respect to $\exp(-V(r)/T)$ vanishes

$$\int d\mathbf{r} y_{\text{eff}}(r) \left\{ \exp \left[ -V(r) / T \right] - \exp \left[ -V_{\text{eff}}(r) / T \right] \right\} = 0$$

- Can calculate $\sigma_{\text{eff}}$ from the soft-sphere potential and hard-sphere properties alone!
- This approximation reproduces captures static quantities beautifully
Relaxation time

- Start with soft spheres at arbitrary pressure
- Use ACW to calculate effective hard sphere diameter $\sigma_{\text{eff}}$
- Obtain new packing fraction for effective hard spheres $\phi_{\text{eff}}$
Relaxation time

- Start with soft spheres at arbitrary pressure
- Use ACW to calculate effective hard sphere diameter $\sigma_{\text{eff}}$
- Obtain new packing fraction for effective hard spheres $\phi_{\text{eff}}$

ACW approx rocks!!
$\tau$ collapses onto
hard-sphere curve
for all finite-ranged
repulsive potentials
and pressures studied
Recall Hard-Sphere Curve

\[
\lim_{T/\varepsilon \to 0} \tau \sqrt{\frac{p\sigma}{m}} = f\left(\frac{T}{p\sigma^3}\right)
\]

Hard spheres

hard-sphere equation of state

fit to Carnahan-Starling eqn
Universal Hard-Sphere Master Curve

- This implies that $\tau \sqrt{p \sigma / m} = \tau_{\text{eff}} \sqrt{p_{\text{eff}} \sigma_{\text{eff}} / m}$ or $\tau = \tau_{\text{eff}} \sqrt{p_{\text{eff}} \sigma_{\text{eff}} / p \sigma}$

- Given
  - hard-sphere master curve
  - pair interaction potential of soft-sphere system
- can calculate relaxation time of soft-sphere system!
- Can also use soft spheres to extend master curve
Two Mechanisms of Relaxation in Soft Spheres

- Temperature opens up free volume against the pressure

\[ T = p \Delta V \]

- hard spheres are fragile glassformers (super-Arrhenius increase of relaxation time)

- Temperature allows soft spheres to overlap so they behave as hard spheres with smaller diameter (less super-Arrhenius with increasing overlap)

- In energy landscape, canyons do not become deeper but become narrower and more convoluted as \( p \uparrow \) or \( T \downarrow \)
Connection to Point J

- Point J corresponds to double limit $\frac{T}{p\sigma^3} \to 0$, $\frac{p\sigma^3}{\varepsilon} \to 0$

- What is

$$\lim_{T/p\sigma^3 \to 0} \lim_{p\sigma^3/\varepsilon \to 0} \tau \sqrt{\frac{p\sigma}{m}} = \lim_{T/p\sigma^3 \to 0} \lim_{p\sigma^3/\varepsilon \to 0} g\left(\frac{T}{p\sigma^3}, \frac{p\sigma^3}{\varepsilon}\right) = \lim_{T/p\sigma^3 \to 0} f\left(\frac{T}{p\sigma^3}\right)$$

- Does $\tau$ diverge at Point J? Or does it diverge at $T/p\sigma^3 > 0$?

- Does Pt J control glass transition? Or is there an underlying thermodynamic glass transition?
Fitting Forms

- **Vogel-Fulcher form**: \[ \frac{\tau}{\tau_0} = \exp\left(\frac{A}{T - T_0}\right) \]

- **Elmatad-Chandler-Garrahan form**:

Form of Scaling Function

\[ f(x) = 0.5 \exp\left(\frac{0.15}{x - 0.05}\right) \]

Vogel-Fulcher form

\[ f(x) = A \exp\left[ B \left( \frac{1}{x} - \frac{1}{x_1} \right)^2 \right] \]

Elmatad-Chandler-Garrahan form

- Hard spheres are very fragile!
- Can't distinguish between V-F form and E-C-G form
- Can't tell if there is a thermodynamic glass transition or not
- But if not, then Point J controls dynamical glass transition
Conclusions

- Point J is a special point
- Hint of connection to glass transition in exponents for jamming transition
- Similarity in form of slow down in dynamics due to equivalence of
  - hard sphere glass transition
  - thermal glass transition of soft spheres at low p
- Hard spheres tell us everything about soft spheres
- Point J controls dynamical glass transition of hard spheres if thermodynamic glass transition does not exist
- Still ahead: attractions
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Bread for Jam:

DOE DE-FG02-03ER46087
German Academic Exchange Service (DAAD)
As $p\sigma^3/\varepsilon$ increases, $\sigma_{\text{eff}}$ decreases.

As $T/p\sigma^3$ increases, $\sigma_{\text{eff}}$ decreases.

$$V(r) = \begin{cases} 
\frac{\varepsilon}{\alpha} \left(1 - \frac{r}{\sigma}\right)^\alpha & r \leq \sigma \\
0 & r > \sigma 
\end{cases}$$
Jamming vs. Glass Transition

(a) Line of J-points
- metastable glassy states
- glass phase

(b) Line of J-points
- metastable glassy states
- liquid
BUT: Real Liquids have Attractions

- Point J only exists for repulsive, finite-range potentials
- Attractions can lead to vapor-liquid transition which preempts Point J

But there is hope:

Attractions serve to hold system at high enough density that repulsions come into play (WCA)
Behavior of liquids is controlled by repulsions, and attractions are perturbation
Behavior of amorphous solids is
- very different from that of crystals
- same in all amorphous solids
- still not understood
Marginally Jammed Solid

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

Density of Vibrational Modes

- Density of states is not Debye-like at low $\omega$
- Result of isostaticity M. Wyart, S.R. Nagel, T.A. Witten, EPL 72, 486 (05)
- Scaling of $\omega^*$ is robust to systems near isostaticity Souslov, Liu, Lubensky, PRL 103, 205503 (2009); Mao, Xu, Lubensky arXiv: 09092616
Boson Peak

- Excess in density of states is tied to peak in heat capacity $C(T)/T^3$
- This frequency/temperature can be tuned in jammed packings by varying $\phi - \phi_c$

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Thermal Conductivity

Kubo formulation

\[ d_i = \frac{\pi}{3h^2\omega_i^2} \sum_{i \neq j} |S_{ij}|^2 \delta(\omega_i - \omega_j) \]

Kittel’s 1949 hypothesis: rise in \( \kappa \) above plateau due to regime of freq-independent diffusivity

\[ \kappa = \frac{1}{V} \sum_i C_i(T)d_i \]

Heat carried by mode \( i \)

Diffusivity of mode \( i \)

Thermal conductivity

Ioffe-Regel Crossover

- Crossover from weak to strong scattering at $\omega^*$
- At Point J, the diffusivity is flat down to $\omega = 0$
- Freq-indep diffusivity originates from Point J

Consequences for Thermal Conductivity

- At $J$, $C/T^3$ is finite in harmonic approx.
- So $\kappa$ saturates up to $T$.
- For $J$, $C/T^3$ of this behavior occurs at $kT^* \sim \hbar \omega^*$.

Boson peak in $C$ and end of plateau in $\kappa$ tied together through $\omega^*$.
Consequences for Thermal Conductivity

 boson peak in $C$
 end of plateau in $\kappa$
 tied together through $\omega^*$
Quasilocalized Modes at $\omega^*$

\[ p_i = \frac{\left( \sum_\alpha |\epsilon_i(\alpha)|^2 \right)^2}{\sum_\alpha |\epsilon_i(\alpha)|^4} \]
Quasilocalized Modes at $\omega^*$

Quasilocalized Modes at $\omega^*$

- Modes become quasilocalized near Ioffe-Regel crossover

Quasilocalized Modes at $\omega^*$

- Modes become quasilocalized near Ioffe-Regel crossover
- High displacements occur in low-coordination regions

The low-frequency quasi-localized modes have the lowest energy barriers to rearrangement
- two-level systems?
- STZ’s?

K-Core Percolation

- **Culling process**
  - Occupied sites with fewer than \( k \) occupied neighbors become vacant
- Repeat culling process until no more can be removed
- Remaining occupied sites called the \( k \)-core

\( k = 3 \)
K-Core Percolation

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Jamming vs k-Core (Bootstrap) Percolation


- Jammed configs at T=0 are mechanically stable.
- For particle to be locally stable, it must have at least \(d+1\) overlapping neighbors in \(d\) dimensions.
- Each of its overlapping nbrs must have at least \(d+1\) overlapping nbrs, etc.
- At \(\phi>\phi_c\) all particles in load-bearing network have at least \(d+1\) neighbors.
- Consider lattice with coord. \(\#Z_{\text{max}}\) with sites independently occupied with probability \(p\).
- For site to be part of “k-core”, it must be occupied and have at least \(k=d+1\) occupied neighbors.
- Each of its occ. nbrs must have at least \(k\) occ. nbrs, etc.
- Look for percolation of k-core.
Long-Ranged Interactions/Attractions

- Point J only exists for repulsive, finite-range potentials
- Real liquids have attractions
- Attractions serve to hold system at high enough density that repulsions come into play (WCA)
- Excess vibrational modes (boson peak) believed responsible for unusual low temp properties of glasses
- These modes derive from the excess modes near Point J

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Repulsion vanishes at finite distance

Effect of Particle Shape

- Ellipsoids

- Introduce new rotational band but onset of translational band still scales as for spheres

- Ellipsoids controlled by Point J for spheres

What happens at $\Sigma > 0$?

Look at rheology: stress $\Sigma$ vs. $T$, $p$, $\dot{\gamma}$

Glasses & colloidal glasses shear thin--is there a connection?
**Dimensional Analysis**

**T. Haxton (2D)**

\[
\frac{\Sigma \sigma^2}{\epsilon} = H \left( \frac{T}{\epsilon}, \dot{\gamma} \sqrt{\frac{m \sigma^2}{\epsilon}}, \frac{p \sigma^2}{\epsilon} \right)
\]

or equivalently,

\[
\frac{\Sigma}{p} = G \left( \frac{T}{p \sigma^2}, \frac{\sqrt{m}}{p}, \frac{p \sigma^2}{\epsilon} \right)
\]

- Stress is indep of potential for small \( T, p \)

\[
\lim_{p \sigma^2 / \epsilon \to 0} \frac{\Sigma}{p} = F \left( \frac{T}{p \sigma^2}, \frac{\sqrt{m}}{p} \right)
\]
Data Collapse for Rheology

\[ \sigma = \gamma m \frac{T}{p} \sigma^2 \]

\[ I = \dot{\gamma} \sqrt{\frac{m}{p}} \]

\[ \lim_{p \sigma^2 / \varepsilon \to 0} \frac{\Sigma}{p} = F \left( \frac{T}{p \sigma^2}, I = \dot{\gamma} \sqrt{\frac{m}{p}} \right) \]

High \( T / p \sigma^2 \), low I: viscous
Low \( T / p \sigma^2 \), low I: elastic
Consequences of Rheology Collapse

Metallic glass (3d)


Equivalence of rheology for colloids and glasses

\[
\lim_{p\sigma^2/\varepsilon \to 0} \frac{\Sigma}{p} = F\left(\frac{T}{p\sigma^2}, I = \dot{\gamma} \sqrt{\frac{m}{p}}\right)
\]

\[
\lim_{p\sigma^2/\varepsilon \to 0} \frac{\tau}{\sqrt{m}} = \tilde{F}\left(\frac{T}{p\sigma^2}, \frac{\Sigma}{p}\right)
\]

describes jamming surface: universal near Point J!