Glass-to-glass transition of hard sphere glasses under external perturbations

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Related talks:
• Misaki Ozawa
• Hajime Yoshino

Workshop on “Avalanches, plasticity, and nonlinear response in nonequilibrium solids”
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Unifying glass and jamming transitions

Initial proposal by Liu and Nagel

Mean-field theory of hard spheres

1-step replica symmetry breaking (1RSB) theory

\[ p = \frac{PV}{NkT} \]

Reduced pressure

Volume fraction \( \phi \)

Jamming (J-line) \([\varphi_{th}, \varphi_{GCP}]\)

Ideal glass transition (Kauzmann point)

Dynamical glass transition

\( \phi_d \), \( \phi_{th} \), \( \phi_K \), \( \phi_{GCP} \)
How good is the 1RSB theory?

Success:
• The predicted transition densities are basically consistent with simulations in large dimensions.
  P. Charbonneau, A. Ikeda, G. Parisi, and F. Zamponi, PRL (2011)
• The prediction of J-line is confirmed by simulations — the jamming transition does not occur at a unique density.
  P. Chaudhuri, L. Berthier, and S. Sastry, PRL (2010)
• The jammed states are isostatic: $Z = 2d$.

Open:
• Does the ideal glass transition (Kauzmann point) exist?

Failure:
• The predicted critical jamming exponents are inconsistent with simulations.
Full-step replica symmetry breaking (fullRSB) theory

**Prediction correct critical exponents at jamming.**


State following calculation: Yoshino’s talk

Basic physical picture

- Liquid
- Stable glass
- Marginal glass
- Gardner transition
- Split of cage
- Single cage

Diagram showing the transition between different states and the J-line (ground states) with key points labeled.
Numerical protocols: following the evolution of hard sphere (HS) glasses under compression and shear

Numerical model: polydisperse hard spheres
Swapping algorithm: Ozawa’s talk
Berthier, Coslovich, Ninarello, and Ozawa, arXiv:1511.06182

dynamical transition

dense equilibrium configurations (swapping algorithm)

glass transition

quasi-static shear

quasi-static compress
Shear of HS glasses

stress-strain

linear response

yielding

liquid

quadratic dilatancy

pressure-strain

\( \varphi_g = 0.598 \)
\( \varphi_g = 0.609 \)
\( \varphi_g = 0.619 \)
\( \varphi_g = 0.630 \)
\( \varphi_g = 0.643 \)
\( \varphi_g = 0.655 \)
Compression of HS glasses

Gardner transition
- aging
- growing time scale
- caging order parameter
- growing length scale
- protocol-dependent shear modulus

Gardner transition

$\varphi_d$

$\varphi_g$

Compress

Decompress

Target density (measure here)
Aging effect

Mean-squared displacement (MSD):

\[ \Delta(t, t_w) = \frac{1}{N} \sum_{i=1}^{N} \langle |r_i(t + t_w) - r_i(t_w)|^2 \rangle \]

waiting time

Gardner transition
Growing time scale

\[ \Delta_{AB}(t) \text{ (lines)} \quad \Delta(t, t_w) \text{ (points)} \]

\[ \Delta_{AB}(t) = \frac{1}{N} \sum_{i=1}^{N} \langle |r_i^A(t) - r_i^B(t)|^2 \rangle \]

State cloning

- Gardner transition
- \( \Delta_{AB} \) is nearly time independent
- \( \Delta_{AB} \approx \Delta(t \to \infty, t_w \to \infty) \)
- Caging order parameter (average cage size)
Growing time scale

\[ \delta \Delta(t, t_w) = \Delta_{AB}(t_w + t) - \Delta(t, t_w) \]

\[ \delta \Delta(t, t_w) \sim 1 - \ln t / \ln \tau \]

Gardner transition

relaxation timescale
Caging order parameter

Gardner transition

(I) stable (1RSB) glass phase

(II) marginal (fullRSB) glass phase

distributions

\[ \Delta_{AB} \]

\[ P(\Delta_{AB}) \]

\[ P(\Delta) \]

\[ P_{eq}(\Delta) \]

Theoretical prediction (qualitative)

\[ \Delta_1 \]

\[ \Delta_0 \]

\[ \Delta_{EA} \]
Caging order parameter

\[ \Delta_{AB} \]

Distributions

Mean cage size (first moment)

Gardner transition

\[ \langle \Delta \rangle, \langle \Delta_{AB} \rangle \]

\[ \varphi = 0.63, 0.67, 0.68 \]

\[ \varphi_g = 0.598, 0.609, 0.619, 0.630, 0.643, 0.655 \]

Gardner transition
Caging order parameter

distributions

$P(\Delta_{AB})$

$\Delta_{AB}$

$10^{-4}$ $10^{-3}$ $10^{-2}$

$P(\Delta)$

$caging susceptibility (second moment)$

Gardner transition

Gardner transition
Spatial organization of cages: visualization of cage fields

\[ u_i = \frac{|r_i^A - r_i^B|^2}{\langle \Delta_{AB} \rangle} - 1 \]

stable glass

marginal glass

Gardner transition

J-line (ground states)

\( \varphi_d \)

\( \varphi_K \)

\( \varphi_{GCP} \)
Growing correlation lengths

\[ u_i = \frac{|r_i^A - r_i^B|^2}{\langle \Delta_{AB} \rangle} - 1 \]

\[ G_L(r) \sim \langle \sum_{\mu=1}^{3} \sum_{i \neq j} u_i u_j \delta(r - |r_{i,\mu}^A - r_{j,\mu}^A|) \rangle \]

\[ G_L(r) \sim \frac{1}{r^\alpha} e^{-(\xi/r)^b} \]

- sizes of cages
- positions of cages
- correlation length

![Graphs showing correlation lengths vs. radius and volume fraction](image)
Protocol-dependent shear modulus

\[ \mu = \frac{\sigma}{\gamma} \]

I. zero-field compression (ZFC)

II. field compression (FC)

\( \varphi_d \)

\( \varphi_g \)

strain

modulus

stress

compress

shear

compress

shear

\( \frac{1}{\rho} \sim T \)
Protocol-dependent shear modulus

Gardner transition

\[ \mu_{ZFC} \sim p^{1.234} \]

\[ \mu_{FC} \sim p^{1.001} \]

mean-field theory:

\[ \mu_{ZFC} \sim p^{1.41574} \]

\[ \mu_{FC} \sim p \]

H. Yoshino and F. Zamponi, PRE (2014)
Compression followed by shear

1RSB phase $\varphi < \varphi_G$

fullRSB phase $\varphi > \varphi_G$

Gardner transition $\gamma_G$?

linear

avalanches

metabasin

sub-basins
Experimental consequences (I)

Anomalous transport properties: anomalous specific heat and thermal conductivity (tunneling two-level systems model).


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glass          crystal (Debye theory)

specific heat: \[ C_p \sim T \]   \[ C_{\text{Debye}} \sim T^3 \]
thermal conductivity: \[ \kappa \sim T^2 \]   \[ \kappa_{\text{Debye}} \sim T^3 \]
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Activated slow dynamics across barriers (Johari-Goldstein relaxation).

Experimental consequences (II)

An abundance of soft vibration modes (Boson peak): isostaticity and marginal stability.


Silbert, Liu, and Nagel, PRL (2005)

Debye density of vibrational modes

\[ D(\omega) \propto \omega^{D-1} \]

Complex irreversible responses to small mechanical deformations.

Conclusions

Four independent ways to detect the Gardner transition:

- The growth of the characteristic relaxation time.
- The growth of the correlation length.
- A non-trivial change in the probability distribution function of a global order parameter.
- Protocol-dependent shear modulus.

Other systems:

- Bidisperse hard disks.
  Berthier, Charbonneau, Jin, Parisi, Seoane, and Zamponi, arXiv:1511.04201

- Mari-Kurchan model (mean-field hard spheres)
Thank you!