Statistical Mechanics of Jamming

- Lecture 1: Timescales and Lengthscales, jamming vs thermal critical points
- Lecture 2: Statistical ensembles: inherent structures and blocked states
- Lecture 3: Example of thermal system with constraints
- Lecture 4: Statistical mechanics of grain packings

Lecture 1

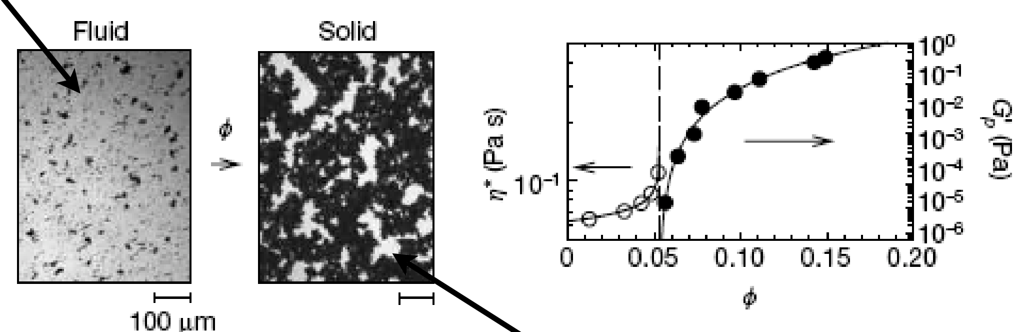
- What falls under the rubric of jamming?
- Universality?
- Signatures of jamming
  - Anomalously slow dynamics
  - Growing length scales?
- Dyamical heterogeneities
- Supercooled liquids (experiments, models)
- Granular packings (experiments, models)

Jamming

"A wide variety of systems, including granular media, colloidal suspensions and molecular systems, exhibit non-equilibrium transitions from a fluid-like to a solid-like state characterized solely by the sudden arrest of their dynamics." [1]

Qualification: No ***obvious*** structural signature

Unjammed phase flows like a liquid

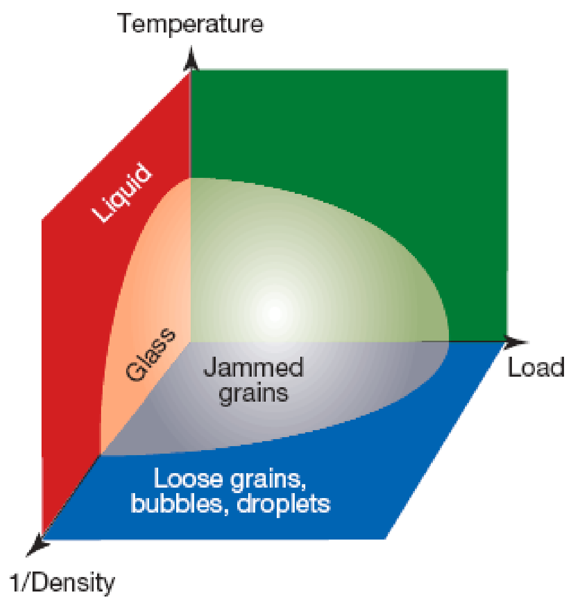


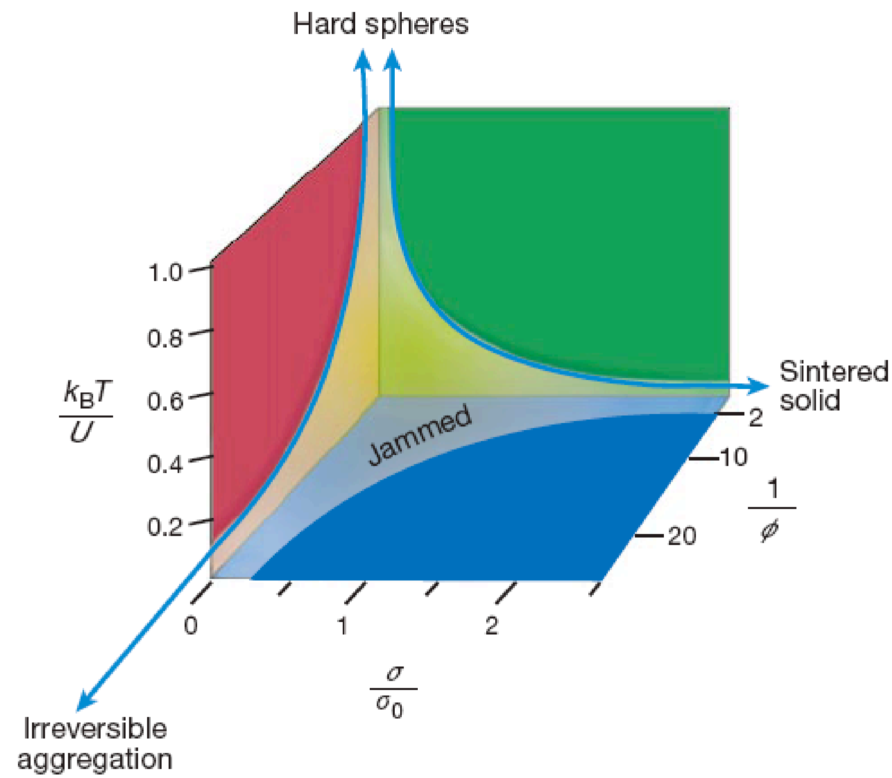
Increasing volume fraction

Jammed Phase has solid-like properties (resists shear)

Jamming is the transition between them: is this a phase transition?

Universal Jamming Phase diagram
Bringing thermal and athermal systems in to same framework





Liu and Nagel [2]

Trappe et al [1]

Signatures of jamming

- Anomalously slow dynamics
- Absence of any purely static, structural signatures
  - Simulations of soft spheres, possible exception
- Dynamical heterogeneities

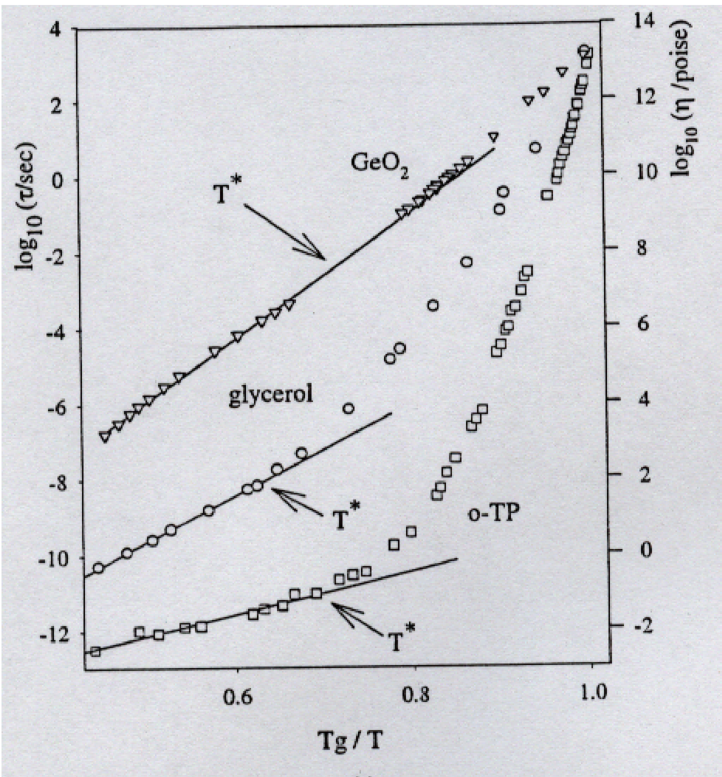
Two schools of thought

- Purely kinetic: arrest of flow with no structural correlations developing
- There is an underlying ideal glass transition

Slow Dynamics

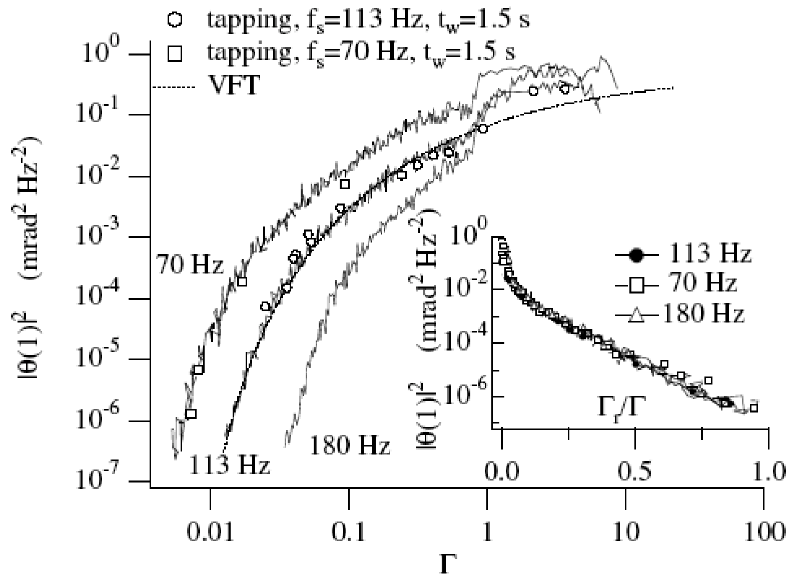
Athermal system

Thermal system



Supercooled liquids

G Tarjus et al J.Phys.C (2000)



Granular packings

G D'Anna & G Gremaud, PRL (2001)

Vogel-Fulcher-Tamann form

$$\tau \sim \mathbf{Exp}((A/\Gamma - \Gamma_0)^p)$$

Why is this anomalously slow?

- Dynamics near a critical point: controlled by a diverging correlation length

$$\xi \simeq (T - T_c)^{-\nu}$$

$$\tau \simeq \xi^{z}$$

$$\tau \simeq (T - T_c)^{-z\nu}$$

(More in Lecture 3)

- Vogel-Fulcher law

$$\xi \simeq (T - T_0)^{-\nu}$$

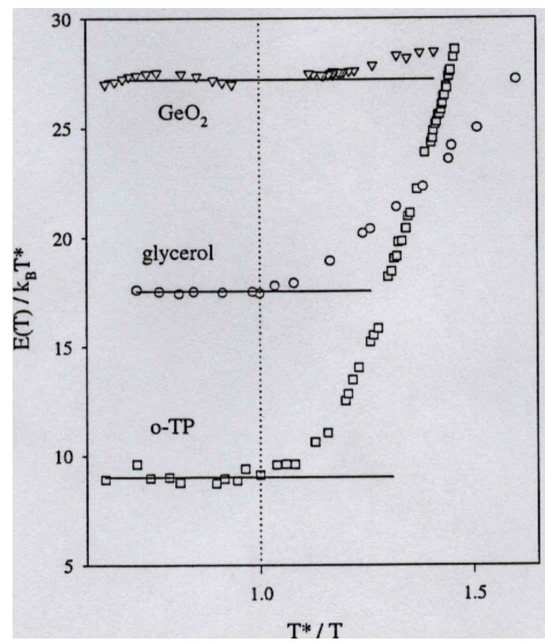
$$\tau \simeq e^{\xi^{\theta}}$$

$$\tau \simeq e^{(T - T_c)^{-z\nu}}$$

Jamming:

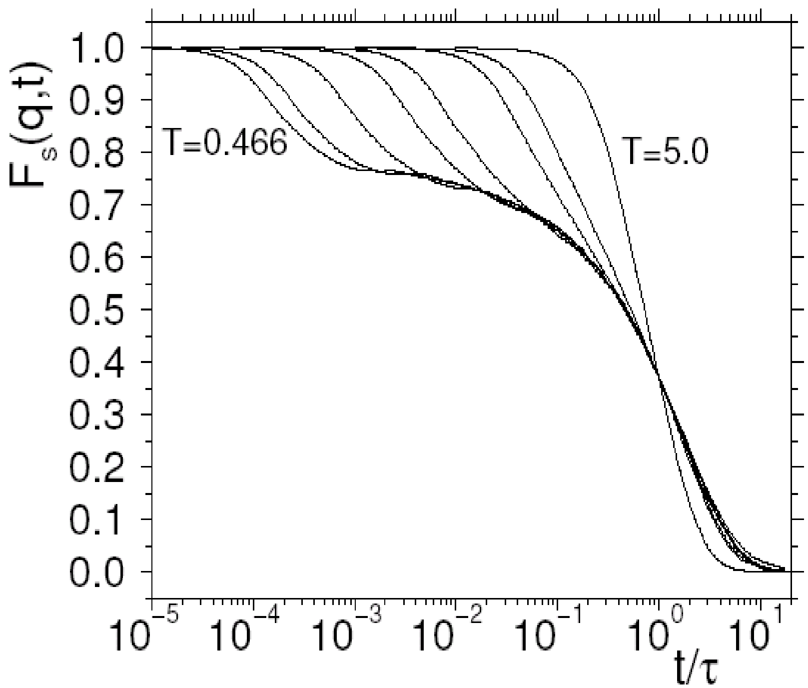
(1) No diverging length scale

(2) Activated scaling



- Models with quenched disorder such as the random field Ising model are described by this type of activated scaling [3]
- Supercooled liquids do not have quenched disorder. Is this type of scaling realized in non-disordered models?
- Granular packings are non-equilibrium systems. Is there a generic mechanism for generating the Vogel-Fulcher scaling?

Supercooled liquids



Non-exponential relaxation in Lennard-Jones fluid (Walter Kob, review)

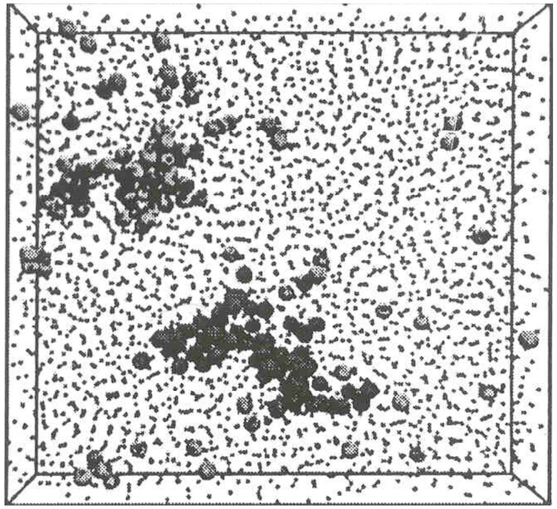
- Incoherent intermediate scattering function [4](density autocorrelation function)

$$\delta\rho_s(\mathbf{q},t) = \exp[-i\mathbf{q}\cdot\mathbf{r}_j(t)]$$

$$F_s(\mathbf{q},t) = < \delta\rho_s(\mathbf{q},t)\delta\rho_s(\mathbf{q},0)^* >$$

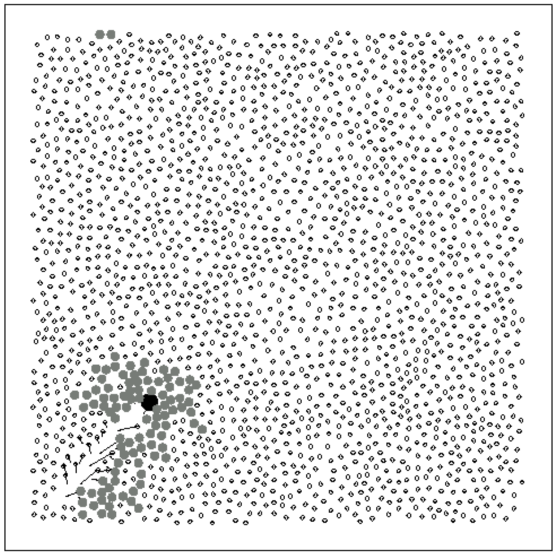
- One of the many successes of mode-coupling theory
  - experiment measures $F_s(\mathbf{q},t)$
- Mode coupling theory does not rely on a static transition it is a purely dynamic theory
- Deficiencies: predicted glass transition temperature too high, absence of activated scaling

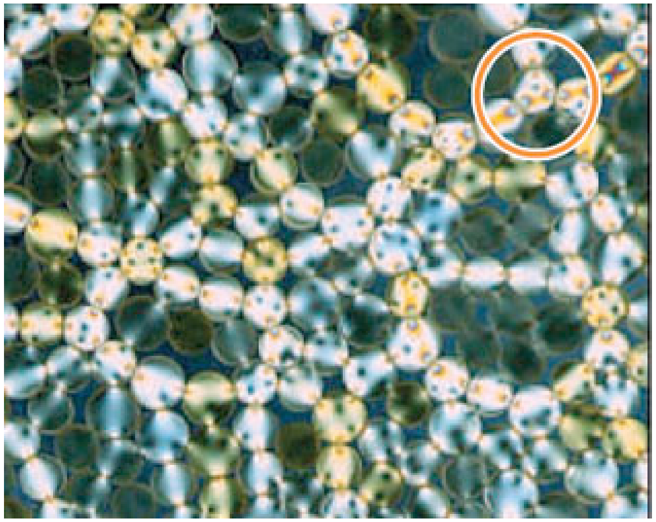
Dynamical heterogeneities



Colloidal glass: Correlation of particles (Weeks et al, Science 287, 627 (2000)

Near the T=0 jamming transition: Number of disks: (Drocco et al, cond-mat/0310291)





Force chains in compressed/ sheared grain packings

Supercooled liquids

- Simulations, measurement and theories of 4-point susceptibility [5-9]

Definition:

$$C((r-r');(t-t')) =< \rho(r',t')\rho(r,t) >$$

Measures how the densities at separated by a certain distance decorrelate with time (remember: incoherent scattering function)

$$G((r-r')) =< \rho(r',t)\rho(r,t) >$$

Static correlation function or equal time, spatial correlation function which is independent of time for a system in equilibrium. Normally, we pick up a diverging length scale from this correlation function

$$G_4((r-r');(t-t')) =< \rho(r',t')\rho(r',t)\rho(r,t')\rho(r,t) >$$

A length scale (time-dependent) obtained from here provides a measure of the extent of correlation between two snapshots separated by time t remain correlated

Supercooled liquids

- Simulations, measurement and theories of 4-point susceptibility [5-9]

$$G_4((r-r');(t-t')) = <\rho(r',t')\rho(r',t)\rho(r,t')\rho(r,t)>$$

This correlation function is related to a susceptibility

$$\chi_4 = <q^2> - <q>^2$$

$$q = \int dr \rho(r,t)\rho(r,t')$$

Compare to the overlap function of spin glasses

$$q_{\alpha\beta}^{parisi} = \sum_i S_i^\alpha S_i^\beta$$

Compare to ferromagnet

$$\chi = \frac{1}{N}(<m^2> - <m>^2)$$

$$m = \sum_i S_i$$

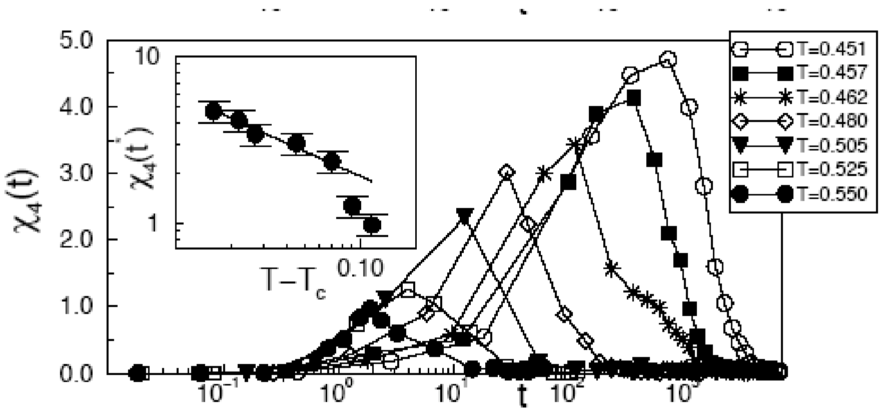
$$<m^2> = \sum_{ij} <S_i S_j> \simeq N + N m_0$$

# of spins correlated with 1

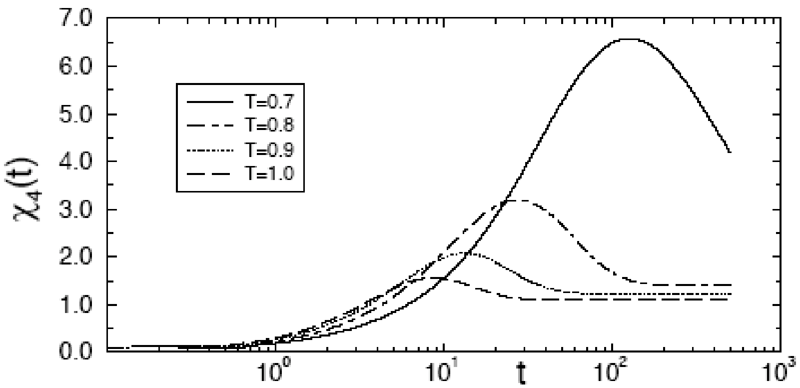
α β are replica indices

Supercooled liquids

- Simulations, measurement and theories of 4-point susceptibility [5-9]



Simulation of binary Lennard Jones[5]



Simulation of p-spin spinglass[5]

Supercooled liquids

- Simulations, measurement and theories of 4-point susceptibility [5-9]

$$\chi_3(\omega, T) = \frac{\chi_s^2}{k_B T} \ell^{2-\overline{\eta}} \mathcal{H}(\omega\tau).$$

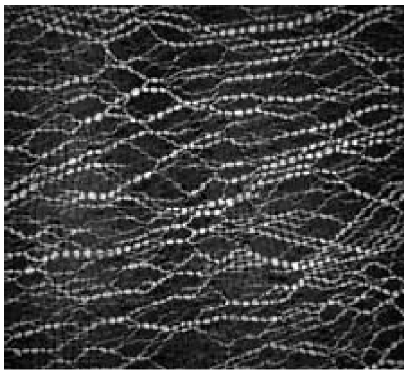
(analog of the dynamical scaling hypothesis for usual critical points)

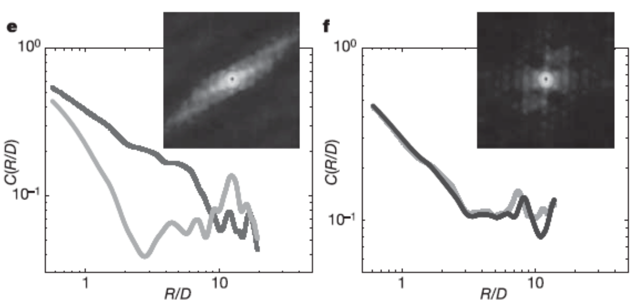
Within mode-coupling theory, this particular response can be related to the dynamical correlation length, l.[6]

Experiments have measured a growing length scale based on this relationship [7]

Granular packings: Length scales ?

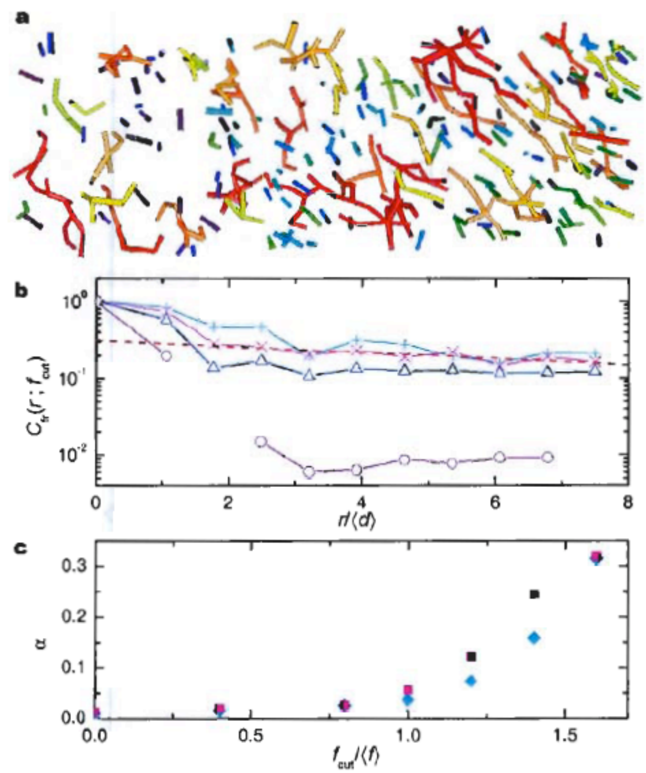
- Behringer's experiments on stress fluctuations [10]





- O'Hern, Silbert simulations [11]: growing length scale from phonon spectrum

- Dinsmore bubble experiments[12]



Blocked states and inherent structures: A promising approach to a unified framework

- Stillinger's construction of inherent structures[13]
- Edwards' idea of blocked states [14]
- Simulations
  - Properties of inherent structures (LJ systems)[15]
  - Properties of inherent structures of purely repulsive systems[16]

Ensemble of Blocked states (inherent structures)

- Consider all mechanically stable states
  - One way in thermal systems is to set an energy scale to infinity
  - athermal systems enforce mechanical stability
- Either way, dealing with constraints
- In thermal ensembles, assume Boltzman distribution
- In athermal systems, what is the appropriate probability distribution? Edwards' ?
- Phase transition in this restricted ensemble, diverging correlation length?
- Is the 4-point correlation a manifestation in the real system of this underlying phase transition?

[1] V. Trappe, V. Prasad, Luca Cipelletti, P. N. Segre and D. A. Weitz, Nature, 411, 772 (2001).

[2] Liu, A. J. and Nagel, S. R.,. Nature 396, (1998)

[3] D. S. Fisher, Phys. Rev. Lett. 56, 416 (1986).

[4] Walter Kob, Lecture notes for LES HOUCHES 2002 SUMMER SCHOOL - SESSION LXXVII; SLOW RELAXATIONS AND NONEQUILIBRIUM DYNAMICS IN CONDENSED MATTER

[5] C. Donati, J. F. Douglas, W. Kob, S. J. Plimpton, P. H. Poole, and S. C. Glotzer, Phys. Rev. Lett. 80, 2338 (1998); W. Kob, C. Donati, S. J. Plimpton, P. H. Poole, and S. C. Glotzer, ibid. 79, 2827 (1997); C. Donati, S. C. Glotzer, P. H. Poole, W. Kob, and S. J. Plimpton, Phys. Rev. E 60, 3107 (1999).

[6] L. Berthier, G. Biroli, J.-P. Bouchaud,, 4 L. Cipelletti, D. El Masri,D. LHote F. Ladieu, and M. Pierno, cond-mat/0512379

[7] Jean-Philippe Bouchaud and Giulio Biroli, cond-mat/051668

[8] David Reichman, K. Minazaki and J.-P. Bouchaud, very recent cond-mat

[9] J. P. Garrahan and D. Chandler, Proc. Natl. Acad. Sci. U.S.A. 100, 9710 (2003).

[10] F. Stillinger, J. Chem. Phys., 88, 7188(1988)

[11] S. Sastry, P. G. Debenedetti, and F. H. Stillinger, Nature London! 393, 554 (1998).

[12] B. Doliwa and A. Heuer, Phys. Rev. E 67, 030501 (2003).

[13] R. A. Denny, D. R. Reichman, and J. P. Bouchaud, Phys. Rev. Lett. 90, 025503 (2003)

[14] C.S. OHearn, L.E. Silbert, A.J. Liu and S.R. Nagel, Phys. Rev. E. 68, 011306, (2003) ;C. S. OHern, S. A. Langer, A. J. Liu, and S. R. Nagel, Phys. Rev. Lett. 88, 075507 (2002).; L. E. Silbert, A. J. Liu and S. R. Nagel, cond-mat/0501616