Glass and jamming transitions of hard spheres in dimension from three to thirteen (and beyond)

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in collaboration with
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A path towards a theory of the glass transition

Theory of second order PT (gas-liquid)

- Qualitative MFT (Landau, 1937)
  Spontaneous Z_2 symmetry breaking
  Scalar order parameter
  Critical slowing down

- Quantitative MFT (exact for $d \to \infty$)
  Liquid-gas: $\beta p/\rho = 1/(1-\rho b) - \beta a \rho$
  (Van der Waals 1873)
  Magnetic: $m = \tanh(\beta J m)$
  (Curie-Weiss 1907)

- Quantitative theory in finite d (1950s)
  (approximate, far from the critical point)
  Hypernetted Chain (HNC)
  Percus-Yevick (PY)

- Corrections around MFT
  Ginzburg criterion, $d_u = 4$ (1960)
  Renormalization group (1970s)
  Nucleation theory (Langer, 1960)

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  Spontaneous replica symmetry breaking
  Order parameter: overlap matrix q_{ab}
  Dynamical transition "à la MCT"

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  Kirkpatrick and Wolynes 1987
  Main topic of this talk

- Quantitative theory in finite d
  DFT (Stoessel-Wolynes, 1984)
  MCT (Bengtzelius-Götze-Sjolander 1984)
  Replicas (Mézard-Parisi 1996)

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Outline

Qualitative MFT of the glass transition

The "standard model" is a Sherrington-Kirkpatrick model with three-spin interactions: $H[S] = \sum_{ijk} J_{ijk} S_i S_j S_k$ with J_{ijk} independent Gaussian random variables

Thouless-Anderson-Palmer (TAP) approach (1977)

- Free energy as a functional of the local magnetizations $F[\{m_i\}]$
- Glassy states are *minima* of $F[\{m_i\}]$
  (see also the potential energy landscape approach of Goldstein-Stillinger-Weber)
- Many glassy minima appear for $T < T_d$

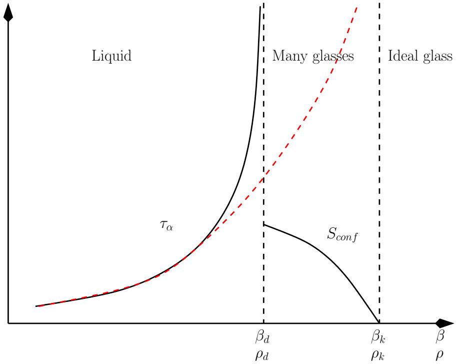
Dynamics (Kirkpatrick-Thirumalai-Wolynes 1987, Cugliandolo-Kurchan 1993)
Full solution of the Langevin dynamics of the model via path integral methods

- $T > T_d$: Ergodic dynamics, full relaxation of spin correlations
  Two step relaxation on approaching T_d, with α-relaxation time $\tau_\alpha \sim (T - T_d)^{-\gamma}$
- $T < T_d$: Non-ergodic dynamics, spin correlations do not decay
  Infinite memory: if the system is started in a spin glass state it will never leave it.
  After a quench from above T_d, the system shows aging

Replica method (Parisi 1979, KTW 1987, Monasson 1995)

- Introduce m coupled copies of the original system
- Allows to study the statistical properties of the glassy states (e.g. count their number) in a much simpler way than TAP
- Thermodynamic (replica symmetry breaking) phase transition à la Kauzmann at $T_k < T_d$

Qualitative MFT of the glass transition



Three temperature regimes (Kirkpatrick-Thirumalai-Wolynes, 1987-1989)

1. $T > T_d$: one single minimum with $m_i = 0$, the liquid state – finite $\tau_\alpha \sim (T - T_d)^{-\gamma}$
2. $T_k < T < T_d$: $S_{conf} > 0$, an exponential number of states – infinite τ_α
   The superposition of all glasses is the liquid: no phase transition
3. $T < T_k$: $S_{conf} = 0$, infinite τ_α
   A thermodynamic transition to the ideal glass happens at T_k

Qualitative MFT of the glass transition

- Spontaneous replica symmetry breaking at T_k
- Order parameter: the overlap between two replicas
- Dynamical transition at $T_d > T_k$ described by schematic MCT

This MFT explains several basic facts of the glass transition...

- Apparent divergence $\tau \sim (T - T_d)^{-\gamma}$ and associated MCT phenomenology
- Finite configurational entropy below T_d that vanishes at T_k
- Specific heat jump at T_k
- Aging and history dependence in the dynamics below T_d

...and makes new predictions

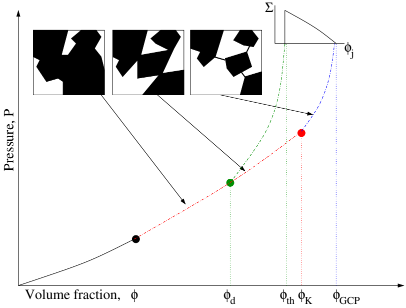
- Diverging dynamical susceptibility at T_d (dynamical heterogeneities)
- Diverging point-to-set correlation (static phase transition)
- Phase coexistence between high overlap and low overlap regions between T_k and T_d

`Kirkpatrick-Thirumalai-Wolynes, 1987-1989`
`Franz-Parisi, 1995-2000`
`Biroli-Bouchaud, 2004`

Outline

Mean field phase diagram of hard spheres

Packing fraction $\varphi = \rho V_d$



Density	Definition
$\varphi_d = \varphi_{MCT}$	The liquid state splits in an exponential number of states
φ_k	Ideal glass phase transition - jump in compressibility
φ_{th}	Divergence of the pressure of the less dense states
φ_{GCP}	Divergence of the pressure of the ideal glass

Finite dimensional approximations

Spin glasses	Hard spheres
TAP approach	Density Functional Theory (DFT) Stoessel and Wolynes, 1984
Dynamics	Mode-Coupling Theory (MCT) Bengtzelius, Gotze, Sjolander, 1984
Replicas	Cloned Liquid Theory (CLT) Mézard and Parisi, 1996

In $d = 3$, each of these theories involves different uncontrolled approximations.
Can we connect them?

Szamel, 2010

For $d \to \infty$, the hard sphere problem simplifies. If A,B,C are three spheres, and AB, BC are in contact, the probability that AC are in contact is very small $\Rightarrow$ Only the first virial term is relevant! (mean field Van der Waals equation)

Frisch and Percus, 1999
Parisi and Slanina, 2000

Are DFT, MCT, CLT equivalent in the mean field limit $d \to \infty$?

Kirkpatrick and Wolynes, 1987

Finite dimensional approximations for large d

Density Functional Theory (Kirkpatrick-Wolynes, 1987)

OK Free energy as a functional of the density field $F[\rho(r)]$ = ideal gas + first virial

Hyp Assume Gaussian density profile $\rho(r) = \sum_i \frac{e^{-\frac{(r-R_i)^2}{2A}}}{\sqrt{2\pi A}^d}$ and optimize over A, $\{R_i\}$

Hyp Assume that $S_0(q) = \frac{1}{N}\sum_{ij} e^{iq(R_i - R_j)} \sim S(q) \Rightarrow \varphi > \varphi_d \propto d\, 2^{-d}$

Mode Coupling Theory (KW 1987, Schmid-Schilling & Ikeda-Miyazaki 2010)

? In the glass phase $\varphi > \varphi_d$, one has $\lim_{t\to\infty} F(q,t) = S(q)f(q) \neq 0$.
MCT provides a self-consistent equation for $f(q)$, but no systematic derivation for large d

? Solution for $f(q)$ gives a non-Gaussian form and $\varphi_d \propto d^2\, 2^{-d}$, but some inconsistencies.

Hyp Assume Gaussian cage shape: $f(q) = e^{-Aq^2}$. Same equation as DFT! ($\varphi_d \propto d\, 2^{-d}$)

Cloned Liquid Theory (Parisi-FZ 2006)

OK Replicated free energy $F[\rho(r_1 \cdots r_m)]$ = ideal gas + first virial

Hyp Gaussian ansatz for cage shape (only A appears, we sum over $\{R_i\}$)
$\varphi_d \propto d\, 2^{-d}$ (with different prefactor) and $\varphi_K \propto d \log d\, 2^{-d}$

So what? We need numerical simulations!

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Outline

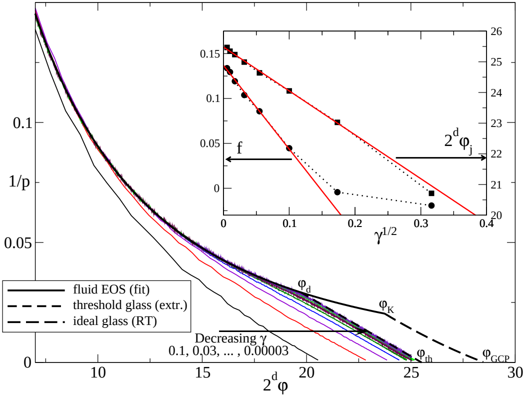
Numerical results - compression

Fluid: Carnahan-Starling EOS

$$p_{\rm fluid}(\varphi) = 1 + 2^{d-1}\varphi\, \frac{1-A_{\rm d}\,\varphi}{(1-\varphi)^d}$$

Glass: free volume EOS

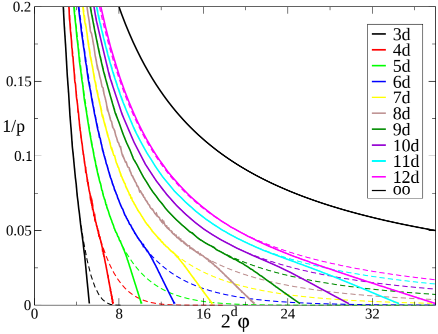
$$p_{\rm fv}(\gamma,\varphi) = \frac{d\,\varphi_{\rm j}(\gamma)[1-f(\gamma)]}{\varphi_{\rm j}(\gamma)-\varphi}$$

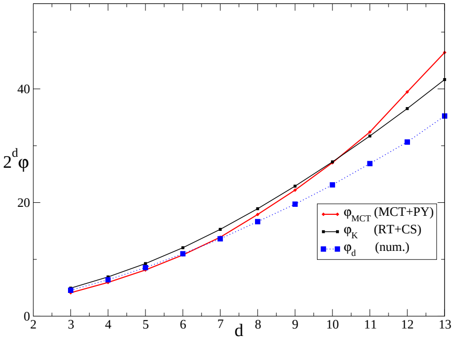


Compression of 9-dimensional hard spheres at constant rate γ
while doing event-driven molecular dynamics

[Skoge, Donev, Stillinger, Torquato, PRE 74, 041127 (2006)]
[Charbonneau, Ikeda, Parisi, FZ, PRL 107, 185702 (2011)]

Numerical results - compression





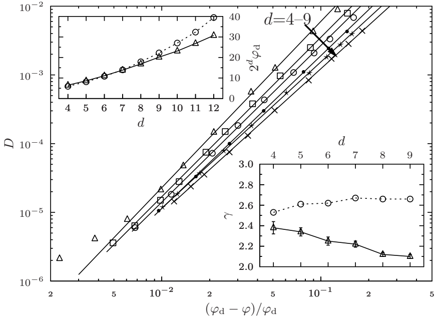
The liquid equation of state approaches the mean field one upon increasing d

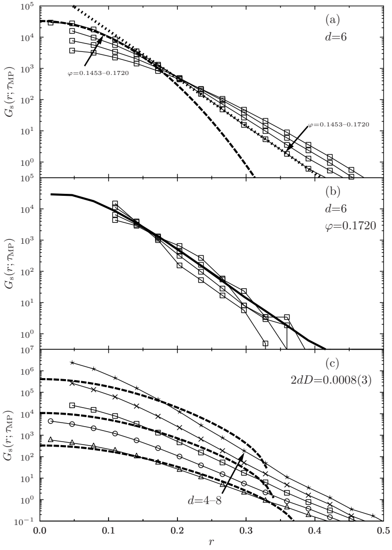
Replica theory gives predictions for φ_k, which is an upper bound to φ_d
These upper bounds follow reasonably well the trend of the numerical data

The results for φ_d are inconsistent with Mode-Coupling Theory

[Charbonneau, Ikeda, Parisi, FZ, PRL 107, 185702 (2011)]

Numerical results - equilibrium dynamics

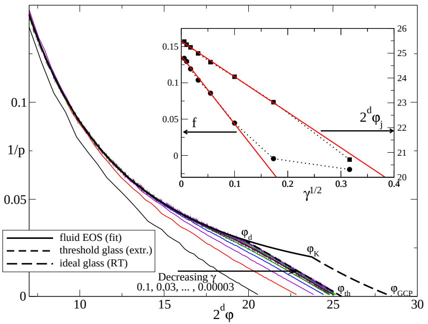


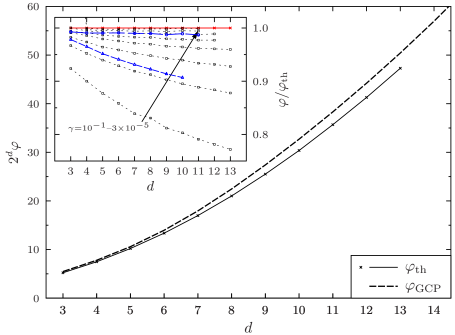


- Power-law fit $D \sim |\varphi - \varphi_d|^\gamma$ is very good
- φ_d coincides with the previous estimate
- φ_d and γ do not follow MCT prediction
- The self Van Hove function is not Gaussian
- *Individual* cages are not Gaussian
- Dynamical heterogeneities are reduced
- MCT's self Van Hove is not good

[Charbonneau, Ikeda, Parisi, FZ, PNAS online August 13]

Numerical results - jamming

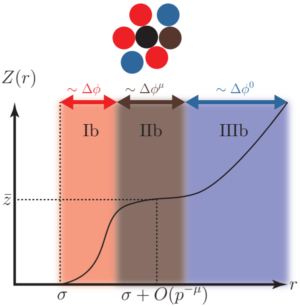


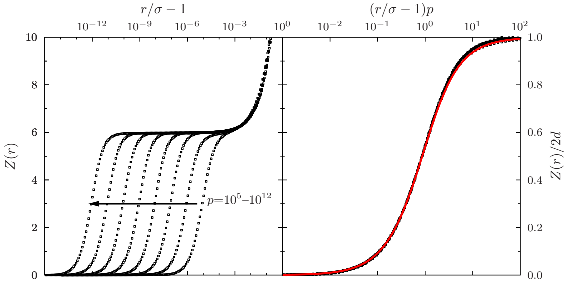


- Jamming happens when pressure becomes infinite and particles touch (transition from entropic rigidity to mechanical rigidity)
- It happens out of equilibrium inside the glass phase
- Its theoretical description requires a good theory of the deep glass phase
  For the moment it can only achieved by the replica method
- The replica prediction for φ_{GCP} provides an upper bound to the numerical φ_{th}
  We can produce jammed packings in a relative density range of $\sim 10\%$ in $d = 13$ (both from compression and from energy minimization)

[Charbonneau, Corwin, Parisi, FZ, submitted]

Numerical results - jamming





- Replica theory provides predictions for the scaling of pair correlation $g(r)$ and $Z(r)$ (both in the pressure and energy protocols)
- Three regimes: I contacts, II matching, III small gaps
- The prediction works very well except on approaching and leaving the plateau where non-trivial exponents are found (mechanical stability and soft modes – `Wyart 2012`)

`[Berthier, Jacquin, FZ, PRE 84, 051103 (2011)]`
`[Charbonneau, Corwin, Parisi, FZ, submitted]`

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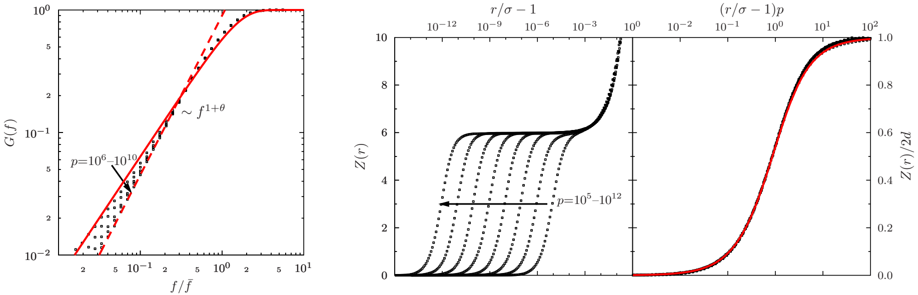

- Force distribution vanishes as $P(f) \sim f^\theta$, $G(f) \sim f^{1+\theta}$.
  Quasi contacts have $Z(r) \sim (r-\sigma)^{1-\alpha}$.
- Hard spheres: $\alpha = 0.40(1)$, $\theta = 0.30(3)$
  Soft spheres: $\alpha = 0.39(1)$, $\theta = 0.42(2)$
  Slight violation of $\alpha \geq 1/(2+\theta)$ in both cases (Wyart 2012)
- All these scalings are independent of dimension and density $\Rightarrow$ mean-field in nature!
  (The upper critical dimension for jamming is 2? – Goodrich, Liu, Nagel, arXiv:1204)

[Charbonneau, Corwin, Parisi, FZ, submitted]

Numerical results - summary

Glass transition

- Data are increasingly consistent with the qualitative MFT upon increasing d (clean power law regime, suppression of activated events, reduced dynamical heterogeneities)
- The transition densities and equation of state are consistent with Gaussian replica theory Yet the cage shape is not Gaussian. Contradiction?
- Although the MCT scenario is qualitatively observed, *quantitative* (non-universal) MCT predictions (transition density, exponents, cage shape) fail

Jamming transition

- The predictions of replica theory for the jamming density and for scaling functions are accurate
- However non-trivial exponents are found, related to soft modes and mechanical stability, that are missed by RT
- All the jamming phenomenology is independent of dimension

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Implications for the theory

The study of the glass and jamming transitions as a function of dimensionality allows to identify their mean field properties and put constraints for the theory

Replicas

- Gaussian replica theory gives a good free energy even if the cage is not Gaussian
- A complete non-Gaussian replica theory can be developed (Kurchan-Parisi-FZ, arXiv:1207)
- It reproduces the Gaussian predictions for the free energy and transition densities
  Explanation: integrals in the free energy are dominated by a single point when $d \to \infty$
- Its predictions for the cage shape still have to be worked out (in slow progress)
- It might capture some non-trivial exponents at jamming (in slow progress)
- It might allow to describe jamming soft modes through full RSB (difficult!)

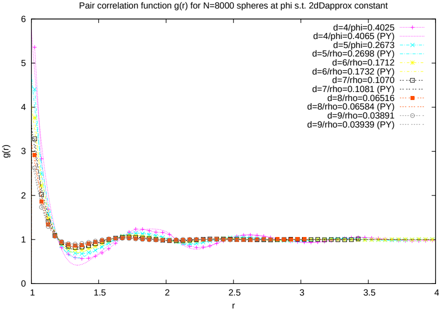
Dynamics

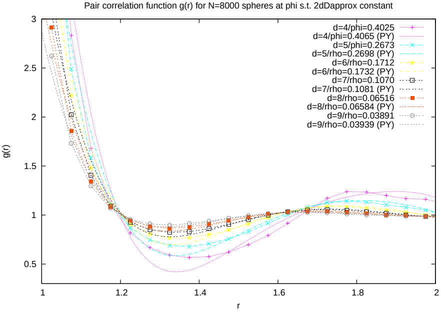
- MCT scenario is well observed: an MCT-like theory should be exact in large d
- Yet the usual form of the MCT kernel does not work - MCT as a Landau theory of the glass transition (Andreanov-Biroli-Bouchaud 2009)
- An exact solution of hard sphere dynamics in $d \to \infty$ (i.e. the good MCT kernel) seems possible, thanks to the replica-dynamics connection (Mari and Kurchan 2011)

Corrections around MFT

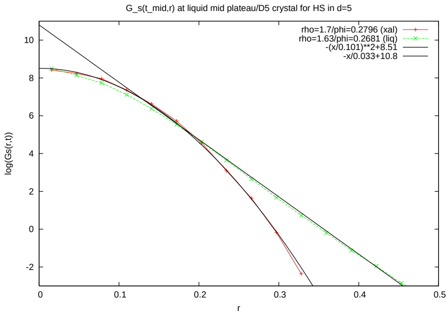
- Glass: corrections appear to be quite small down to $d = 4$, slightly bigger in $d = 3$
- Consistent with a quantitative Ginzburg criterion (Franz-Jacquin-Parisi-Urbani-FZ, 2012)
- They should be understandable through RG and perturbative expansions around MF
- Jamming: no corrections are observed, mean field theory should be enough!

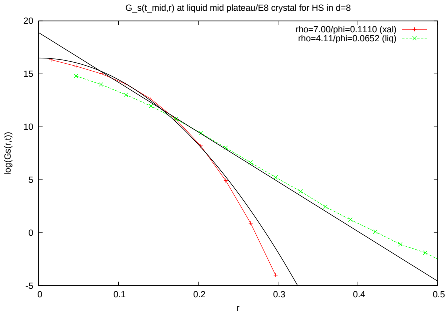
Comparison of PY and numerics for $g(r)$



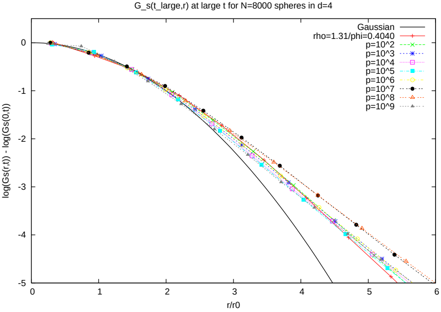


Comparison of glass and crystal self Van Hove function





The cage remains non-Gaussian at high pressure



The cage remains non-Gaussian at high pressure deep in the glass phase, where hopping out of the cage is completely absent. Hence the non-Gaussianity cannot be attributed to hopping or other cage instabilities.