Theory of simple glasses and jamming

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WARNING: this talk is going to be sloppy!

Outline

1. Glass and jamming transitions
   - The glass transition
   - The jamming transition
   - Marginality and criticality at jamming
   - Glass/jamming phase diagram

2. A theory of the glass and jamming transitions
   - Expansion around $d = \infty$ in statistical mechanics
   - Exact solution of the hard sphere model in $d = \infty$
   - Exact solution of the hard sphere model in $d = \infty$

3. Predictions of the theory, and numerical tests
   - Phase diagram
   - Critical dynamics at the dynamic glass transition
   - Critical scaling at jamming
   - The large d packing problem
   - Random close packing of binary mixtures

Outline

The liquid-glass transition

Macroscopically well-known for thousands of years. . .

Dynamical arrest of a liquid into an amorphous solid state
No change in structure, $g(r)$ unchanged
Driven by thermal fluctuations: entropic effects, entropic rigidity

The liquid-glass transition

Macroscopically well-known for thousands of years. . .

. . . yet constructing a first-principle theory is a very difficult problem!

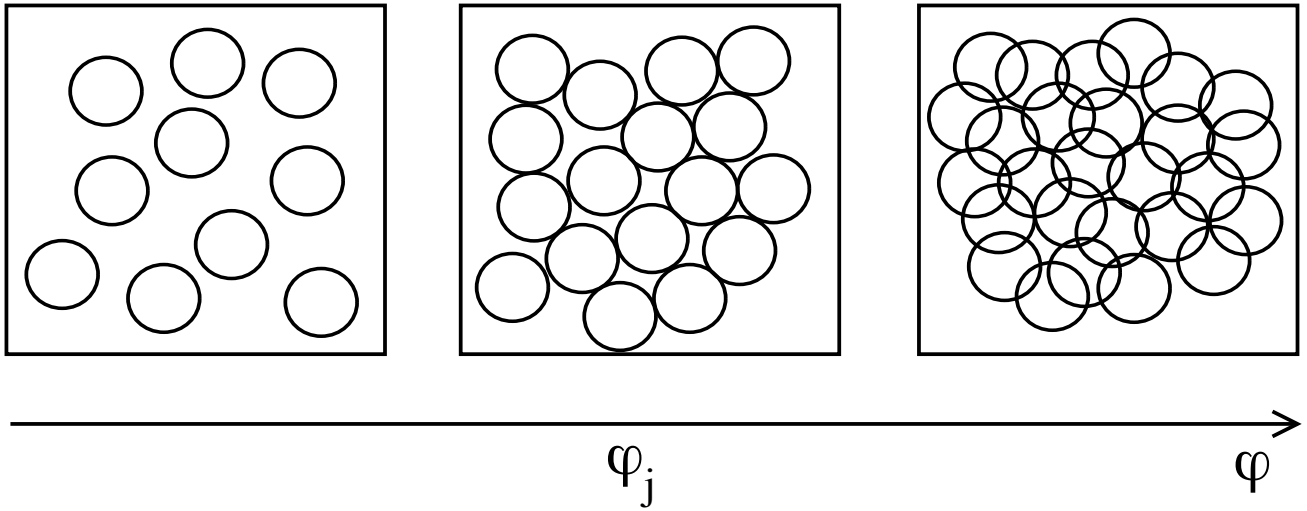
- No natural small parameter to construct a perturbative expansion
  Low density virial expansion: fails, too dense
  Harmonic expansion: fails, reference positions are not known
- Several processes simultaneously at work: crystal nucleation, ergodicity breaking, activated barrier crossing, dynamic facilitation
- Laboratory glasses are very far from criticality (if any)
  Theory must take into account strong pre-critical corrections

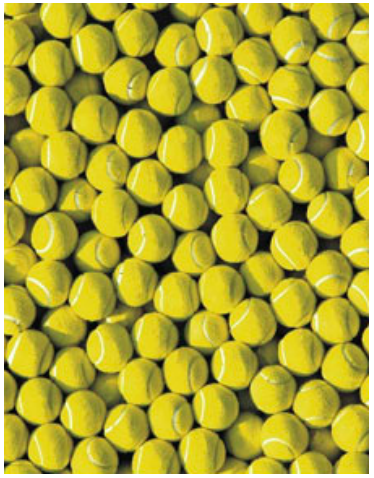
[Berthier, Biroli, RMP 83, 587 (2011)]

The jamming transition

Another transition that is observed in everyday experience

An *athermal* assembly of repulsive particles
Transition from a loose, floppy state to a mechanically rigid state
Above jamming a mechanically stable network of particles in contact is formed



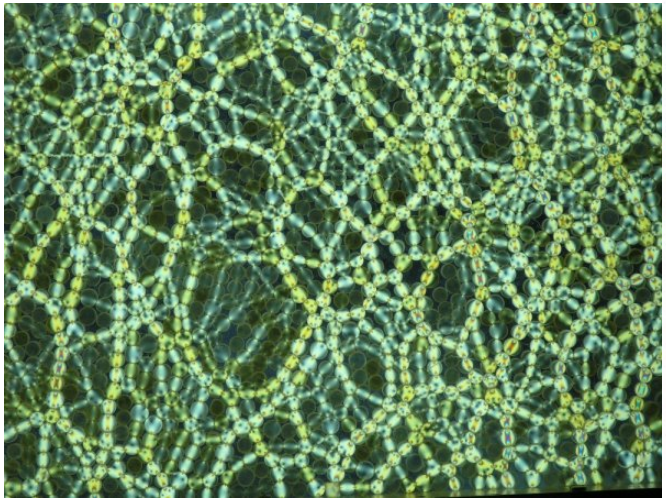


For hard spheres, φ_j is also known as *random close packing*: $\varphi_j(d = 3) \approx 0.64$

[Bernal, Mason, Nature 188, 910 (1960)]
[O'Hern, Langer, Liu, Nagel, PRL 88, 075507 (2002)]

The jamming transition

Granular materials, emulsion droplets, colloidal suspensions, powders, . . .



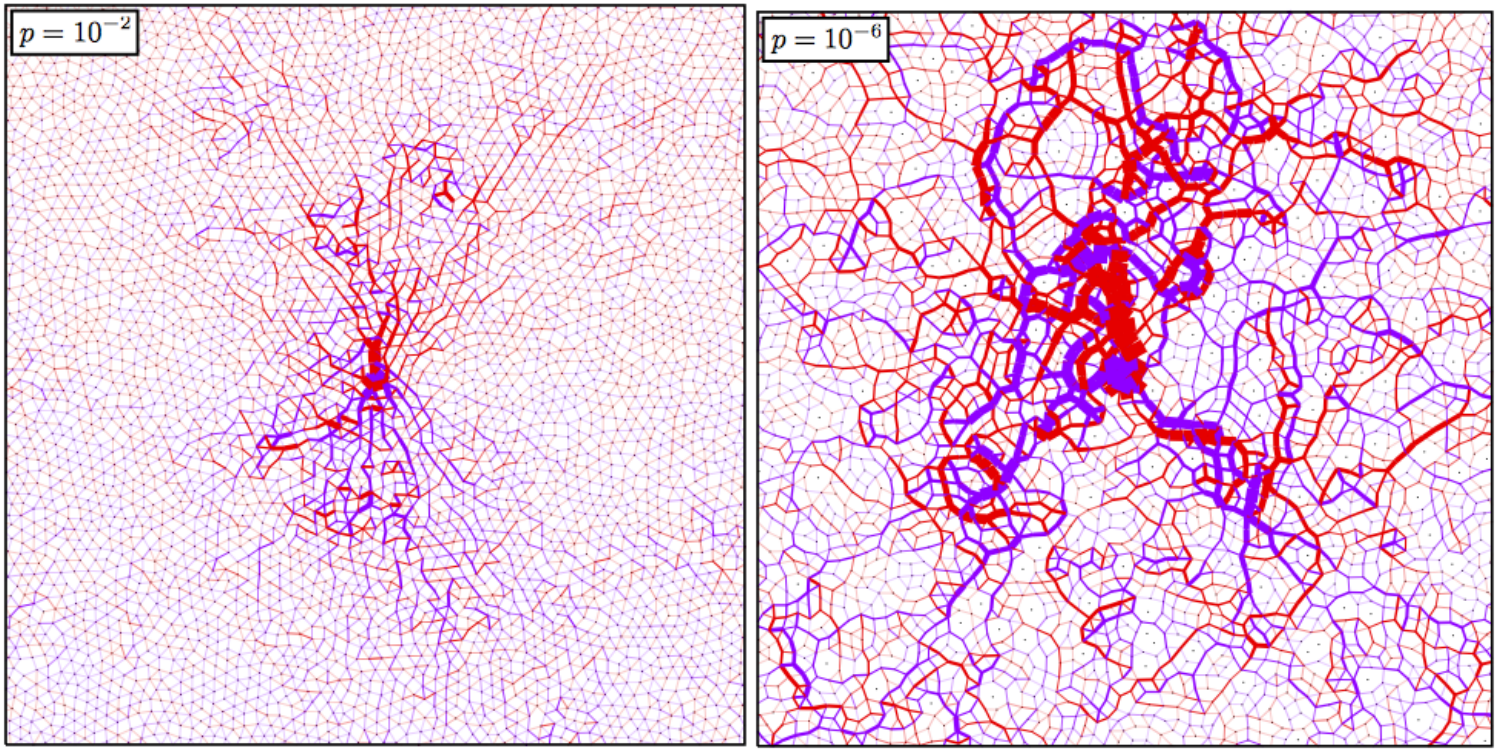
. . . , board games, . . .

Photoelastic disks from B.Behringer's group
ZipZap courtesy of O.Dauchot

The jamming transition

Granular materials, emulsion droplets, colloidal suspensions, powders, ...

- criticality of jamming is easily observed:
  e.g. for hard spheres, $p = \beta P/\rho \sim |\varphi - \varphi_j|^{-1}$ and $\Delta \sim p^{-\kappa}$ with $\kappa < 2$
- robustly universal properties, independent of d
- anomalous "soft modes" associated to a diverging correlation length



[Van Hecke, J.Phys.: Cond.Mat. 22, 033101 (2010)]
[Ikeda, Berthier, Biroli, JCP 138, 12A507 (2013)]

Marginality and criticality at jamming

- Force balance on each particle: $\vec{F}_i = \sum_j \vec{f}_{ij} = \sum_j f_{ij}\hat{r}_{ij} = 0$
  Given packing $\{\hat{r}_{ij}\}$: dN linear equations for $zN/2$ variables f_{ij}
  To have a solution $z \geq 2d$
  Numerical simulations: at φ_j, $z = 2d$, *isostatic packings*

- Open one contact $\rightarrow$ remove one variable f_{ij} $\rightarrow$ no solution, unstable $\rightarrow$ floppy mode

- Stable system of N particles with $(z + \delta z)N/2$ contacts, $N = L^d$
  Cut in two parts: remove cL^{d-1} contacts
  $\Delta z = \delta z\, L^d/2 - cL^{d-1} > 0 \quad \leftrightarrow \quad \delta z > 2/(cL)$
  Stable packing only for $L > L^* = 2/(c\,\delta z)$ where continuum elasticity holds

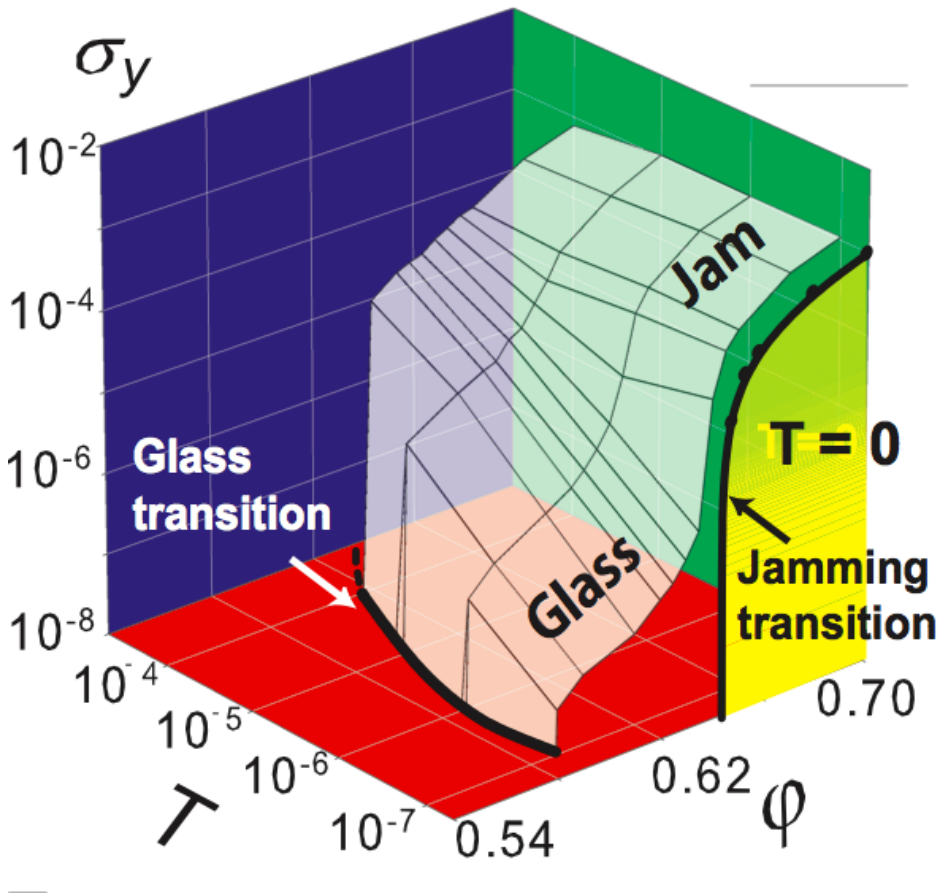
- Numerical simulations: $\delta z \sim |\varphi - \varphi_j|^\nu \rightarrow L^* \sim |\varphi - \varphi_j|^{-\nu}$, $\nu \approx 1/2$

Criticality and a divergent L^* are direct consequences of *isostaticity* and *marginal stability*

[Wyart, Nagel, Silbert, Witten, PRE 72, 051306 (2005)]

Glass/jamming phase diagram

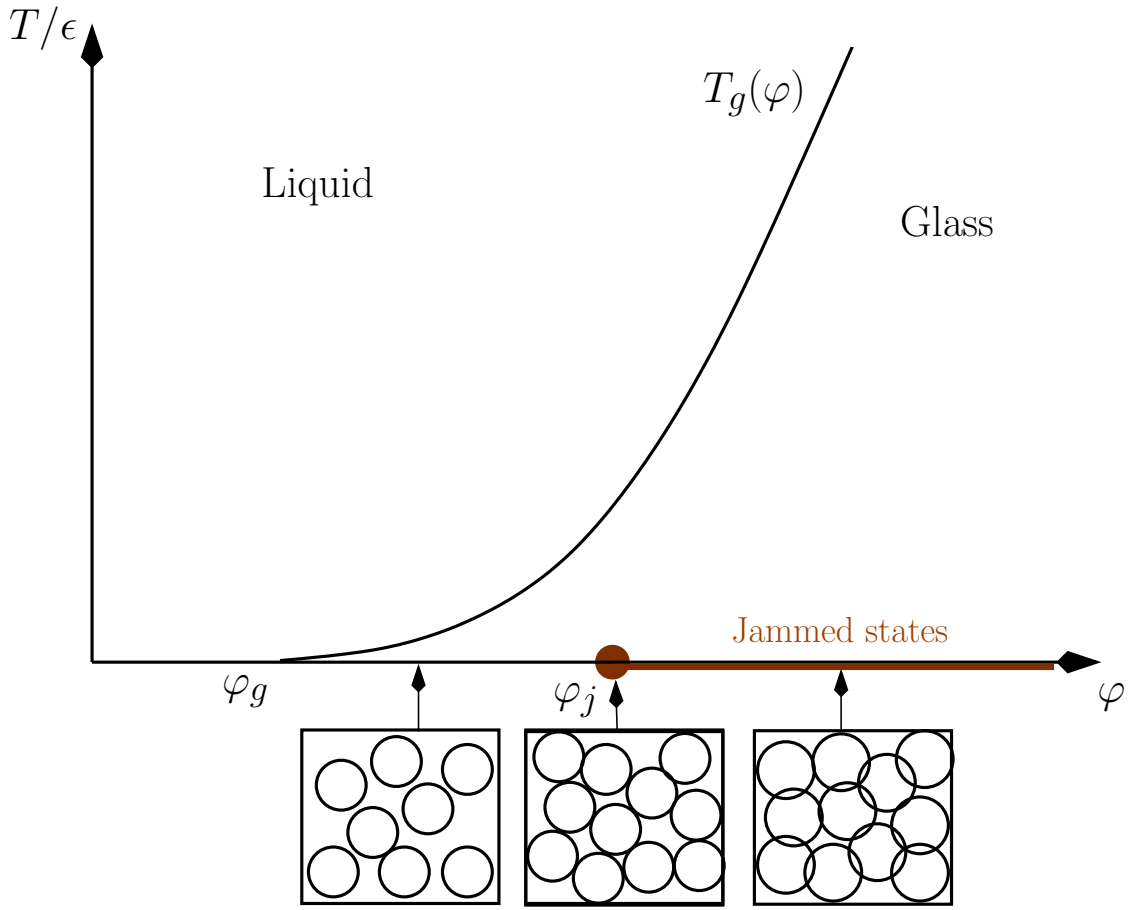
- The soft sphere model:
  $v(r) = \epsilon(1 - r/\sigma)^2\theta(r - \sigma)$
- Two control parameters:
  T/ϵ and $\varphi = V_\sigma N/V$
- $T/\epsilon = 0 \leftrightarrow$ hard spheres



The glass transition goes from liquid to an "entropically" rigid solid
Jamming is a transition from "entropic" rigidity to "mechanical" rigidity

[Ikeda, Berthier, Sollich, PRL 109, 018301 (2012)]

Glass/jamming phase diagram



A theoretical description of the glass transition is difficult; and jamming happens inside the glass!
Problem: $T_g(\varphi)$ and φ_j depend on the numerical/experimental protocol
Remark: same phase diagram as random optimization problems, e.g. qCOL

[Berthier, Jacquin, FZ, PRE 84, 051103 (2011)]

Glass/jamming transitions: summary

- Liquid-glass and jamming are new challenging kinds of phase transitions
- Disordered system, no clear patter of symmetry breaking
- Unified phase diagram, jamming happens at $T = 0$ inside the glass phase
- Criticality at jamming is due to *isostaticity* and associated anomalous response

Outline

Expansion around $d = \infty$ in statistical mechanics

"But suppose that we were unable to diagonalize the Hamiltonian [of QCD] exactly, and that even a computer solution were formidably difficult or impossible. How then might we proceed? To make progress, we must make an expansion of some kind. Since there is no obvious expansion parameter we must find a hidden one. [...] We may take a cue from the spectacular developments [...] in critical phenomena [...] [and] regard the number of spatial dimensions not as a fixed number, three, but as a variable parameter."

[E.Witten, Physics Today 33, 38 (1980)]

Many fields of physics (QCD, turbulence, critical phenomena, non-equilibrium ... glasses!) struggle because of the absence of a small parameter

Proposal: $1/d$ is a small parameter

Exact solution for $d = \infty$ is possible, using your favorite mean field method:
for hard spheres, it predicts distinct glass ($\leftarrow$RFOT) and jamming transitions

Question: which features of the $d = \infty$ solution translate smoothly to finite d?

For the glass transition, the answer is very debated!

For the jamming transition, numerical simulations show that the properties of the transition are *independent of d*

[Goodrich, Liu, Nagel, PRL 109, 095704 (2012)]
[Charbonneau, Corwin, Parisi, FZ, PRL 109, 205501 (2012)]

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Expansion around $d = \infty$ in statistical mechanics

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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- Qualitative MFT (Parisi, 1979; KTW, 1987)
  Spontaneous replica symmetry breaking
  Order parameter: overlap matrix q_{ab}
  Dynamical transition "à la MCT"

- Quantitative MFT (exact for $d \to \infty$)
  Kirkpatrick and Wolynes 1987
  Kurchan, Parisi, Urbani, FZ 2006-2013

- Quantitative theory in finite d
  DFT (Stoessel-Wolynes 1984)
  MCT (Bengtzelius-Götze-Sjolander 1984)
  Replicas (Mézard-Parisi 1996, +FZ 2010)

- Corrections around MFT
  Ginzburg criterion, $d_u = 8$ (2007, 2012)
  Renormalization group (2011–)
  Nucleation (RFOT) theory (KTW 1987)

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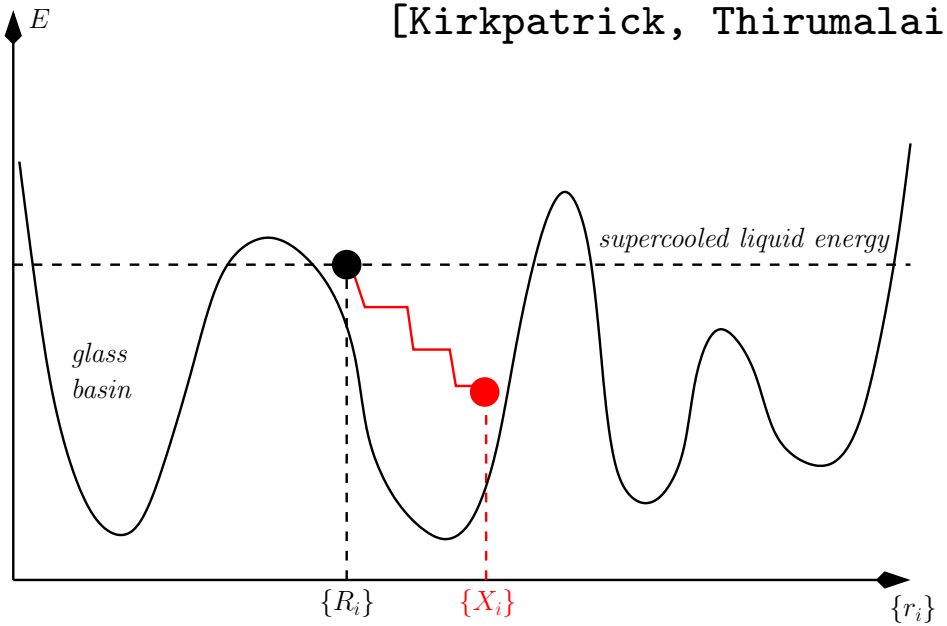
The RFOT picture

[Goldstein, Stillinger, Weber et al. 1969 - ...]
[Kirkpatrick, Thirumalai, Wolynes 1987-1989]



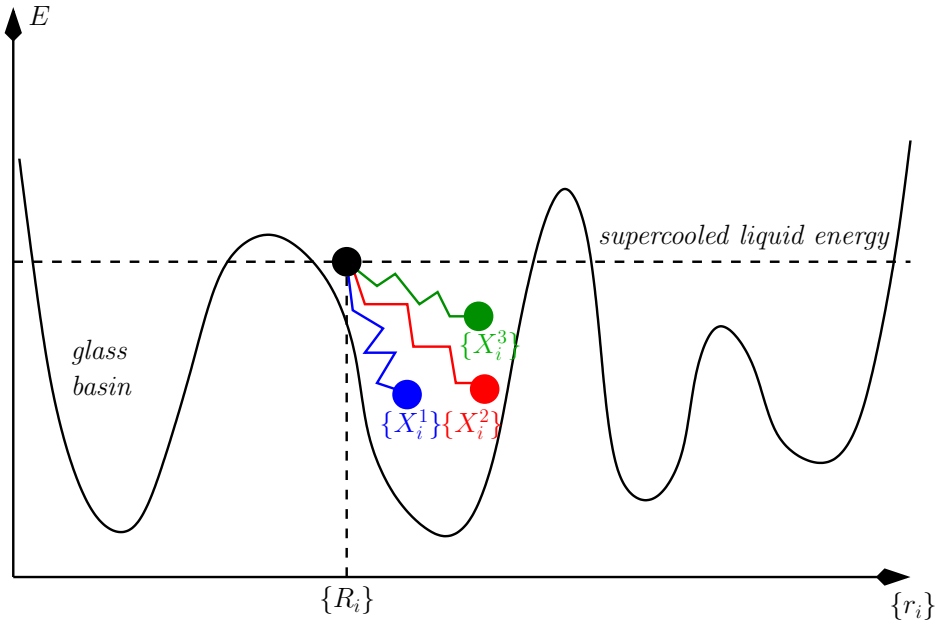
The supercooled liquid is a collection of glasses
Each equilibrium liquid configuration R belongs to a metastable glass state

X is a copy of the system. If $X(t = 0) = R$, either $X \sim R$ at all times (glass), or X diffuses away from R (liquid). The dynamics of X is the equilibrium dynamics of the liquid.

Relaxation in the supercooled liquid is like escaping from a metastable state – except that the process is repeated over and over

[Krzakala and Zdeborova, JCP 134, 034513 (2011)]

Why replicas?



A modified, constrained equilibrium replaces dynamics

$$F_g = -k_B T \int dR \frac{e^{-\beta H[R]}}{Z} \log Z[X|R] \qquad Z[X|R] = \int dX e^{-\beta' H[X] + \beta' \varepsilon \sum_i (X_i - R_i)^2}$$

Need replicas: $F_g = -k_B T \lim_{n\to 0} \log \left[\int dR e^{-\beta H[R]} Z[X|R]^n \right] - F_{\rm liq}$

The replicated system is a homogeneous and isotropic "molecular liquid" that can be treated by standard liquid theory

[Franz, Parisi, J. de Physique I 5, 1401 (1995)]
[Monasson, PRL 75, 2847 (1995)]

Solution of the hard sphere model in $d = \infty$

- A liquid of molecules, each made by m atoms: $\bar{x} = \{x_1 \cdots x_m\}$
  In $d \to \infty$ only the first virial coefficient survives
  The entropy is:
  $S[\rho(\bar{x})] = \int d\bar{x}\rho(\bar{x})[1 - \log \rho(\bar{x})] + \frac{1}{2}\int d\bar{x}d\bar{y}\rho(\bar{x})\rho(\bar{y})f(\bar{x},\bar{y})$
- Rotational and translational invariance: $\rho(\bar{x}) = \rho(q_{ab})$, $q_{ab} = u_a \cdot u_b$, $u_a = x_a - \frac{1}{m}\sum_b x_b$
  From $d\,m$ to $(m-1)(m-2)/2$ coordinates
- Saddle-point evaluation for $d \to \infty$: $S[q_{ab}]$
  q_{ab} determined by the saddle-point equation
- No hope to solve for generic $q_{ab} \to$ use hierarchical matrices introduced by Parisi
- Exact solution within the "full replica symmetry breaking" structure of q_{ab}

[Kurchan, Parisi, FZ, JSTAT (2012) P10012]
[Kurchan, Parisi, Urbani, FZ, J.Phys.Chem. B 117, 12979 (2013)]
[Charbonneau, Kurchan, Parisi, Urbani, FZ, arXiv:1310.2549]

Approximate solution in finite d:
- a Gaussian assumption for $\rho(\bar{x})$ (exact for $d = \infty$)
- resummation of virial diagrams (through HNC or similar)

[Parisi, FZ, RMP 82, 789 (2010)]

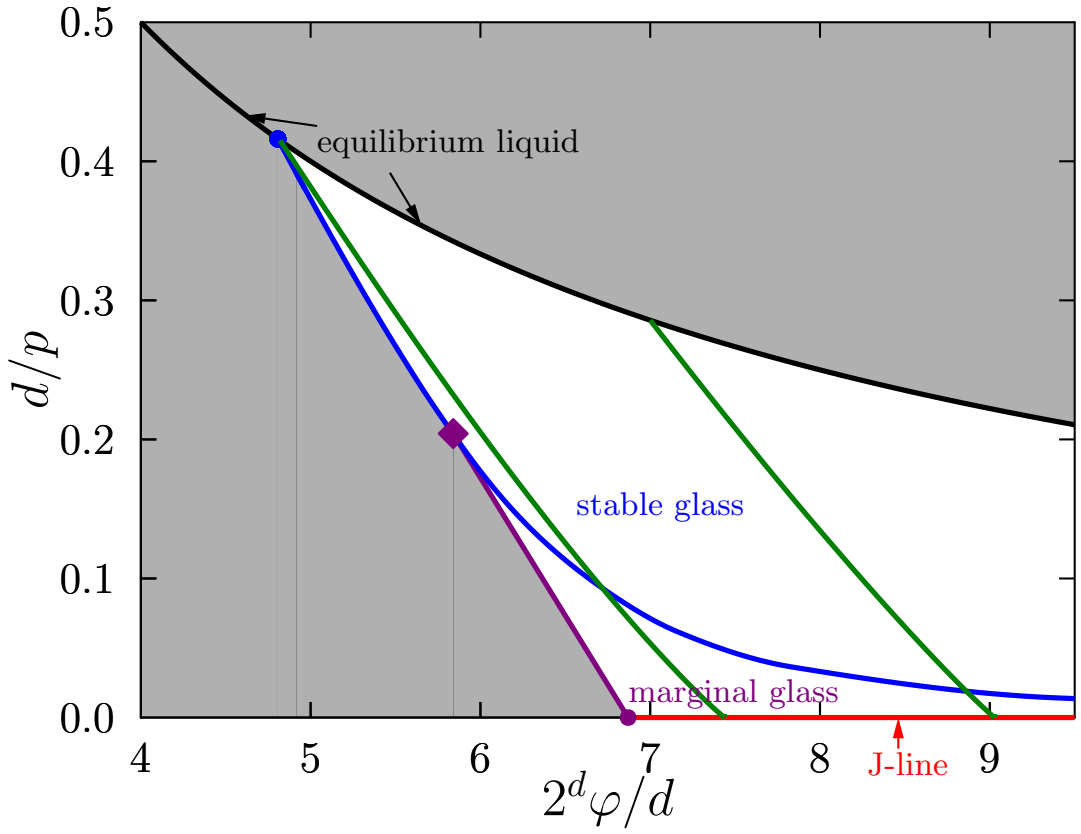
Theory of glass/jamming: summary

- A $1/d$ expansion around a mean-field solution is a standard tool when the problem lack a natural small parameter
- Hard spheres are exactly solvable when $d \to \infty$
  They have a glass phase and a jamming transition
- You can choose your preferred method of solution: replicas are convenient
- An approximate mean field solution in finite d is obtained by resumming virial diagrams

Outline

The phase diagram (theory)

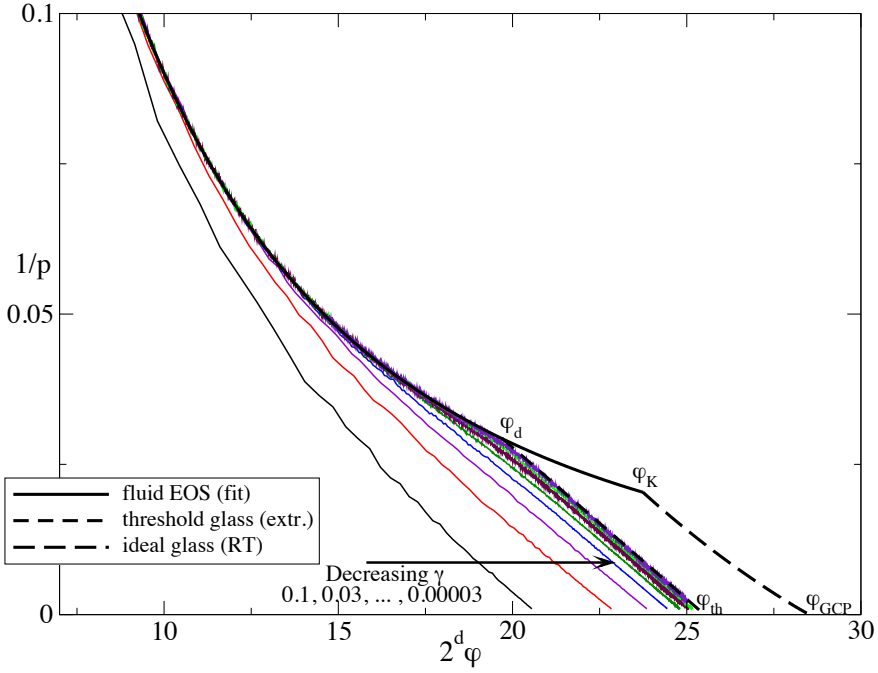
Prediction of the theory for $d = \infty$:

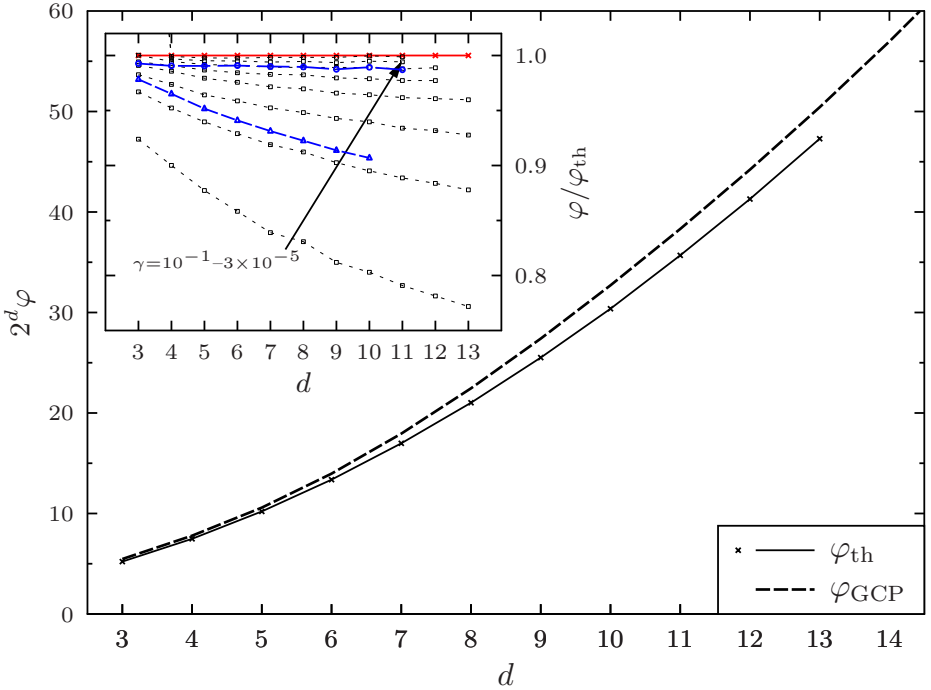


- Distinct glasses, depending on initial equilibrium density → A *range* of jamming densities
- A Gardner transition, stable glass → marginal glass

[Charbonneau, Kurchan, Parisi, Urbani, FZ, arXiv:1310.2549]

The phase diagram (simulation)





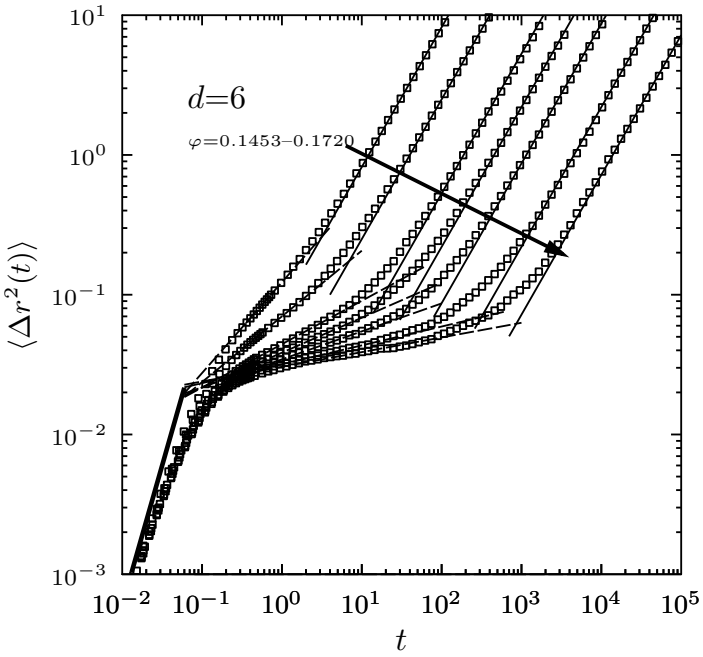
Compression of d-dimensional hard spheres at rate γ (Lubachevsky-Stillinger event-driven MD)

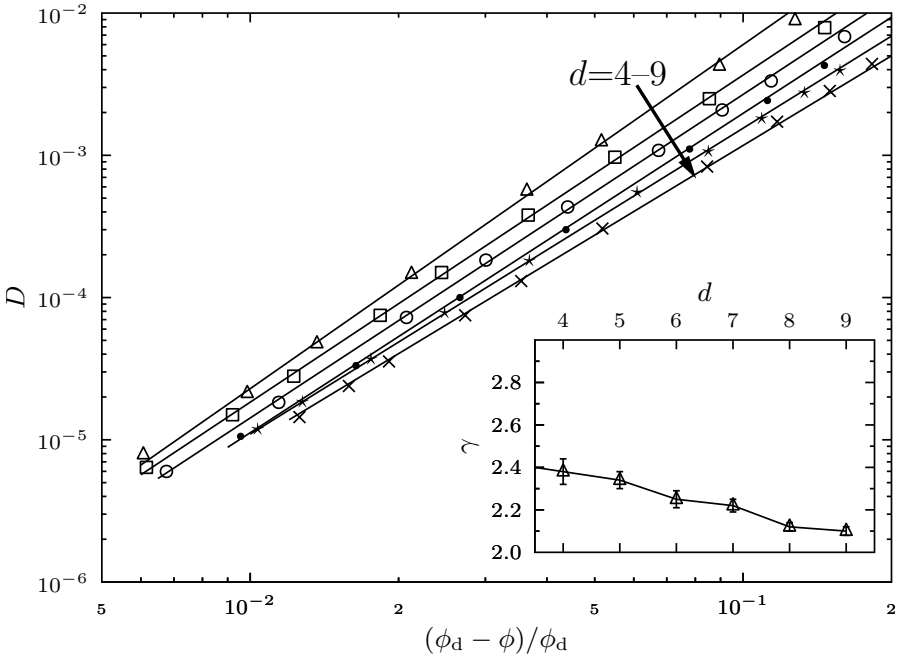
$$p_{\rm fluid}(\varphi) = 1 + 2^{d-1}\varphi\,\frac{1-A_{\rm d}\,\varphi}{(1-\varphi)^d} \qquad p_{\rm glass}(\gamma,\varphi) = \frac{d\,\varphi_{\rm j}(\gamma)[1-f(\gamma)]}{\varphi_{\rm j}(\gamma)-\varphi}$$

A range of jammed packings depending on compression speed: OK
Analytic computation of the glass EOS is possible: work in progress

[Charbonneau, Ikeda, Parisi, FZ, PRL 107, 185702 (2011)]
[Charbonneau, Corwin, Parisi, FZ, PRL 109, 205501 (2012)]

Critical dynamics at the dynamic glass transition





Equilibrium MD simulation in the liquid close to φ_d
MCT-like dynamical criticality: $D \sim |\varphi - \varphi_d|^\gamma$

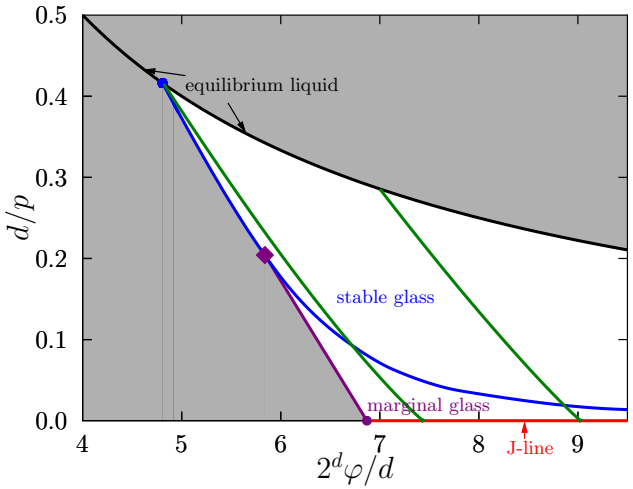
[Charbonneau, Ikeda, Parisi, FZ, PNAS 109, 13939 (2012)]

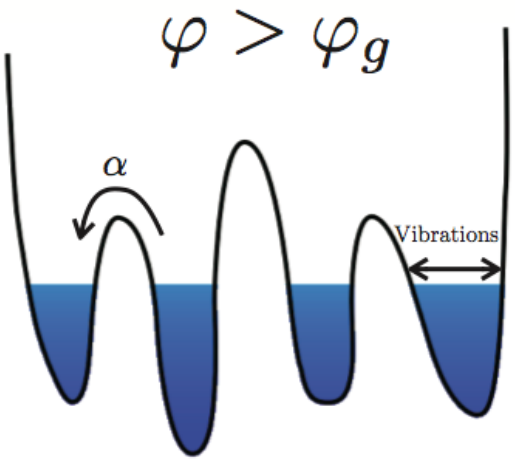
Analytic computation in $d = \infty$ of the exponent $\lambda_{\rm MCT} = 0.70698 \to \gamma = 2.33786$
Finite d computation in progress

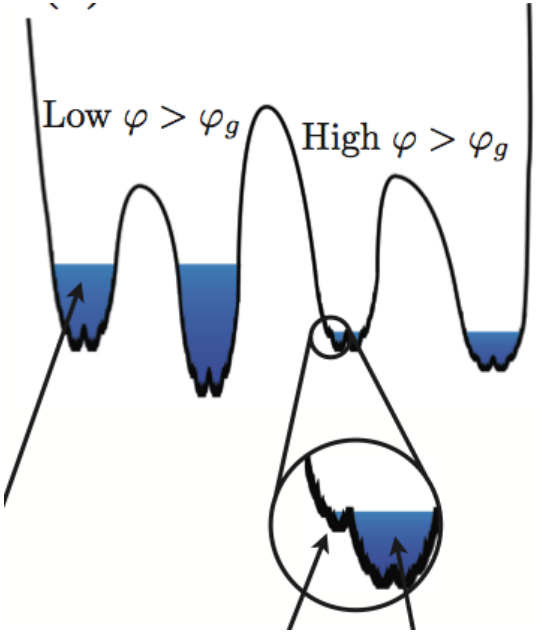
[Kurchan, Parisi, Urbani, FZ, J.Phys.Chem. B 117, 12979 (2013)]

The Gardner transition

- Theory predicts a *Gardner transition* in the glass phase
- Gardner transition: stable → marginally stable glass
- The J-line falls inside the marginal phase

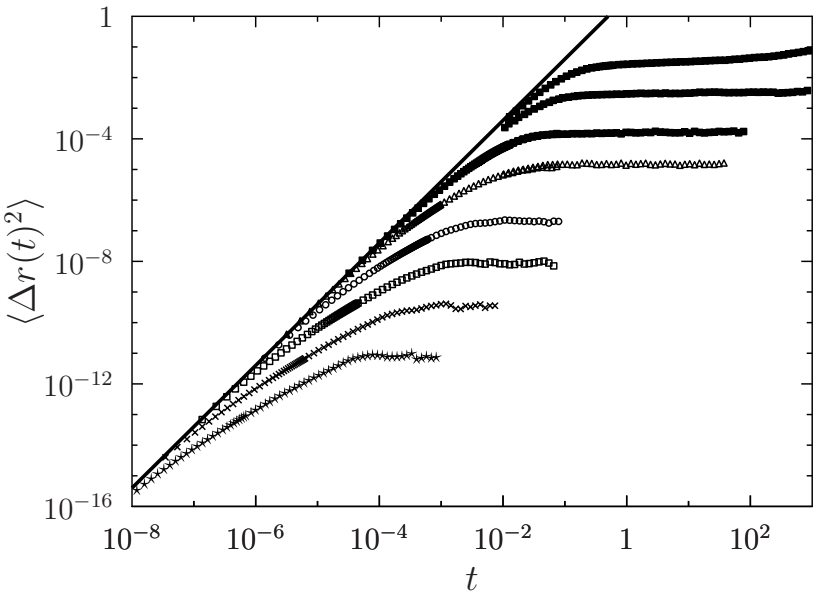


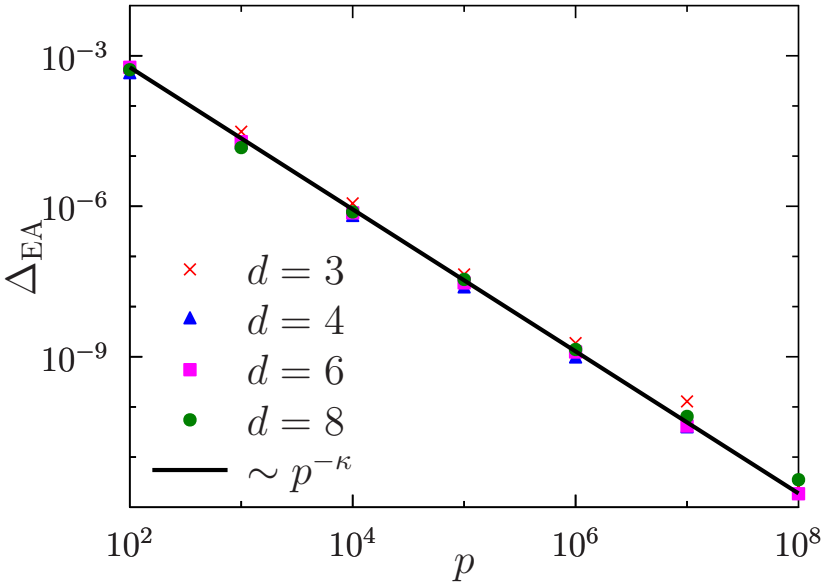




[Charbonneau, Kurchan, Parisi, Urbani, FZ, arXiv:1310.2549]

Mean square displacement in the glass

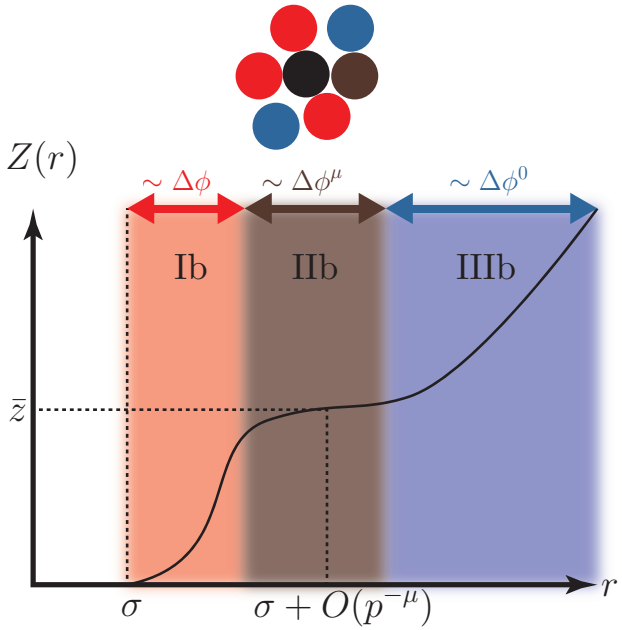


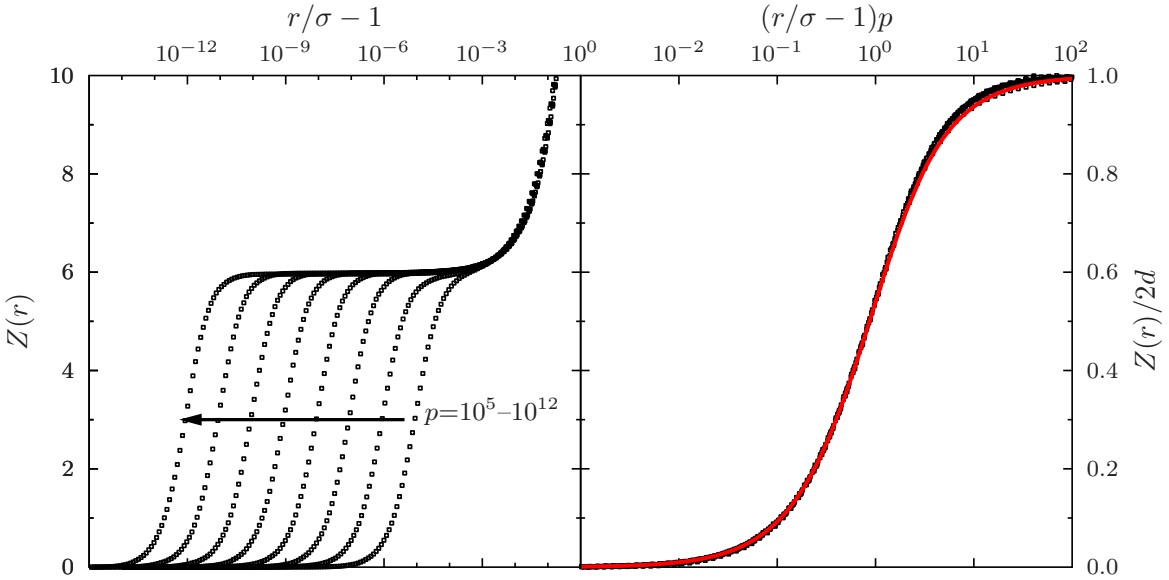


- In the glass the MSD has a plateau: diffusion is arrested, only vibrations
- The plateau value $\Delta_{\rm EA}$ is the Debye-Waller factor
- Independent caging: $\Delta_{\rm EA} \sim p^{-2}$ (e.g. crystal)
- Theory: $\Delta_{\rm EA} \sim p^{-\kappa}$ with $\kappa = 1.416$; excellent agreement with MD
- $\Delta_{\rm EA} \gg p^{-2}$: anomalously large vibrations $\rightarrow$ correlated vibrations, soft modes
- Ignoring the Gardner transition leads to $\kappa = 1$, wrong!

[Ikeda, Berthier, Biroli, JCP 138, 12A507 (2013)]
[Charbonneau, Kurchan, Parisi, Urbani, FZ, arXiv:1310.2549]

Pair correlation at jamming



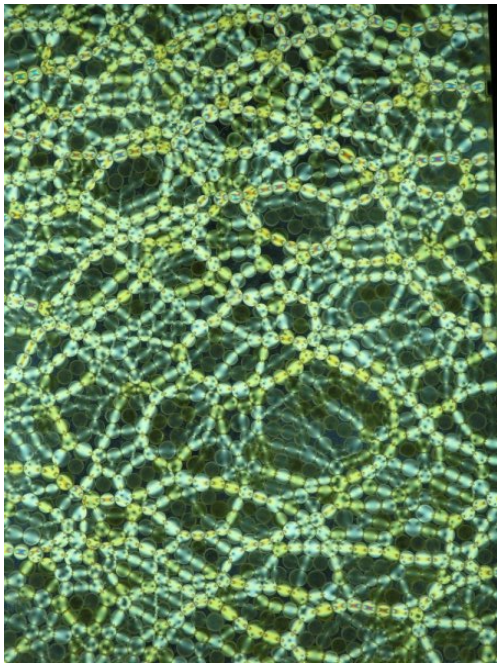


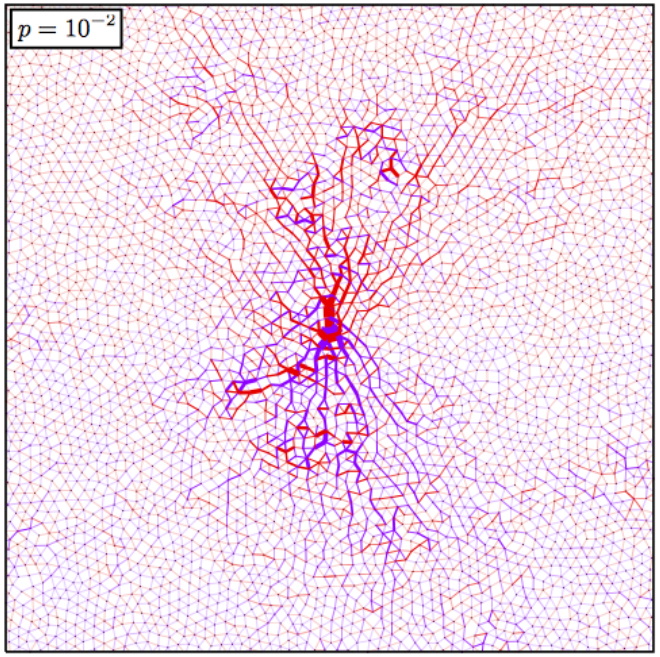
- Predictions for the scaling of pair correlation $g(r)$ and $Z(r) = d\,2^d\phi \int_0^r ds\, s^{d-1} g(s)$
- Three regimes: I contacts, II matching, III small gaps
- Contact regime: $Z(r) = 2d\mathcal{Z}[(r-\sigma)/\sigma p]$
- $\mathcal{Z}(\lambda) = 1 - \int_0^\infty df\, P(f) e^{-\lambda f}$
- $P(f) \sim f^{\theta} \quad \leftrightarrow \quad \mathcal{Z}(\lambda \to \infty) \sim 1 - \lambda^{-1-\theta}$ with $\theta = 0.4231$
- $Z(r > \sigma) \sim 2d + (r-\sigma)^{1-\alpha}$ with $\alpha = 0.413$

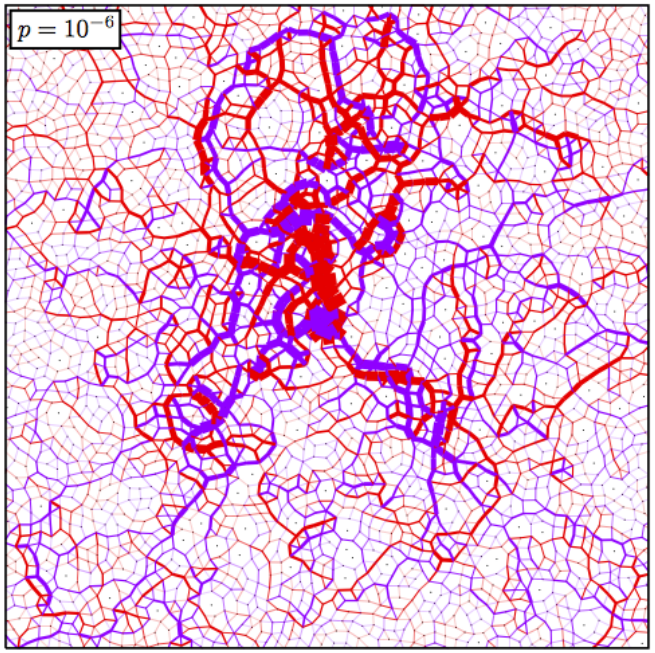
[Charbonneau, Corwin, Parisi, FZ, PRL 109, 205501 (2012)]
[Charbonneau, Kurchan, Parisi, Urbani, FZ, arXiv:1310.2549]

Marginal stability and mechanical stability

- The exponent θ describes small forces: contacts that *break* first
- The exponent α describes quasi-contacts: contacts that *form* first
- These exponents play a crucial role for the mechanical stability of random packings
  [Wyart, PRL 109, 125502 (2012)]
- Neglecting the Gardner transition gives $\theta = 0$ and $\alpha = 1$: plain wrong!
- Taking into account the Gardner transition gives the correct values: amazing!
- Marginal stability, isostaticity and mechanical stability are intimately connected
  [Charbonneau, Kurchan, Parisi, Urbani, FZ, arXiv:1310.2549]







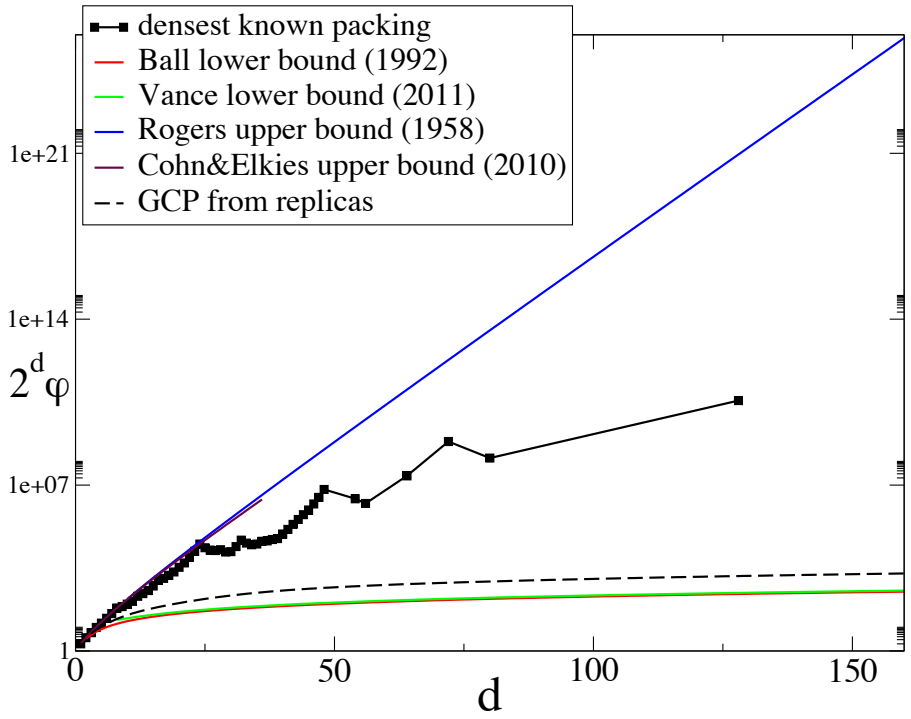
The packing problem

- An elegant mathematical problem with connections to many others (number theory, ...)
- Applications in information & communication theory (coding, ...)
- Applications in physics (granulars, colloids, glasses, ...)

[Torquato, Stillinger, RMP 82, 2633 (2011)]

The packing problem in large spatial dimension

- Best rigorous upper bound $2^d \varphi \leq 2^{0.4010\ldots\, d}$
- Best rigorous lower bound $2^d \varphi \geq (6/e)\, d$ (20 years to gain a factor $3/e$!)
- Good lattice packings only known up to $d = 128$
- Lattice packings density seems to beat the lower bound by an exponential factor (?)

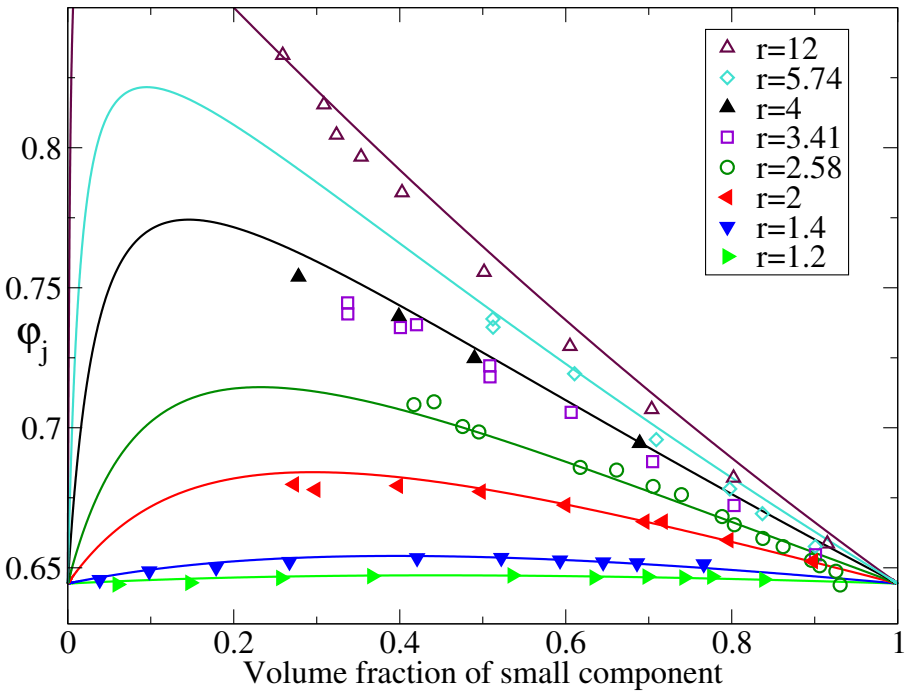


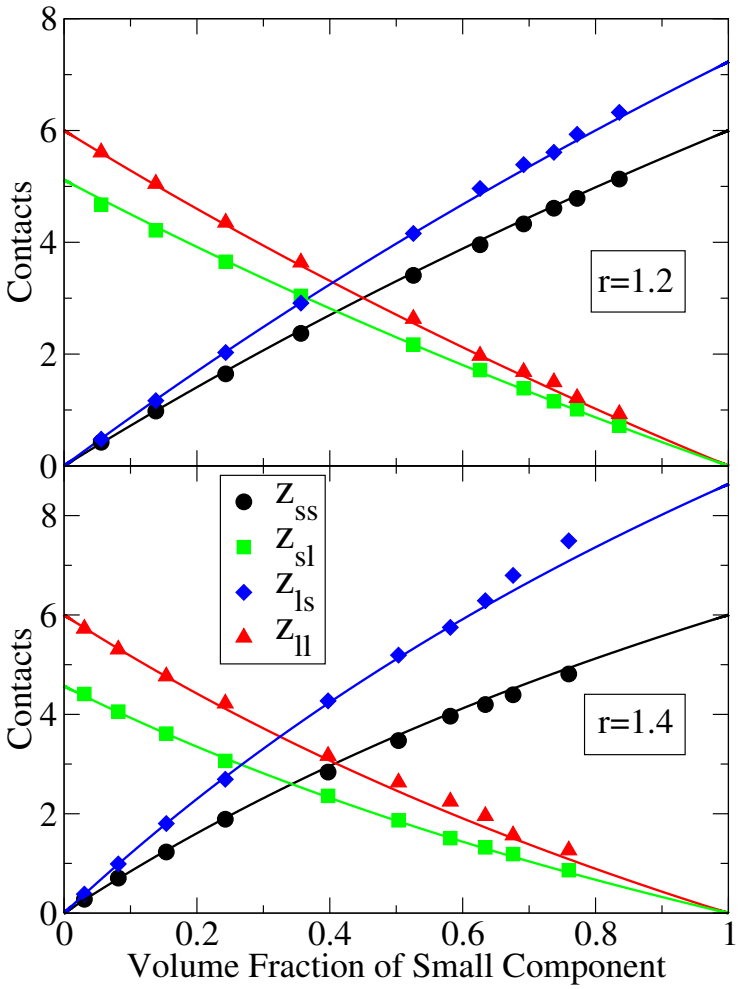
- Non-rigorous replica result: amorphous packings exist for $\varphi \leq 2^{-d}\, d \log d$
- Non-rigorous replica result: amorphous packings can be constructed in polynomial time in N for $\varphi \leq 7.4\, d\, 2^{-d}$, via simulated annealing

Any rigourous justification of these results
would be extremely welcome by the mathematical community

[Parisi, FZ, RMP 82, 789 (2010)]

Random close packing of binary mixtures





$r = D_A/D_B$

All packings are predicted to be globally isostatic
Partial contact numbers are almost independent of φ_j

[Biazzo, Caltagirone, Parisi, FZ, PRL 102, 195701 (2009)]

Results: summary

- The $d = \infty$ phase diagram is qualitatively realized in finite d
  Quantitative computation are possible, in progress
- MCT-like dynamics at the glass transition, exponents can be computed
- Critical properties of jamming are obtained only by taking into account the Gardner transition to a marginal phase
  Analytic computation of the non-trivial critical exponents α, θ, κ
- New (non-rigorous, but constructive) bounds on the packing problem in large d
- Extension to binary mixtures: prediction of jamming density and partial contacts

THANK YOU FOR YOUR ATTENTION