Exact computation of the critical exponents of the jamming transition

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Special thanks E. DeGiuli, E. Lerner, M. Wyart

Kyoto, 11/08/2015

Outline

1. Reminder of the basics

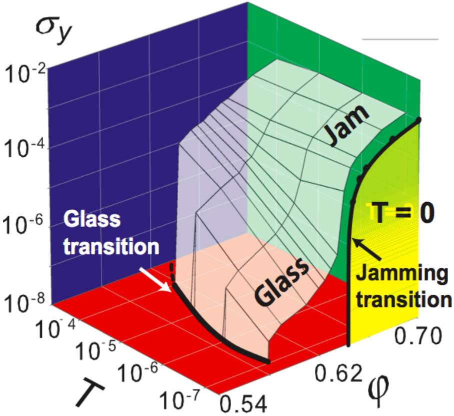
2. Exact solution of hard spheres in infinite dimensions

3. The critical exponents of jamming

Outline

Glass/jamming phase diagram

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

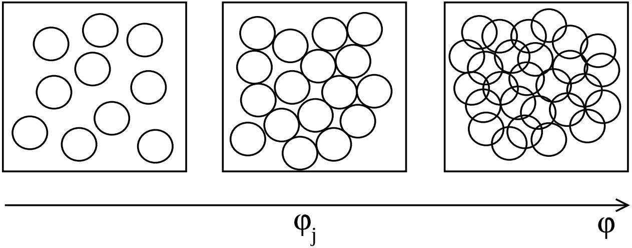


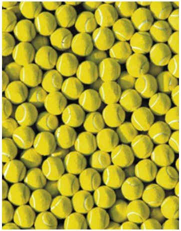
The glass transition goes from liquid to an “entropically” rigid solid
Jamming is a transition from “entropic” rigidity to “mechanical” rigidity

[Liu, Nagel, Nature 396, 21 (1998)]
[Berthier, Witten, PRE 80, 021502 (2009)]
[Ikeda, Berthier, Sollich, PRL 109, 018301 (2012)]

The jamming transition

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





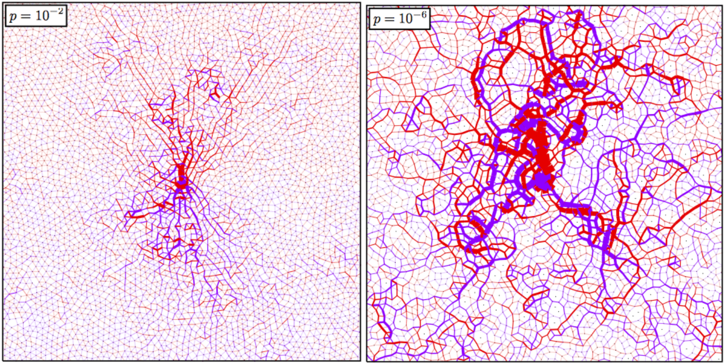
Hard sphere limit $T/\epsilon \to 0$:
For $\varphi < \varphi_j$: pressure $P \propto T \to 0$ and reduced pressure $p = P/(\rho T)$ is finite
For $\varphi > \varphi_j$: pressure $P \propto \epsilon(\varphi - \varphi_j)$

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)]
[Liu, Nagel, Nature 396, 21 (1998)]
[O'Hern, Langer, Liu, Nagel, PRL 88, 075507 (2002)]

The jamming transition

Anomalous "soft modes" associated to a diverging correlation length of the force network



[Wyart, Silbert, Nagel, Witten, PRE 72, 051306 (2005)]
[Van Hecke, J.Phys.: Cond.Mat. 22, 033101 (2010)]

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:
  to make a theory of jamming we first need to make a theory of glass
- Criticality at jamming is due to *isostaticity* and associated anomalous response

Outline

Expansion around $d = \infty$ in statistical mechanics

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

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

In $d = \infty$, exact solution using mean-field theory

Proposal: use $1/d$ as a small parameter $\rightarrow$ RFOT theory

[Kirkpatrick, Thirumalai, Wolynes 1987-1989]

[Kirkpatrick, Wolynes, PRA 35, 3072 (1987)]

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

For the glass transition, the answer is very debated!

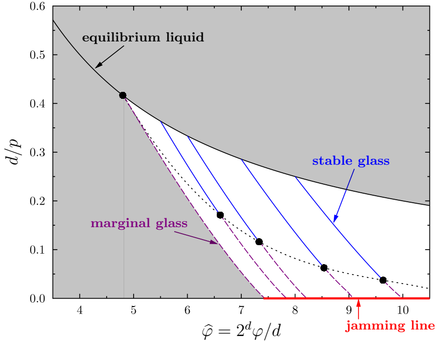
For the jamming transition, numerical simulations show that the properties of the transition are *very weakly dependent on d*

[Goodrich, Liu, Nagel, PRL 109, 095704 (2012)]

[Charbonneau, Corwin, Parisi, FZ, PRL 109, 205501 (2012)]

Exact phase diagram of hard spheres in $d = \infty$

[Charbonneau, Kurchan, Parisi, Urbani, FZ, Nature Comm. 5, 3725 (2014)]
[Rainone, Urbani, Yoshino, FZ, PRL 114, 015701 (2015) & in progress]



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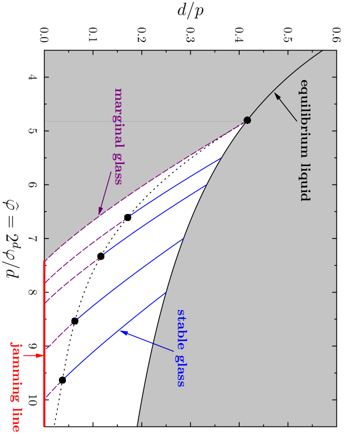
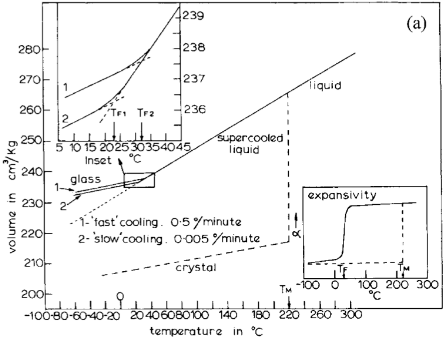
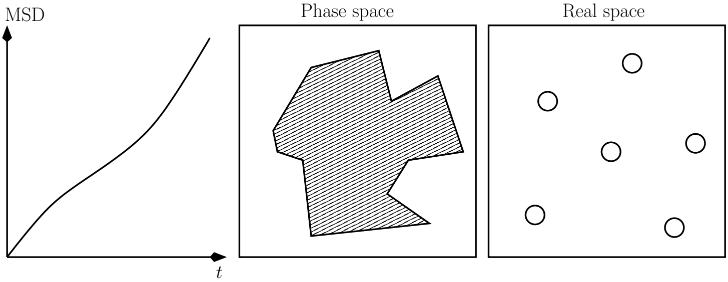
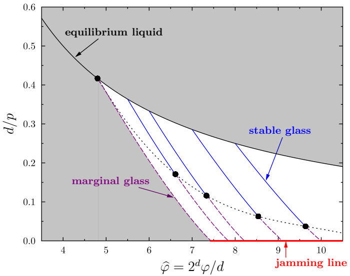




Constant pressure P
Horizontal axis: $1/p = \rho/(\beta P) = T\rho/P \propto T$: *temperature*
Vertical axis: $\varphi \downarrow \equiv v \uparrow$: *specific volume*

Exact phase diagram of hard spheres in $d = \infty$

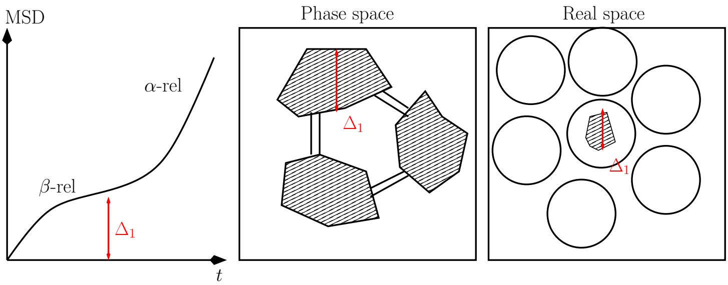


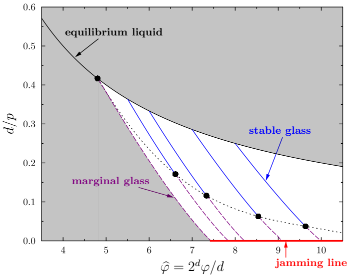


1. Low-density liquid

- Dynamics: diffusive MSD
- Phase space: $\{x_i\} \in \mathbb{R}^{Nd}$. Allowed configurations have no overlaps.
- Real space: $x_i \in \mathbb{R}^d$ hard sphere position

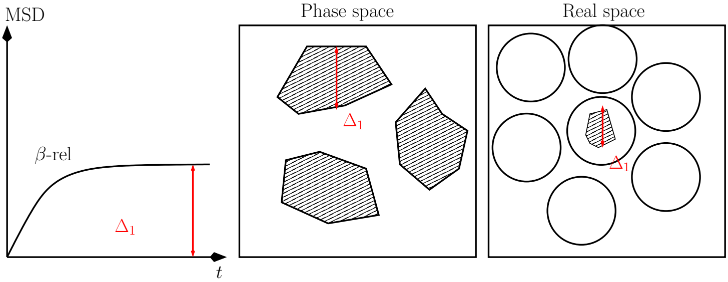
Exact phase diagram of hard spheres in $d = \infty$

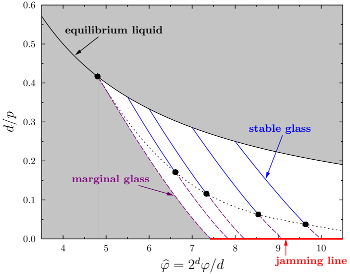




2. **Supercooled liquid approaching $\varphi_{\rm d}$**
   - Almost disconnected phase space
   - Slow α relaxation
   - Critical β relaxation to plateau Δ_1
   - MCT/RFOT-like caging

Exact phase diagram of hard spheres in $d = \infty$

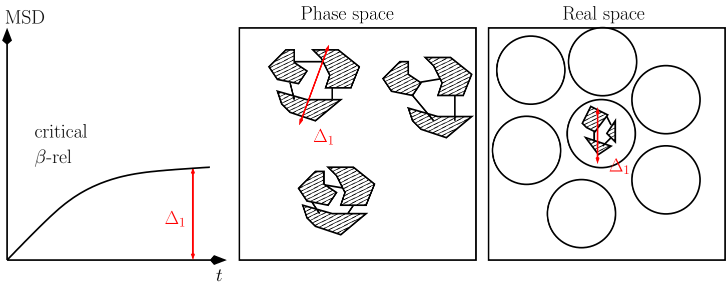


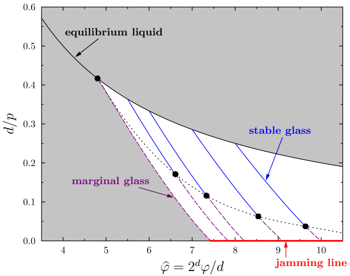


3. Equilibrium above φ_{d}: trapped in a glass

- Disconnected phase space
- Completely arrested α relaxation
- Non-critical β relaxation to a plateau
- Complete caging with short range correlations

Exact phase diagram of hard spheres in $d = \infty$

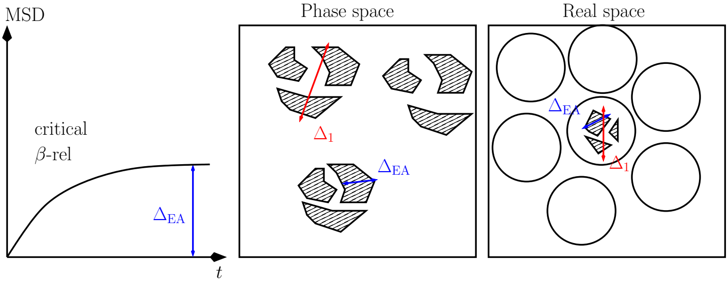


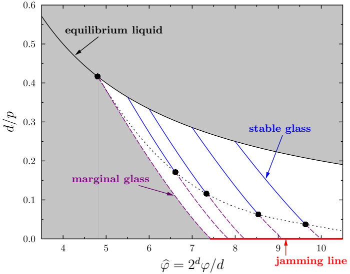


4. Glass approaching the Gardner point

- Glass basin fractures
- Critical β relaxation to a plateau
- Caging with long range correlations

Exact phase diagram of hard spheres in $d = \infty$

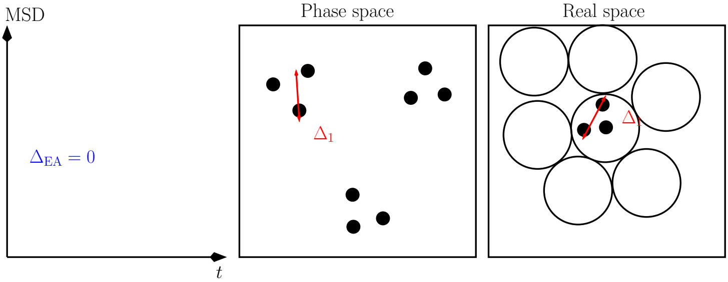


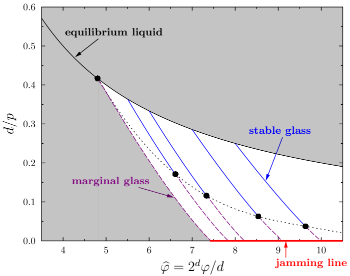


5. Gardner (fullRSB) glass

- Glass meta-basin fractured in sub-basins
- Sub-basins are *marginally stable*
- Critical β relaxation to a plateau $\Delta_{\rm EA} < \Delta_1$
- Caging with infinite range correlations

Exact phase diagram of hard spheres in $d = \infty$

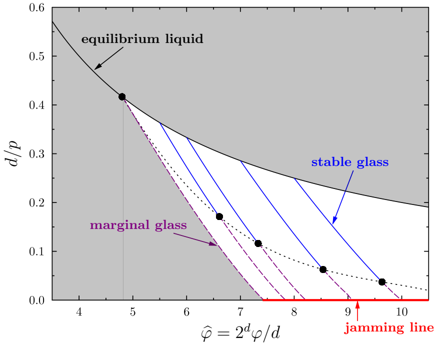




6. Jamming

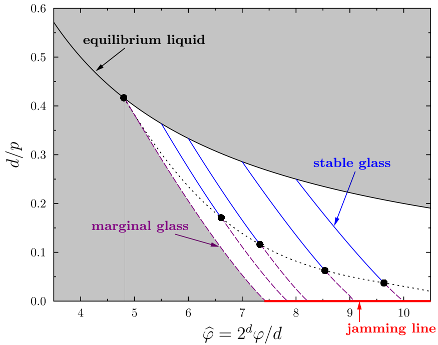
- No motion of particles (infinite pressure)
- Sub-basins shrink to points (single configurations)
- The jamming line falls in the Gardner phase

Solution in $d = \infty$: summary



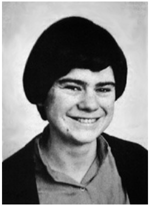
- A $1/d$ expansion around a mean-field solution is a standard tool when the problem lack a natural small parameter
- Hard spheres are exactly solvable when $d \to \infty$
  You can choose your preferred method of solution: replicas are convenient
- They follow the RFOT scenario with protocol-dependent glass and jamming transitions

Solution in $d = \infty$: summary



Crucial new result:

- A *Gardner transition* inside the glass phase with critical β-relaxation and diverging χ_4 – ending at the MCT point
- Stable $\rightarrow$ marginally stable glass
  `[Gardner, Nucl.Phys.B 257, 747 (1985)]`
- The jamming line falls inside the marginal phase



Solution in $d = \infty$: FAQ

- How did you make the computations? $\Rightarrow$ arXiv:1411.0826
- How can I detect the Gardner transition in my simulations? $\Rightarrow$ Beatriz Seoane's poster
- How universal is all this stuff? $\Rightarrow$ arXiv:1501.03397, 1506.01997
- What about rheological properties? $\Rightarrow$ Hajime Yoshino's talk

Outline

Criticality around jamming

- The plateau value $\Delta_{\rm EA}$ goes to zero at jamming, $\Delta_{\rm EA} \sim p^{-\kappa}$
- At $p = \infty$, gap distribution $g(h) \sim h^{-\gamma}$ and force distribution $P(f) \sim f^{\theta}$

[Wyart, PRL 109, 125502 (2012)]

- Three critical exponents κ, γ, θ
- Scaling relations based on *marginal mechanical stability of the packing*
- $\gamma = 1/(2+\theta)$ and $\kappa = 2 - 2/(3+\theta)$
- Only one exponent remains undetermined
- Numerically $\gamma \approx 0.4$ in all dimensions, which implies $\theta \approx 0.5$ and $\kappa \approx 1.4$

[DeGiuli, Lerner, Brito, Wyart, PNAS 111, 17054 (2014)]

The jamming transition is a new kind of zero-temperature "critical" point, characterized by scaling and non-trivial critical exponents

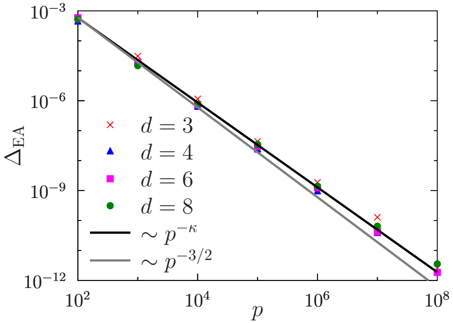
Critical exponents of jamming

- Neglecting the Gardner transition gives $\theta = 0$ and $\gamma = 1$: plain wrong
- Taking into account the Gardner transition gives correct values: $\kappa = 1.41574\ldots$, $\gamma = 0.41269\ldots$, $\theta = 0.42311\ldots$
- Consistent with scaling relations $\gamma = 1/(2+\theta)$ and $\kappa = 2 - 2/(3+\theta)$
- Marginal stability in phase space and marginal mechanical stability are intimately connected

[Charbonneau, Kurchan, Parisi, Urbani, FZ, Nature Comm. 5, 3725 (2014)]

Critical exponents of jamming

$\kappa = 1.41574\ldots$, $\gamma = 0.41269\ldots$, $\theta = 0.42311\ldots$
Perfectly compatible with the numerical values in all dimensions $d = 2\cdots 10$
[Charbonneau, Kurchan, Parisi, Urbani, FZ, Nature Comm. 5, 3725 (2014)]



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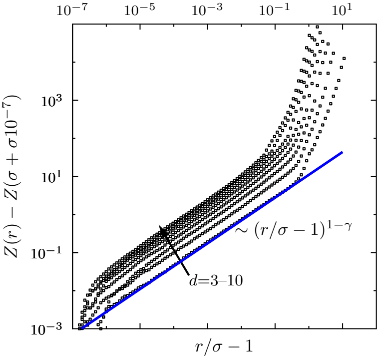

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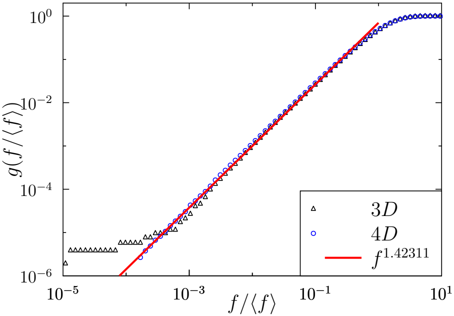


Summary

- The jamming transition is a new kind of zero-temperature critical point, characterized by scaling and non-trivial critical exponents

- Critical properties of jamming are obtained only by taking into account the Gardner transition to a marginal fullRSB phase
  Analytic computation of the non-trivial critical exponents γ, θ, κ

- An unexpected connection between hard spheres in $d \to \infty$ and the SK model
  An instance where the fullRSB structure gives quantitative predictions for critical exponents in finite dimensions!

Perspectives

The Gardner transition is known since 1985 in spin glasses, but it has always been considered as an exotic phenomenon. Its existence in structural glasses proves that it is instead a new *Unifying Concept in Glass Physics*.

- It explains the criticality of the jamming transition and the abundance of soft modes in low-temperature glasses
- It implies that zero-field-cooled (ZFC) and field-cooled (FC) responses are different
- It implies a critical β-relaxation and non-trivial β-aging *inside a glass basin* – which could explain the anomalous behavior of the β-relaxation observed in some polymer experiments
- It could explain the presence of dynamical heterogeneities (divergent χ_4) in low-temperature glasses
- It could explain the anomalies of quantum glasses ("two-level systems")

THANK YOU FOR YOUR ATTENTION

Additional material

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)

Theory of the liquid-glass transition

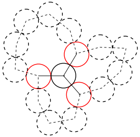
- Qualitative MFT (Parisi, 1979; KTW, 1987)
  Spontaneous replica symmetry breaking
  Order parameter: overlap matrix q_{ab}
  Dynamical transition "à la MCT"

- 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)

$1/d$ as a small parameter – amorphous hard spheres



- Geometric argument:
  kissing number $e^d \gg$ coordination at jamming $2d$
  $\Rightarrow$ uncorrelated neighbors
  Uncorrelated neighbors correspond to a mean field situation
  (like Ising model in large d)
- Statistical mechanics argument:
  third virial (three body terms) $\ll$ second virial (two-body term).
  Rigorously true for $2^d \varphi \lesssim 1$
  Re-summation of virial series (in the metastable liquid state) gives a pole at $2^d \varphi \sim e^d$.
  Glass transition is around $2^d \varphi \sim d$ `Percus, Kirkwood`

Keep only ideal gas + second virial term (as in TAP equations of spin glasses):

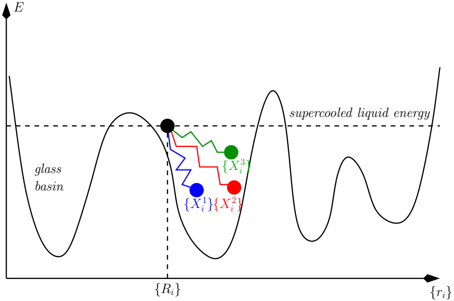
$$-\beta F[\rho(x)] = \int dx \rho(x)[1 - \log \rho(x)] + \frac{1}{2} \int dxdy \rho(x)\rho(y)[e^{-\beta v(x-y)} - 1]$$

Solve $\frac{\delta F[\rho(x)]}{\delta \rho(x)} = 0$ to find minima of $F[\rho(x)]$

Exact* solution for $d = \infty$ is possible, using your favorite method (we used replicas)

* *Exact for theoretical physics, not rigorous for the moment*

Why replicas? (no quenched disorder!)



Gibbs measure split in many glass states

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

Need replicas to average the log, self-induced disorder

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

Critical exponents of jamming

A short technical detour on the computation of exponents:

- In the replica language the Gardner phase is decribed by the Parisi fullRSB structure
  unexpected analogy between HS in $d \to \infty$ and the SK model!
  [Wyart, PRL 109, 125502 (2012)]
  [Muller, Wyart, arXiv:1406.7669]
- Order parameter is $\Delta(y)$ for $y \in [1, 1/m]$, the overlap probability distribution
- Coupled Parisi equation for $\Delta(y)$ and a function $P(y, f)$, probability of the forces
- At jamming, $m \to 0$, $y \in [1, \infty)$
- Scaling solution at large y: $\Delta(y) \sim y^{-1-c}$ and $P(y, f) \sim y^a p(f\, y^b)$
- a, b and c are related to κ, γ and θ
- Equation for $p(t)$ in scaling limit: boundary conditions give scaling relations for a, b, c
- One free exponent is fixed by the condition of marginal stability of the fullRSB solution

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