Exact computation of the critical exponents of the jamming transition

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Special thanks

Edan Lerner and Matthieu Wyart

Rome 3, June 5, 2014
Outline

1. Glass and jamming transitions

2. A theory of the jamming transition: large $d$ expansion

3. The Gardner transition and the critical exponents
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1. Glass and jamming transitions

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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

A 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, $\varphi_j$ 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)]
The jamming transition

Granular materials, emulsion droplets, colloidal suspensions, powders, ...
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)]
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 \( \varphi_j \), \( z = 2d \), 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 and jamming transitions

**Glass/jamming phase diagram**

- Statistical mechanics: introduce temperature $T$ and eventually send $T \to 0$

- The soft sphere model: $v(r) = \epsilon(1 - r/\sigma)^2 \theta(r - \sigma)$

- Two control parameters: $T/\epsilon$ and $\varphi = v_\sigma N/V$

- $T/\epsilon = 0$ & $\varphi < \varphi_j \leftrightarrow$ hard spheres

Jamming is a transition from “entropic” rigidity to “mechanical” rigidity
A theoretical description of the glass transition is difficult; and jamming happens inside the glass!

[Berthier, Jacquin, FZ, PRE 84, 051103 (2011)]
[Ikeda, Berthier, Sollich, PRL 109, 018301 (2012)]
Criticality around jamming

- In the glass the MSD has a plateau: diffusion is arrested, only vibrations
- The plateau value $\Delta_{EA}$ is the Debye-Waller factor
- Scaling $\Delta_{EA} \sim T^{\kappa/2} D[(\varphi - \varphi_j)/\sqrt{T}]$
- Shear modulus of the glass $\mu \sim T/\Delta_{EA}$ has a similar scaling
- At $\varphi = \varphi_j$ & $T = 0$, gap distribution $g(h) \sim h^{-\alpha}$ and force distribution $P(f) \sim f^\theta$

[Donev, Torquato, Stillinger, PRE 71, 011105 (2005)]
[Wyart, PRL 109, 125502 (2012)]
[Charbonneau, Corwin, Parisi, FZ, PRL 109, 205501 (2012)]
[Ikeda, Berthier, Biroli, JCP 138, 12A507 (2013)]
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- Three critical exponents $\kappa$, $\alpha$, $\theta$
- Scaling relations based on marginal mechanical stability of the packing
- $\alpha = 1/(2 + \theta)$ and $\kappa = 2 - 2/(3 + \theta)$
- Only one exponent remains undetermined
- Numerically $\alpha \approx 0.4$ in all dimensions, which implies $\theta \approx 0.5$ and $\kappa \approx 1.4$


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

- Liquid-glass and jamming are new challenging kinds of phase transitions

- Disordered system, no clear pattern 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
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Expansion around $d = \infty$ in statistical mechanics

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

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

Proposal: use $1/d$ as a small parameter [E. Witten, Physics Today 33, 38 (1980)].

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 and the values of $\kappa, \alpha, \theta$ are very weakly dependent on $d$.

[Goodrich, Liu, Nagel, PRL 109, 095704 (2012)]
[Charbonneau, Corwin, Parisi, FZ, PRL 109, 205501 (2012)]
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: $m = \tanh(\beta Jm)$
    (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

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  - DFT (Stoessel-Wolynes 1984)
  - MCT (Bengtzeliu-Götze-Sjolander 1984)
  - Replicas (Mézard-Parisi 1996, +FZ 2010)

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  - Ginzburg criterion, $d_u = 8$ (2007, 2012)
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  - Nucleation (RFOT) theory (KTW 1987)
Expansion around $d = \infty$ in statistical mechanics

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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):

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

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
1/d as a small parameter – amorphous hard spheres

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Why replicas? (no quenched disorder!)

Gibbs measure split in many glass states

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

Need replicas to average the log, self-induced disorder

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

Crucial result:

- A *Gardner transition* inside the glass phase
- Stable → marginally stable glass *in phase space*  
  \[ \text{[Gardner, Nucl.Phys.B 257, 747 (1985)]} \]
- The jamming line falls inside the marginal phase

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

- Neglecting the Gardner transition gives $\theta = 0$ and $\alpha = 1$: plain wrong
- Taking into account the Gardner transition gives correct values:
  $\kappa = 1.41574 \ldots$, $\alpha = 0.41269 \ldots$, $\theta = 0.42311 \ldots$
- Consistent with scaling relations $\alpha = 1/(2 + \theta)$ and $\kappa = 2 - 2/(3 + \theta)$
- $\alpha$ and $\kappa$ are perfectly compatible with the numerical values
- Some debate on $\theta$ in low dimensions
- 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

A short technical detour on the computation of exponents:

- In the replica language the Gardner phase is described by the Parisi fullRSB structure.
  Unexpected analogy between HS in $d \to \infty$ and the SK model!
  [Wyart, PRL 109, 125502 (2012)]

- 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 $\kappa$, $\alpha$ and $\theta$.

- 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]
Summary

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

- The $d = \infty$ phase diagram is qualitatively realized in finite $d$. Quantitative computations in finite $d$ are possible, in progress.

- 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 $\alpha, \theta, \kappa$.

- An unexpected connection between hard spheres in $d \to \infty$ and the SK model.

THANK YOU FOR YOUR ATTENTION.