Exact computation of the critical exponents of the jamming transition

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Special thanks Edan Lerner and Matthieu Wyart

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Outline

1. Glass and jamming transitions
2. A theory of the jamming transition: large d expansion
3. The Gardner transition and the critical exponents

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!

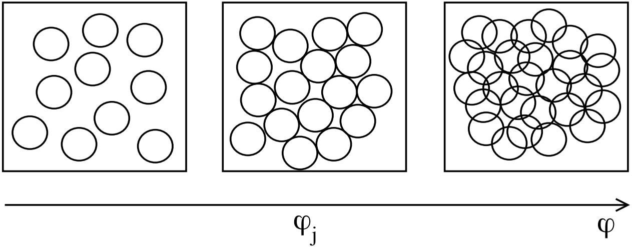
- No natural small parameter to construct a perturbative expansion
  Low density virial expansion: fails, too dense
  Harmonic expansion: fails, reference positions are not known
- Several processes simultaneously at work: crystal nucleation, ergodicity breaking, activated barrier crossing, dynamic facilitation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

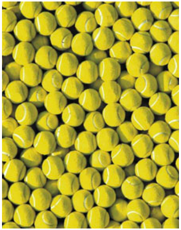
[Berthier, Biroli, RMP 83, 587 (2011)]

The jamming transition

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



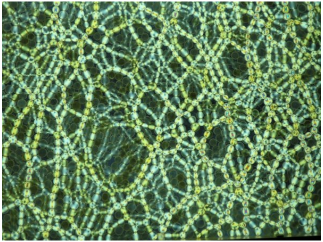


For hard spheres, φ_j is also known as *random close packing*: $\varphi_j(d = 3) \approx 0.64$

[Bernal, Mason, Nature 188, 910 (1960)]
[Liu, Nagel, Nature 396, 21 (1998)]
[O'Hern, Langer, Liu, Nagel, PRL 88, 075507 (2002)]

The jamming transition

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

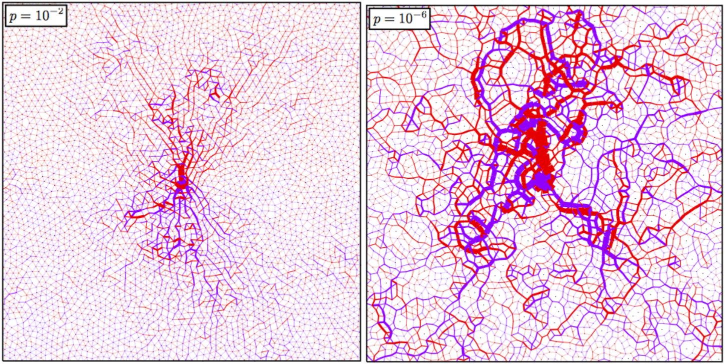


..., board games, ...

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

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 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

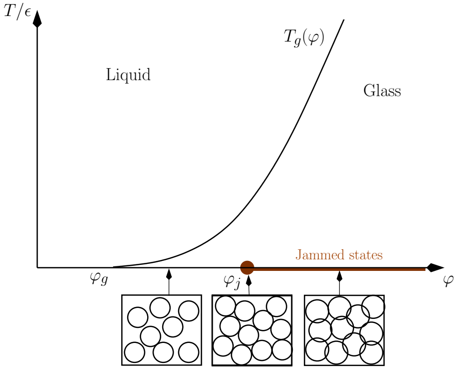
- Numerical simulations: $\delta z \sim |\varphi - \varphi_j|^\nu \rightarrow L^* \sim |\varphi - \varphi_j|^{-\nu}$, $\nu \approx 1/2$

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

- 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/ϵ and $\varphi = v_\sigma N/V$
- $T/\epsilon = 0$ & $\varphi < \varphi_j$ $\leftrightarrow$ hard spheres



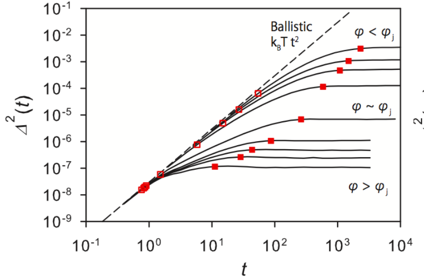
Jamming is a transition from "entropic" rigidity to "mechanical" rigidity
A theoretical description of the glass transition is difficult; and jamming happens inside the glass!

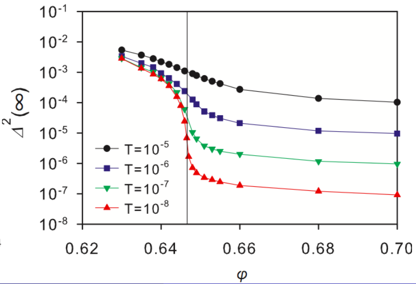
[Berthier, Jacquin, FZ, PRE 84, 051103 (2011)]
[Ikeda, Berthier, Sollich, PRL 109, 018301 (2012)]

Criticality around jamming

- In the glass the MSD has a plateau: diffusion is arrested, only vibrations
- The plateau value $\Delta_{\rm EA}$ is the Debye-Waller factor
- Scaling $\Delta_{\rm EA} \sim T^{\kappa/2} \mathcal{D}\big[(\varphi - \varphi_j)/\sqrt{T}\big]$
- Shear modulus of the glass $\mu \sim T/\Delta_{\rm EA}$ 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 κ, α, θ
- 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 $\kappa \approx 1.4$

`[DeGiuli, Lerner, Brito, Wyart, arXiv:1402.3834]`

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

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

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 κ, α, θ 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: $m = \tanh(\beta J m)$
  (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)
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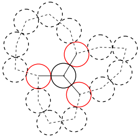
$1/d$ as a small parameter – amorphous hard spheres



- 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):

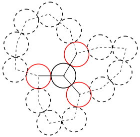
$$-\beta F[\rho(x)] = \int dx \rho(x)[1-\log\rho(x)] + \frac{1}{2}\int dxdy\rho(x)\rho(y)[e^{-\beta v(x-y)} - 1]$$

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*

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



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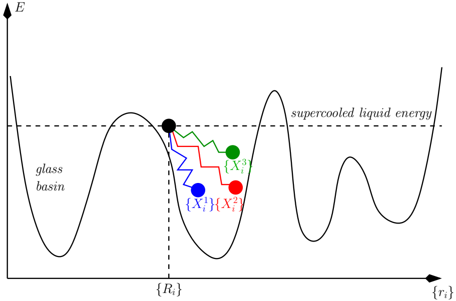
Why replicas? (no quenched disorder!)



Gibbs measure split in many glass states

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

Need replicas to average the log, self-induced disorder

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

Theory of glass/jamming: summary

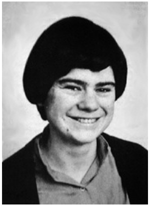
- A $1/d$ expansion around a mean-field solution is a standard tool when the problem lack a natural small parameter
- Hard spheres are exactly solvable when $d \to \infty$
  They have a glass phase and a jamming transition
- You can choose your preferred method of solution: replicas are convenient
-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

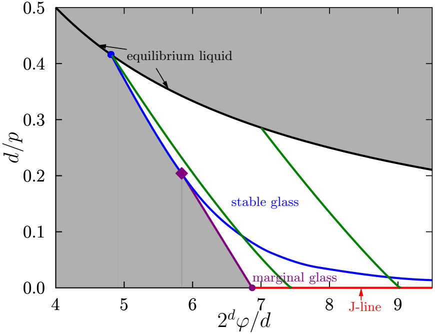
Outline

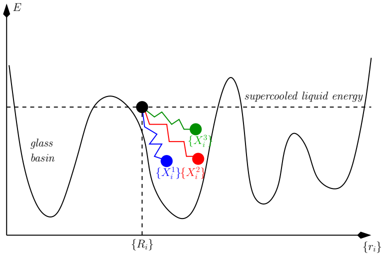
The phase diagram

Crucial result:

- A *Gardner transition* inside the glass phase
- Stable → marginally stable glass *in phase space*
  [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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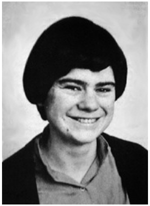

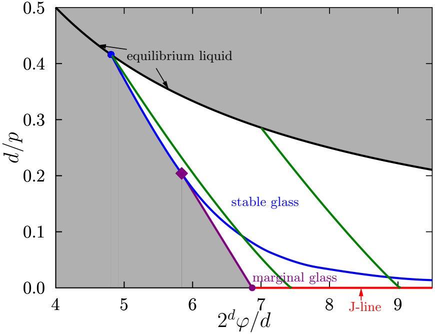

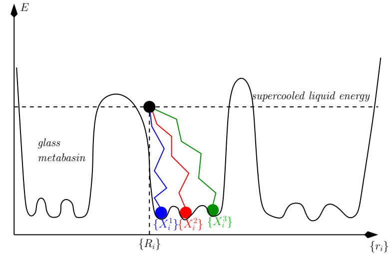

[Charbonneau, Kurchan, Parisi, Urbani, FZ, Nature Comm. 5, 3725 (2014)]

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 $\kappa = 2 - 2/(3+\theta)$
- α and κ are perfectly compatible with the numerical values
- Some debate on θ 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 decribed 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 κ, α 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]

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 α, θ, κ
- An unexpected connection between hard spheres in $d \to \infty$ and the SK model

THANK YOU FOR YOUR ATTENTION