Mean field theory of plasticity and yielding of glasses

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SIMONS FOUNDATION

Outline

1 Introduction

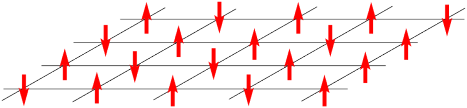
2 Methodology

3 Results: jamming and yielding of hard spheres

4 Conclusions

Introduction

A theoretical physicist's view of Magnetite: the Ising model



2−D Ising Model

I will talk about glasses at the same level of abstraction...

A logical 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

- 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)

- Large-scale fluctuations
  Ginzburg criterion, $d_u = 4$ (1960)
  Renormalization group (1970s)
  Nucleation theory (1960s)

Theory of the liquid-glass transition

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  Spontaneous replica symmetry breaking
  Order parameter: overlap matrix q_{ab}

- Quantitative MFT (exact for $d \to \infty$)
  Kirkpatrick and Wolynes 1987
  Kurchan, Parisi, FZ 2012

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

- Large-scale fluctuations
  Ginzburg criterion, $d_u = 8$ (2011)
  Renormalization group (in progress)
  Nucleation (RFOT) theory (KTW 1987)

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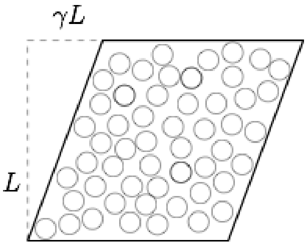
Goal

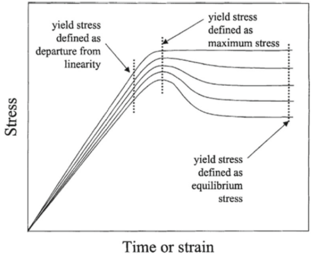
Plasticity and yielding of glasses are extremely interesting... you know why!

Goal: construct a *microscopic* statistical mechanics treatment of glasses under shear

In this talk I will focus on the solid phase, to which a fixed shear strain γ is applied adiabatically: a thermodynamic formulation is possible [Mezard, Yoshino, 2010]

I will not consider the flow regime where $\dot{\gamma} > 0$: need a fully dynamical treatment. Work in progress. Contact with MCT?
[Fuchs, Cates 2002, $\cdots$, Agoritsas, Biroli, Urbani, FZ, 2017]





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Main methodological ingredients

1. General scheme for thermodynamics in glasses: the “state following” formalism

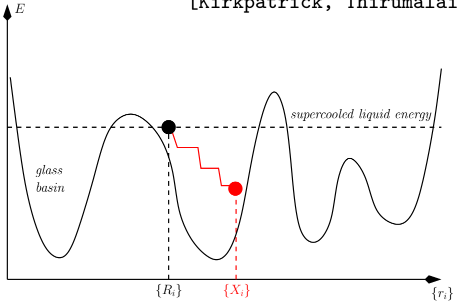
[Kirkpatrick, Thirumalai, Wolynes 1987-1989]
[Franz&Parisi, Monasson 1995]

2. Practical implementation: exact solution of glasses in the mean field limit $d \to \infty$

[Charbonneau, Kurchan, Parisi, Urbani, FZ 2012-2015]

The RFOT/MCT/energy landscape scenario for glasses

[Goldstein, Stillinger, Weber, Heuer et al. 1969 - ...]
[Bengtzelius, Gotze, Sjolander et al. 1984 - ...]
[Kirkpatrick, Thirumalai, Wolynes 1985-1989]



Consider an equilibrium liquid configuration $R = \{R_i\}$ of N particles: $P(R) \propto e^{-\beta_g H(R)}$

Make a copy of the system undergoing some dynamics, $X(t)$, such that $X(t=0) = R$.

- Supercooled liquid: $\langle [X(t) - R]^2 \rangle \to Dt$
- Glass: $\langle [X(t) - R]^2 \rangle \to \Delta_r$

In the glass, $X(t \to \infty)$ reaches an equilibrium *restricted* to a metastable state
This restricted equilibrium can be *followed* at different temperature, density, strain...

State following

- Restricted equilibrium with constraint $\langle (X-R)^2 \rangle = \Delta_r$
  $Z[T,\Delta_r|R] = \int dX e^{-\beta H[X]} \delta[(X-R)^2 - \Delta_r]$

- Glass free energy:
  $F_g[T,\Delta_r|T_g] = -T \int dR \frac{e^{-\beta H[R]}}{Z} \log Z[\Delta_r|R]$

  [Franz&Parisi, Monasson 1995]

- Technically, the average of the logarithm is computed using the replica method

- The problem becomes analytically tractable in the mean field limit of $d \to \infty$
  Only the first virial correction survives in this limit

  [Frisch, Rivier, Wyler 1985-1988]

- Generalised to the state following scheme, exact computation of F_g for arbitrary potential

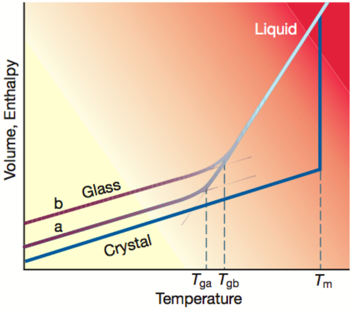
  [Charbonneau, Kurchan, Parisi, Urbani, FZ 2012-2015]
  [Rainone, Urbani, Yoshino, FZ 2015]

- The dynamics can also be solved exactly $\Rightarrow$ MCT-like equations

  [Barrat, Burioni, Mezard 1997]
  [Maimbourg, Kurchan, FZ 2015]

Practical implementation: simulation and experiment

- Main difficulty: by definition, we cannot equilibrate in the deeply supercooled liquid phase
- However: play with time scales
- Cool the system slowly; lowest equilibrium temperature when $\tau_\alpha(T_g) = \tau_{prod}$
- Use smart techniques (vapor deposition, swap algorithm...) to access lower T_g
- Once the system is equilibrated at T_g, work on time scales $\tau_{exp} \ll \tau_{prod} = \tau_\alpha(T_g)$
- The system is effectively confined in the glass state selected by the last equilibrated configuration R



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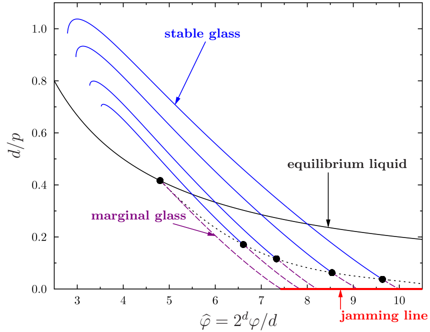
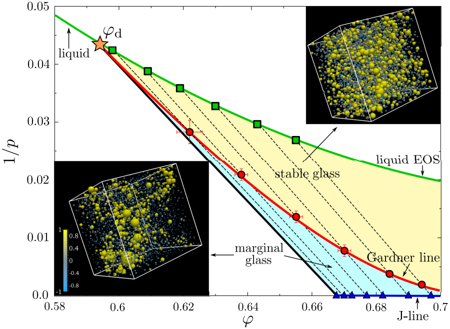
Phase diagram of unstrained hard spheres





Theory: monodisperse HS in $d = \infty$, state following

[Rainone, Urbani, Yoshino, FZ 2015]

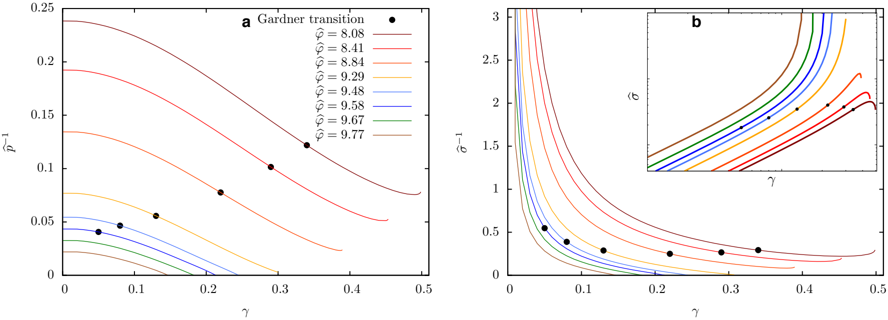
Numerical simulation: polydisperse HS in $d = 3$, swap + MD

[Berthier, Charbonneau, Jin, Parisi, Seoane, FZ 2016]

Experiment: shaken bidisperse granular system

[Seguin, Dauchot 2016]

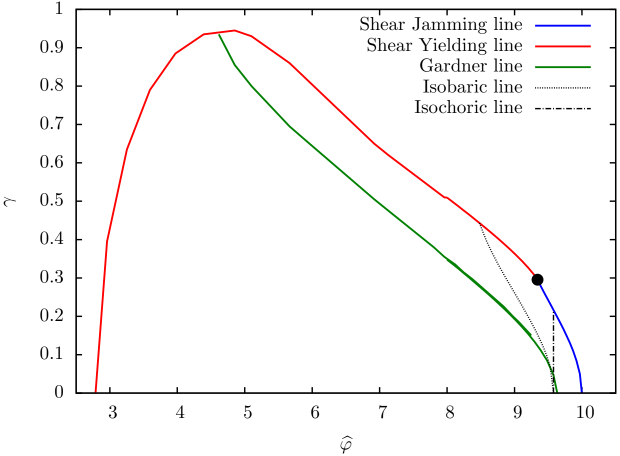
Applying shear strain to the glass: theory



Dilatancy, shear yielding, shear jamming, marginal stability

[Urbani, FZ 2017]

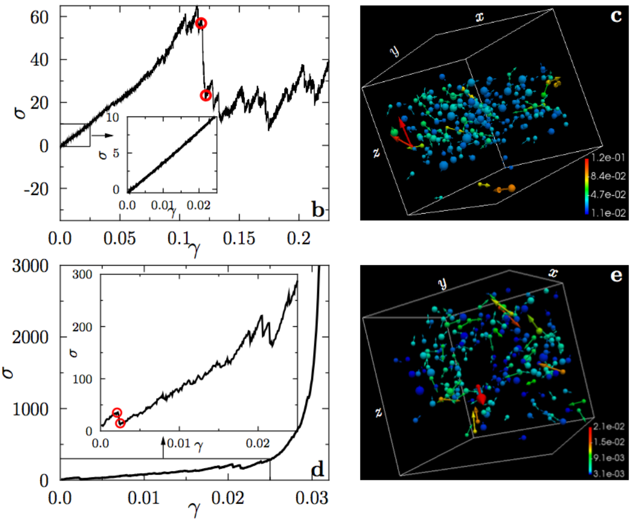
Applying shear strain to the glass: theory



Phase diagram of strained glass – a new critical point

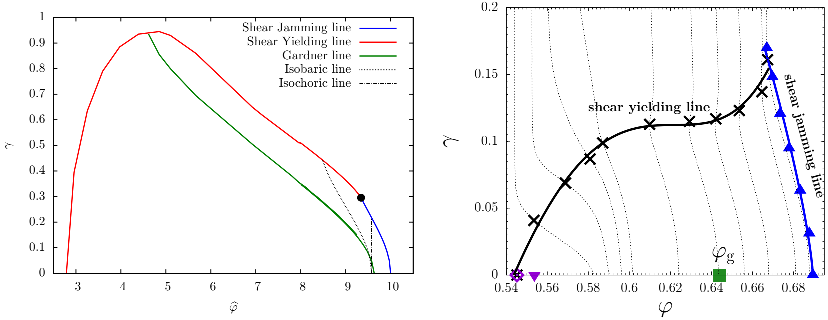
[Urbani, FZ 2017]

Applying shear strain to the glass: numerical simulations



[Jin, Yoshino 2017]

Applying shear strain to the glass: numerical simulations



[Jin, Urbani, Yoshino, FZ, preliminary]

The shear yielding point is a homogeneous spinodal in mean field
A first order transition in 3d? (shear banding = nucleation?)

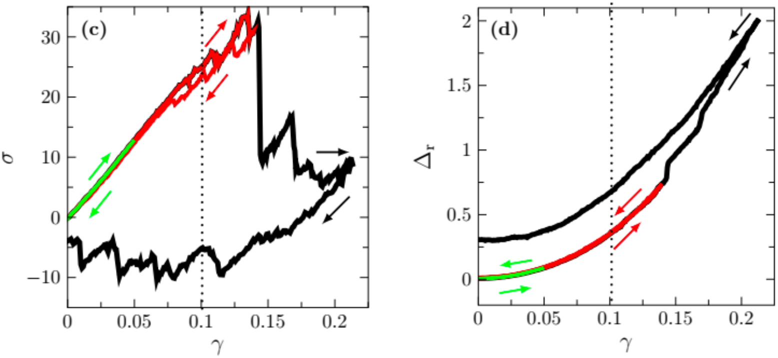
[Jaiswal, Procaccia, Rainone, Singh 2017]

Applying shear strain to the glass: numerical simulations

■ Reversibility to HOME (the reference liquid state)

$\varphi_g = 0.655 \qquad \varphi = 0.66 \qquad \gamma_G = 0.1$

MSD to the initial state



[Jin, Urbani, Yoshino, FZ, preliminary]

The marginally stable phase: additional results

Analytical prediction about the behavior of non-linear elastic moduli $\sigma = \sum_n \mu_n \gamma^n$:

$$\overline{(\delta\mu_n)^2} \sim \frac{V^{(2n-1)/3}}{V}$$

Breakdown of standard elasticity

[Biroli, Urbani, 2016]

Analytical prediction for the distribution of avalanches, with $P(S) \sim S^{-\tau}$ at small S
$\tau = 1$ above jamming, $\tau = 1.41$ exactly at jamming
Compares well with numerics around jamming

[Franz, Spigler, 2017]

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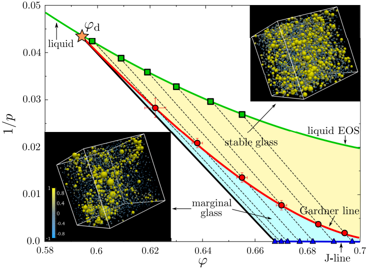
Summary

- A single mean-field theoretical framework ($d = \infty$) to describe: dilatancy, shear yielding, shear jamming, marginal stability, plasticity, avalanches, non-linear elasticity...
- Yielding is a homogeneous spinodal: challenging to go beyond mean field
- Theory relies on a very strong separation of time scales: $\tau_{exp} \ll \tau_{prod} = \tau_\alpha(\varphi_g)$
- Achieved in numerical simulations by swap algorithm: agreement with theory, sharp phase transitions
- Difficult to achieve in colloidal/granular glasses: much more difficult to separate the various phenomena



Perspectives

Extension to soft spheres:

- Localised excitations in low d
- High energy states: localised plasticity, then soft yielding
- Low energy states: no plasticity, sharp yielding

Extension to sticky hard spheres:

- Gel phases, two step yielding, ...

Dynamical regime:

- Write dynamical equations in $d \to \infty$, out of equilibrium with finite $\dot{\gamma}$: almost done
- Solve these equations... very difficult!

Field theory of the yielding transition:

- Spinodal with disorder: study upper critical dimension, susceptibilities...

Thank you for your attention!

THE END