2014 Sept 12th "Critical Phenomena in Random and Complex Systems" Capri

# Twisting and breaking glasses: a replica approach

#### Hajime Yoshino Cybermedia Center, Osaka Univ.

HY and F. Zamponi, "The shear modulus of glasses: results from the full replica symmetry breaking solution", Phys. Rev. E 90, 022302 (2014).

See also the Poster by Corrado Raione

Collaborators

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Replica trick to compute shear-modulus ex. 3D soft-core system  $v(r) \sim r^{-12}$ 

Shear-modulus of Hard-sphere glass in large-D limit

Finite temperature MD simulation of aging in a jamming system

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State following approach via Franz-Parisi potential

#### Financial Supports

Synergy of Fluctuation and Structure : Quest for Universal Laws in Non-Equilibrium Systems 2013-2017 Grant-in-Aid for Scientific Research on Innovative Areas, MEXT, Japan



JPS Core-to-Core program 2013-2015 Non-equilibrium dynamics of soft matter and information





# Outline

## Introduction:

- Shear on the cloned liquid in the large-d limit (theory)
- Second Second
- Discussions

## Glass transition



Supercooled liquids

Vibrations within cages  $\beta$  - relaxation



Structural relaxation α-relaxation

Confocal scope image (E. Weeks and D. Weitz (2002))

#### Shear modulus: a paradox and a lesson



Intra-state and inter-state responses under shear (IRSB)

H.Yoshino and M. Mézard, Phys. Rev. Lett. 105, 015504 (2010).



C.F. step-wise magnetic response in spin-glasses : H.Y. and T. Rizzo, Phys. Rev. B 77, 104429 (2008).

stress-strain curve



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#### Introduction:

- Shear on the cloned liquid in large-d limit (theory)
- Aging around the jamming point (simulation)

## Discussions

J. Kurchan, G. Parisi and F. Zamponi, J. Stat. Mech. P10012 (2012).

J. Kurchan, G. Parisi, P. Urbani and F. Zamponi, J. Chem. Phys. B117, 1279 (2013).

P. Charbonneau, J. Kurchan, G. Parisi, P. Urbani, F. Zamponi, arXiv:1310.2549 .

P. Charbonneau, J. Kurchan, G. Parisi, P. Urbani, F. Zamponi, Nature Communications 5, 3725 (2014).

H. Yoshino and F. Zamponi, Phys. Rev. E 90, 022302 (2014).

#### Basic idea of cloned liquid

m-replicas obeying the same Hamiltonian

$$\begin{array}{ll} \mathbf{x}_{i}^{a} & i=1,2,\ldots,N & a=1,2,\ldots,m \\ & \text{``Cage size''} & \Delta = \langle (x_{i}^{a}-x_{i}^{b})^{2} \rangle & {}^{H}={}^{H_{0}}-\frac{\epsilon}{4}\sum_{i}\sum_{a,b}\langle (\mathbf{x}_{i}^{a}-\mathbf{x}_{i}^{b})^{2} \rangle \\ & \text{liquid} & \Delta = \infty & \text{solid} & \Delta < \infty \end{array}$$



Edwards-Andeson Order Parameter (non-ergodicity order parameter)

$$q_{\rm EA} = \lim_{t \to \infty} \frac{1}{N} \sum_{i=1}^{N} \langle s_i(t) s_i(0) \rangle = \frac{1}{N} \sum_{i=1}^{N} \langle s_i \rangle^2$$

#### Repulsive contact systems

Repulsive colloids, emulsions, granular matter,..

Model potential energy





E. R. Weeks, in "Statistical Physics of Complex Fluids", Eds. S Maruyama & M Tokuyama (Tohoku University Press, Sendai, Japan, 2007).

$$U = \sum_{\langle ij \rangle} v(r_{ij}) \qquad r_{ij} = |\mathbf{r}_i - \mathbf{r}_j|$$
$$v(r) = \epsilon (1 - r/D)^{\alpha} \theta (1 - r/D)$$

$$\lim_{T \to 0} e^{-v(r)/k_{\rm B}T} = \theta(r/D - 1)$$

Essentially "hard-spheres" at low temperatures.

## Mean-field phase diagram

Cloned liquid theory (replica + liquid theory)

G. Parisi and F. Zamponi, Rev. Mod. Phys. 82, 789 (2010)

L. Berthier, H. Jacquin and Z. Zamponi, Phys. Rev. Lett. 106, 135702 (2011) and Phys. Rev. E 84, 051103 (2011).



#### Experiment: rigidity of emulsions

T. G. Mason, Martin-D Lacasse, Gary Grest, Dov Levine, J Bibette, D Weitz, Physical Review E 56, 3150 (1997)



Interaction between emulsions:  $v(r)/\epsilon = (1 - r/\sigma)^{\alpha}$   $\alpha > 2?$ M-D. Lacasse, G. S. Grest, D. Levin, T. G. Mason and D. A. Weitz, PRL **76**,3448 (1996)  $\alpha = 2$ I. J. Jorjadze, L-L. Pontani and J. Brujic, PRL **111**, 048302(2013). Istep RSB approximation

H. Yoshino, AIP Conference Proceedings 1518, 244 (2013)

S. Okamura and H. Yoshino, arXiv:1306.2777 (2013).

$$\lim_{T \to 0} \beta \hat{\mu} = \frac{1}{m^*} \left( \frac{A^*}{m^*} \right) \frac{6\phi}{\pi} y_{\text{liq}}^{HS} (\phi_{\text{GCP}})^3 \left[ c_1 - c_2 \sqrt{\frac{A^*}{m^*}} + \dots \right]$$

ex. Soft-particle case  $\alpha = 2$  (3-dim) Berthier-Jacquin-Zamponi (2011)  $\phi_{\rm GCP} = 0.633353..$   $A^*/m^*(\phi_{\rm GCP}) \simeq 9.72187 \times 10^{-5}$   $y_{\rm liq}^{\rm HS}(\phi_{\rm GCP}) \simeq 23.6238$ 

|Harmonic approx.vs IRSB approx. (2012)  $\delta \phi = \phi_{\rm J} - \phi \quad P \propto T/|\delta \phi|$ "unjammed" side  $\delta \phi < 0$ "inherent structures" 'meta-basins" (1RSB)  $\mu_{
m harmonic} \propto T/|\delta\phi|^{3/2}$  shear-modulus  $\lim_{T \to 0} \mu(T) \propto T/|\delta\phi|$ Yoshino (2012), Okamura-Yoshino (2013) Brito-Wyart (2006)  $\lim_{T \to 0} \Delta(T) \propto |\delta \phi|$  $\Delta_{\rm harmonic} \propto |\delta \phi|^{3/2}$ cage size Berthier-Jacqin-Zamponi (2011) Ikeda-Berthier-Birol (2013) **Emulsion experiments:** T. G. Mason et al (1997). Guerra-Weitz (2013)

Gardner transition! J. Kurchan, G. Parisi and F. Zamponi, J. Stat. Mech. P10012 (2012).



Emulsion experiments: T. G. Mason et al (1997). Guerra-Weitz (2013)

#### • AT instability - Gardner's transition

JRL De Almeida and D. J. Thouless, Journal of Physics A: Math. Gen. 11, 938 (1978) E. Gardner, Nucl. Phys. B 257, 747 (1985).

J. Kurchan, G. Parisi, P. Urbani, and F. Zamponi, J. Phys. Chem. B 117, 12979 (2013).



# Replicated liquid theory of hard spheres $\ d ightarrow \infty$

molecule made of replicas

J. Kurchan, G. Parisi and F. Zamponi, J. Stat. Mech. P10012 (2012).

P. Charbonneau, J. Kurchan, G. Parisi, P. Urbani, F. Zamponi, Nature Communications 5, 3725 (2014).

$$\overline{x} = \{x_1 \cdots x_m\}$$
  $x_a = ((x_a)_1, (x_a)_2, \dots, (x_a)_m)$ 

$$-\beta F = \int d\overline{x}\rho(\overline{x})[1 - \log\rho(\overline{x})] + \frac{1}{2} \int d\overline{x}d\overline{y}\rho(\overline{x})\rho(\overline{y})f(\overline{x},\overline{y})$$
Replicated Mayer function
$$f(\overline{x},\overline{y}) = -1 + \prod_{a=1}^{m} e^{-\beta v(|(x_a - y_a)|)}$$
Contact potential

## 1+continuous Replica Symmetry Breaking



(note) Spinglass case : G. Parisi (1980) massless "replicon" mode, marginal stability

#### Response in hierarchical energy landscape



#### Response of "cloned system" in hierarchical energy landscape

RSB case : H. Yoshino and M. Me´zard, Phys. Rev. Lett. 105, 015504 (2010)



# Twist on the replicated liquid

$$\begin{split} u^{a} & & & \\ & & & \\ & & & \\ & & & \\ & & & \\ & & -\beta F(\{\gamma_{a}\}) = \int d\overline{x}\rho(\overline{x})[1 - \log\rho(\overline{x})] + \frac{1}{2}\int d\overline{x}d\overline{y}\rho(\overline{x})\rho(\overline{y})f_{\{\gamma_{a}\}}(\overline{x},\overline{y}) \\ & &$$

$$-\beta F(\hat{\alpha}, \{\gamma_a\})/N = 1 - \log \rho + d\log m + \frac{d}{2}(m-1)\log(2\pi eD^2/d^2) + \frac{d}{2}\log\det(\hat{\alpha}^{m,m}) \\ -\frac{d}{2}\widehat{\varphi}\int\frac{d\lambda}{\sqrt{2\pi}}\mathcal{F}\left(\Delta_{ab} + \frac{\lambda^2}{2}(\gamma_a - \gamma_b)^2\right)$$

Small strain expansion

$$F(\{\gamma_a\})/N = F(\{0\})/N + \sum_{a=1}^{m} \sigma_a \gamma_a + \frac{1}{2} \sum_{a,b}^{1,m} \mu_{ab} \gamma_a \gamma_b + \cdots$$

yields shear-modulus matrix

$$\beta \mu_{ab} = \frac{d}{2} \widehat{\varphi} \begin{bmatrix} \delta_{ab} \sum_{c(\neq c)} \frac{\partial \mathcal{F}}{\partial \Delta_{ac}} - (1 - \delta_{ab}) \frac{\partial \mathcal{F}}{\partial \Delta_{ab}} \end{bmatrix} \quad \text{``sum rule''} \quad \sum_{b} \mu_{ab} = 0$$
$$\beta \widehat{\mu}(y) = \frac{1}{m\gamma(y)} \quad \Delta(y) = \frac{\gamma(y)}{y} - \int_{y}^{1/m} \frac{dz}{z^{2}} \gamma(z) \quad \text{for} \quad y = x/m$$

Hierarchical RSB



Hierarchical rigidity

$\mu_2$	$\mu_1$	$\mu_0$	
$\mu_1$	$\mu_2$		
$\mu_0$		$\mu_2$	$\mu_1$
		$\mu_1$	$\mu_2$

IRSB case : HY and M. Mezard (2010), HY (2012)

m < x < 1



$$\beta \widehat{\mu}_{ab} = \beta \widehat{\mu}_{\rm EA} \left( \delta_{ab} - \frac{1}{m} \right)$$

step RSB

H. Yoshino and M. M'ezard, PRL 105, 015504 (2010).

H. Yoshino, The Journal of Chemical Physics 136, 214108 (2012).

$$\beta \hat{\mu}_{\text{EA}} = \widehat{\Delta}_{\text{EA}}^{-1} \qquad \widehat{\Delta}_{\text{EA}} \sim \widehat{\Delta}_d - C(\widehat{\varphi} - \widehat{\varphi}_d)^{1/2}$$

in agreement with MCT

W. Gotze, Complex dynamics of glass-forming liquids: A mode-coupling theory, vol. 143 (Oxford University Press, USA, 2009).G. Szamel and E. Flenner, PRL 107, 105505 (2011).



#### $\widehat{\varphi}_{\mathrm{Gardner}} < \widehat{\varphi} < \widehat{\varphi}_{\mathrm{GCP}}$



+continuous RSB

Effective medium approach + numerical simulation

E DeGiuli; E Lerner; C Brito; M Wyart, arXiv: I 4023834

"'Following glassy states" under perturbation

$$S. Franz and G. Parisi, J. Phys. I France 5 (1995) 1401.$$
F. Krzakala and L. Zdeborova, Eur. Phys. Lett., 90 (2010) 66002.  

$$\sum_{\substack{i=a \to 0^+ N \to \infty}} \sum_{slave : "m+1"th replica} \sum_{i=a \to \infty} \sum_{j=1}^{m} \frac{1}{Z_m} \int_{\mathbf{r}^1, \dots, \mathbf{r}^m} e^{-\beta \sum_{a=1}^m H[\mathbf{x}^a]} \log Z^e(\gamma)$$
Franz-Parisi potential  

$$NV_{FP}(\gamma) = \langle \log Z^e(\gamma) \rangle_m \equiv \frac{1}{Z_m} \int_{\mathbf{r}^1, \dots, \mathbf{r}^m} e^{-\beta \sum_{a=1}^m H[\mathbf{x}^a]} \log Z^e(\gamma)$$

$$Z^e(\gamma) = \log \int_{\mathbf{r}^m + 1} e^{-\beta H[\{\mathbf{r}_i^{m+1}\}; \gamma]} H[\{\mathbf{r}_i\}] = \sum_{i < j} v(\mathbf{r}_i - \mathbf{r}_j)$$

$$-\beta F_{FP}(\gamma) = \log \int_{r^1 \dots r^m, r^{m+1} \dots r^{m+s}} e^{-\beta \sum_{a=1}^m H[\{\mathbf{r}^a\}] - \beta \sum_{b=m+1}^{m+s} H[\{\mathbf{r}^b\}, \gamma]}$$

$$= \log \int_{r^1 \dots r^m} e^{-\beta \sum_{a=1}^m H[\mathbf{r}^a]} (Z^e(\gamma))^s$$

$$-\beta F_{FP}(\gamma) = \log Z_m + sNV_{FP}(\gamma) + O(s^2).$$

#### Nonlinear response - yielding

"state following under (de)compression/shear" via Franz-Parisi potential

C. Raione, P. Urbani, H. Yoshino and F. Zamponi, submitted



See the Poster by Corrado Raione



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$$\varphi = 0.67 \quad k_{\rm B}T/\epsilon = 10^{-5}$$



 $t_{\rm w} = 3 \times 10^2, 10^3, 3 \times 10^3, 5 \times 10^3, 10^4, 3 \times 10^4, 10^5$ 

$$\varphi = 0.67 \quad k_{\rm B}T/\epsilon = 10^{-5}$$

$$\sigma(\tau; t_{\rm w})/\gamma \qquad \text{FDT}$$

$$\sigma(\tau; t_{\rm w})/\gamma \qquad \text{FDT}$$

$$0.1 \qquad 0.1 \qquad$$

7

 $t_{\rm w} = 3 \times 10^2, 10^3, 3 \times 10^3, 5 \times 10^3, 10^4, 3 \times 10^4, 10^5$ 

#### Discussion : fluctuation within meta-basin





# Summary

# Response to shear of a hard-sphere glass in large-dimensional limit

- 1. Exact free-energy functional under shear
- 2. Analysis of shear-modulus

\* 1RSB - jump + square-root singularity at Td \*1+continuous RSB - (1) hierarchy of rigidities (2) anomalous scaling as  $\widehat{\varphi} \to \widehat{\varphi}_J$ 

3. State following under shear - observation of the yield process