“Physics of glassy and granular materials” Satellite meeting of STATPHYS25

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On the rigidity of jamming systems at finite temperatures

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Satoshi Okamura and Hajime Yoshino, arXiv:1306:2777

科研費 KAKENHI

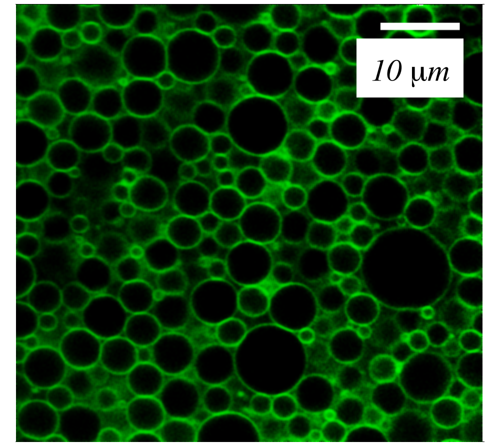
Outline

- Background
- Shear-modulus of a thermalized jamming system : cloned liquid approach
- MD simulations of stress-relaxations : response and correlation
- Discussions

Repulsive contact systems

Room temperature

$$k_{\mathrm{B}}T/\epsilon \sim 10^{-5}$$

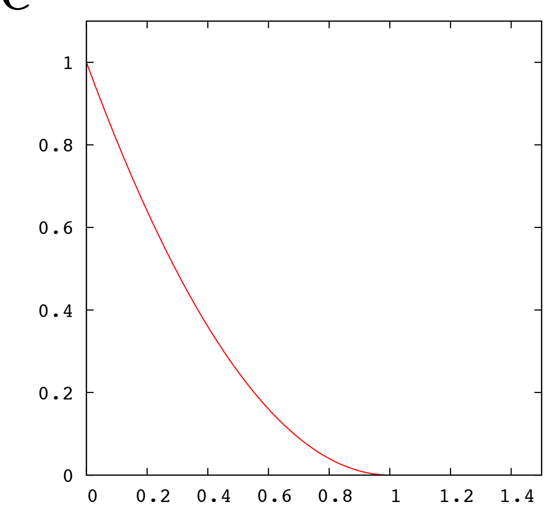


Emulsions

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

A simplified model

$v(r)/\epsilon$



r/σ

$$U = \sum_{\langle ij \rangle} v(r_{ij}) \qquad r_{ij} = |\mathbf{r}_i - \mathbf{r}_j|$$

$$v(r) = \epsilon(1 - r/\sigma)^2 \theta(1 - r/\sigma)$$

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

Essentially “hard-spheres” at low temperatures.

Unharmonicity, floppiness, marginal stability..

C. F. Schreck, T. Bertrand, C. S. O’Hern, and M. D. Shattuck, Phys. Rev. Lett. 107, 078301 (2011).

M. Wyart, Phys. Rev. Lett. 109, 125502 (2012).

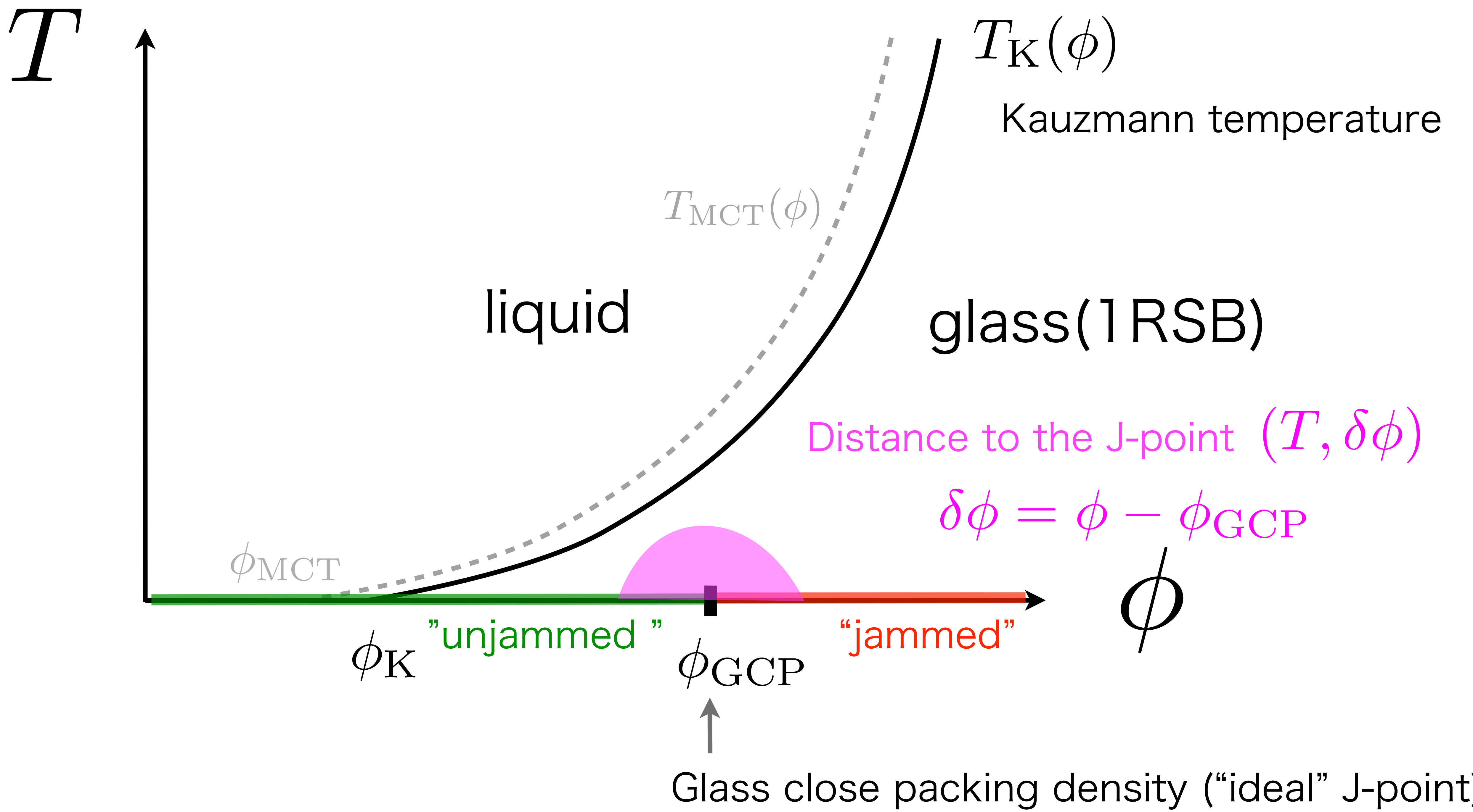
E. Lerner, G. During and M. Wyart arXiv.1302.3990

J. Kurchan, G. Parisi, P. Urbani and F. Zamponi, arXiv.1303.1028

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).

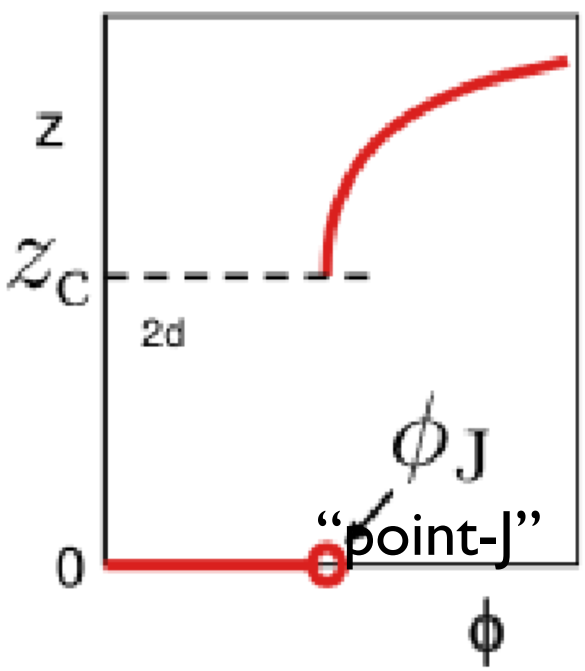


Possibility of 1+continuous RSB: J. Kurchan, G. Parisi, P. Urbani and F. Zamponi, arXiv.1303.1028

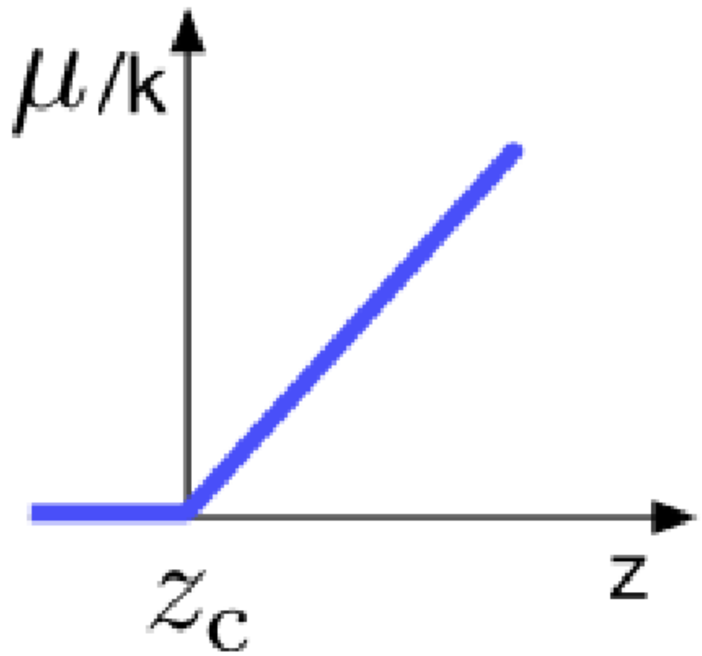
Behavior of static quantities at T=0 (Friction less systems)

Review: M. Van Hecke, J. Phys.: Condens. Matter 22 033101 (2010).

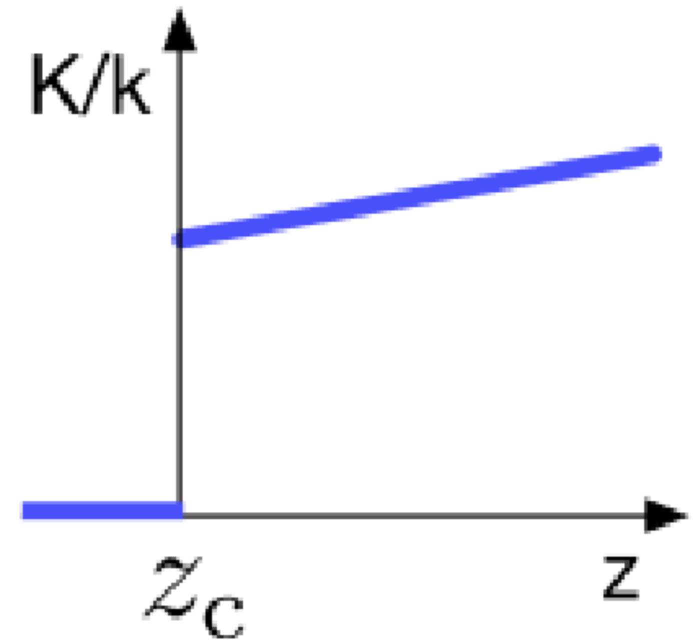
Average contact number



Shear-modulus



Bulk modulus



$$z - z_c \propto \sqrt{\phi - \phi_J}$$

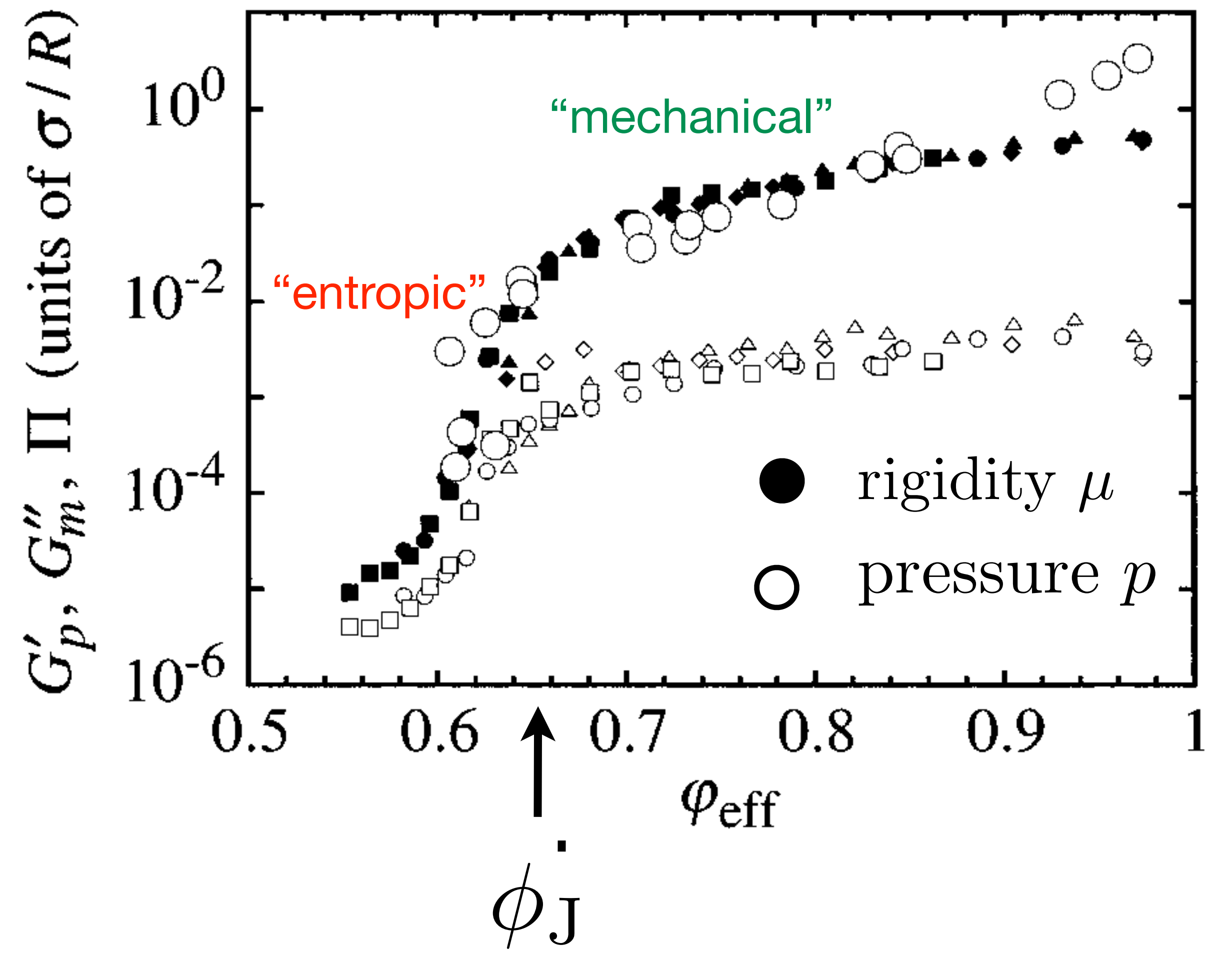
$k = \epsilon$ in the present system (harmonic sphere)

$$\mu \propto \sqrt{\phi - \phi_J} \qquad P = \phi - \phi_J$$

$$\mu \gg P$$

Experiment: rigidity of emulsions

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



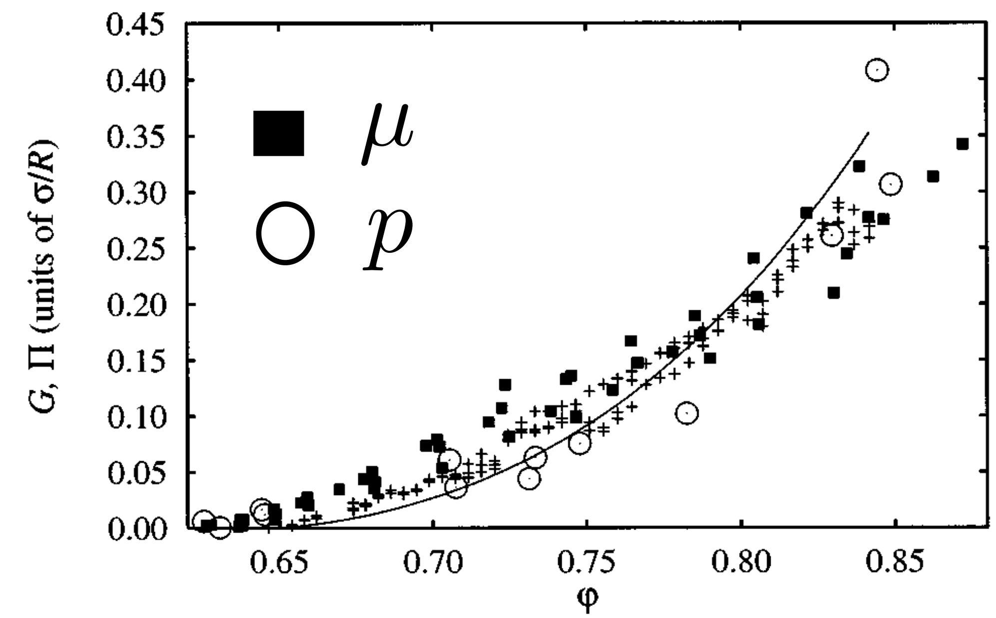


FIG. 1. The scaled shear modulus and osmotic pressure as a function of φ. The computed scaled static shear modulus $G/(\sigma/R)$ (+) and osmotic pressure $\Pi/(\sigma/R)$ (line), as obtained from the model presented in Sec. IV B 2, are compared with the experimental values of $G'_p(\varphi_{\rm eff})$ (■) and $\Pi(\varphi_{\rm eff})$ (○).

rigidity (shear-modulus) pressure

$$\mu \sim p$$

measurements at room temperature

$$k_{\rm B}T/\epsilon \sim 10^{-5}$$

Why not $\mu \propto \sqrt{\phi - \phi_{\rm J}}$?

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).

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The fluctuation formula of the rigidity and its T=0 limit

Rigidity — Born term — non-Affine correction

$$\mu = b - N\beta\left(\langle\sigma^2\rangle - \langle\sigma\rangle^2\right)$$

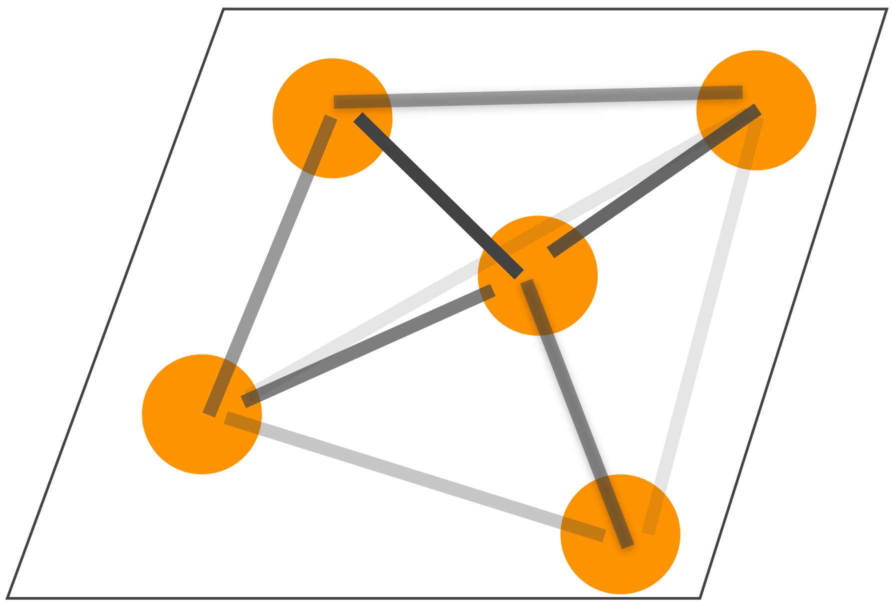
Harmonic expansion around energy minima (Lutsko 1989, Maloney-Lemaitre 2004,..)

$$\beta\left(\langle\sigma^2\rangle - \langle\sigma\rangle^2\right) = \frac{1}{N}\sum_{i=1}^{N}\vec{\Xi}_i\cdot(H^{-1}\vec{\Xi})_i + O(T) + \cdots$$

unharmonic corrections

corrections via "plasticity"

effective random spring model



$$\sigma = \frac{1}{N}\sum_{i<j}\sigma_{ij} \qquad \sigma_{ij} = r\frac{dv(r)}{dr}\bigg|_{r=r_{ij}} \frac{x_i - x_j}{r_{ij}}\frac{z_i - z_j}{r_{ij}}$$

$$\vec{\Xi}_i = \sum_{j(\neq i)}\nabla\sigma_{ij} \qquad H_{ij}^{\mu\nu} = \sum_{k<l}\frac{\partial^2 v(r_{kl})}{\partial x_i^{\mu} x_j^{\nu}}$$

rigidity of an inherent structure

$$\mu_{\rm IS} = b_{\rm IS} - \frac{1}{N}\sum_{i=1}^{N}\vec{\Xi}_i\cdot(H^{-1}\vec{\Xi})_i$$

Reformulation of the fluctuation formula

D. R. Squire and A. C. Holt and W. G. Hoover Physica 42, 388(1969).

$$\mu = \mu_{\mathrm{born}} - \frac{\beta}{V} \sum_{\langle kl \rangle} \sum_{\langle mn \rangle} \left(\langle \sigma(\mathbf{r}_{kl}) \sigma(\mathbf{r}_{mn}) \rangle - \langle \sigma(\mathbf{r}_{kl}) \rangle \langle \sigma(\mathbf{r}_{mn}) \rangle \right)$$

$$\mu_{\mathrm{born}} \equiv \frac{1}{V} \sum_{\langle ij \rangle} \hat{z}^2 [r^2 \frac{d^2 v(r)}{dr^2} \hat{x}^2 + r \frac{dv(r)}{dr} (1 - \hat{x}^2)].$$

$$\sigma(\mathbf{r}) \equiv \hat{z} \hat{x} r \frac{dv(r)}{dr}$$

↓

(c.f) G. Farago and Y. Kantor, PRE, 2478 (2000).

H. Yoshino, AIP Conf. Proc, 1518, 244 (2013) (arXiv:2012.6826).
(Simplification in Isotropic systems)

$$\beta\mu = \frac{1}{V} \left[\sum_{\langle kl \rangle} \langle \beta\sigma(\mathbf{r}_{kl}) \rangle^2 - \sum_{\langle kl \rangle} \sum_{\langle mn \rangle \neq \langle kl \rangle} \left(\langle \beta\sigma(\mathbf{r}_{kl}) \beta\sigma(\mathbf{r}_{mn}) \rangle - \langle \beta\sigma(\mathbf{r}_{kl}) \rangle \langle \beta\sigma(\mathbf{r}_{mn}) \rangle \right) \right]$$

Computation of the shear-modulus via cloned liquid approach

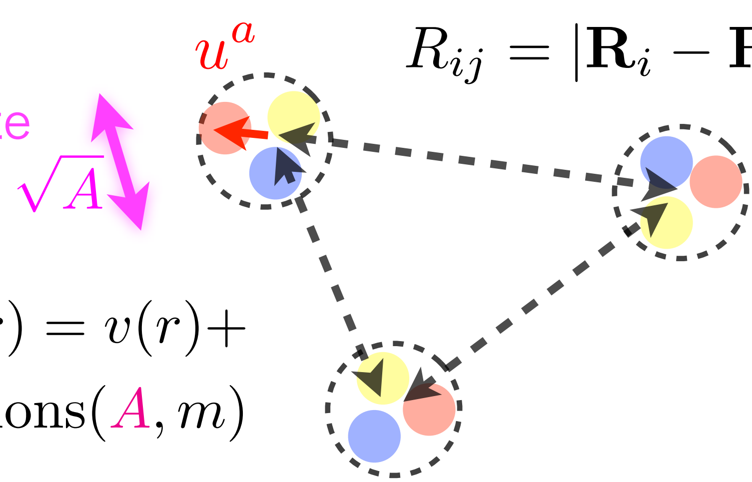
Put shear on replicated liquid

M. Mezard and G. Parisi, J. of Chem. Phys. 111 (1999) 1076
G. Parisi and F. Zamponi, Rev. Mod. Phys. 82, 789 (2010).

$$\beta\mu_{ab} = \frac{1}{V}\left[\sum_{\langle kl\rangle}\langle\beta\sigma(\mathbf{r}^a_{kl})\rangle\langle\beta\sigma_b(\mathbf{r}^b_{kl})\rangle\right.$$

$$\left.-\sum_{\langle kl\rangle}\sum_{\langle mn\rangle\neq\langle kl\rangle}(\langle\beta\sigma(\mathbf{r}^a_{kl})\beta\sigma(\mathbf{r}^b_{mn})\rangle - \langle\beta\sigma(r^{\mathbf{a}}_{kl})\rangle\langle\beta\sigma(r^b_{mn})\rangle)\right]$$

switch-on cloning (1step RSB)..



$$R_{ij} = |\mathbf{R}_i - \mathbf{R}_j|$$

$$\mathbf{r}^a_i = \mathbf{R}_i + \mathbf{u}^a_i \qquad \mathbf{R}_i \equiv \frac{1}{m}\sum_{a=1}^{m}\mathbf{r}^a_i$$

$$v_{\rm eff}(r) = v(r) + \text{corrections}(A, m)$$

$$\langle(\mathbf{u}^a_i)^\mu\rangle_{\rm cage} = 0 \qquad \langle(\mathbf{u}^a_i)^\mu(\mathbf{u}^b_j)^\nu\rangle_{\rm cage} = A(\delta_{ab} - \frac{1}{m})\delta_{\mu\nu}\delta_{ij}$$

the rigidity matrix becomes..

Intra-state modulus (plateau modulus)

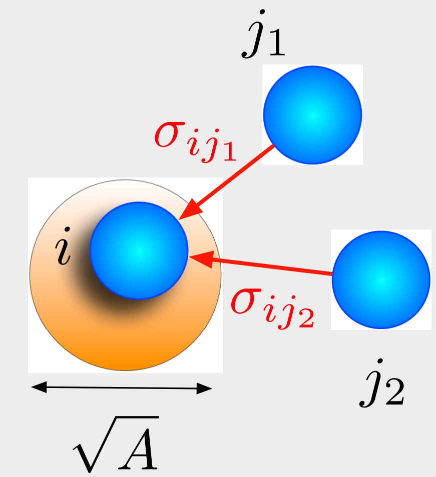
$$\mu_{ab} = \hat{\mu}(\delta_{ab} - \frac{1}{m})$$

Hajime Yoshino and Marc Mézard, Phys. Rev. Lett. 105, 015504 (2010),
Hajime Yoshino, J. Chem. Phys. 136, 214108 (2012).

See also Talk by G. Szamel, tomorrow

Rigidity at low temperatures

Intra-state modulus (plateau modulus)



$$T^* = \frac{T}{m}$$

At 0-th order, no rigidity!

The non-vanishing contribution starts at first order of the cage expansion.

$$\beta\hat{\mu} = -A\frac{\rho}{V}\int d^d r_0 d^d r_1 d^d r_2 \left(\nabla_0^a \cdot \nabla_0^b\right) \beta\sigma(\mathbf{r}_{01}^a)\beta\sigma(\mathbf{r}_{02}^b) g_3(r_{01}^a, r_{02}^b, r_{12}; T^*)\Big|_{\mathbf{r_{01}^a}=\mathbf{r}_{01}, \mathbf{r_{02}^b}=\mathbf{r}_{02}} + \ldots \qquad (a \neq b)$$

$$\simeq -\frac{A}{m^2}\rho\int dr_1 dr_2 d\Omega_1 d\Omega_2 \nabla_1 \left[\hat{x}_1\hat{z}_1 r_1 \Delta(r_1;T^*)y(r_1;T^*)\right] \cdot \nabla_2 \left[\hat{x}_2\hat{z}_2 r_2 \Delta(r_2;T^*)y(r_2;T^*)\right] y(r_{12};T^*)e^{-\beta^*\phi(r_{12}}$$

Kirkwood approx. $(g_{\rm liq})_3(T/m, \phi; \mathbf{r}_1, \mathbf{r}_2) = g_{\rm liq}(T/m, \phi, r_1) g_{\rm liq}(T/m, \phi, r_2) g_{\rm liq}(T/m, \phi, |\mathbf{r}_1 - \mathbf{r}_2|)$

cavity function $y(r;T) \equiv e^{\beta\phi(r)} g(r;T)$ $\qquad \Delta(r;T) \equiv \frac{d}{dr} e^{-\beta\phi(r)} \xrightarrow[T\to 0]{} \delta(r-a)$

effective potential $e^{-\beta\phi_{\rm eff}(r)} \simeq \theta(r-a) + \sqrt{\pi A/m}\,\delta(r-a) + \ldots$

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

$$c_1 = (113/120)\pi^2,\; c_2 = (376709/22050)\pi^2$$

Rigidity of "contact force" systems at low temperatures

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

ex. Soft-particle case $\alpha = 2$ (3-dim) Berthier-Jacquin-Zamponi (2011)

$\phi_{\rm GCP} = 0.633353..$ $A^*/m^*(\phi_{\rm GCP}) \simeq 9.72187\times 10^{-5}$ $y_{\rm liq}^{\rm HS}(\phi_{\rm GCP}) \simeq 23.6238$

$\phi < \phi_{\rm GCP}$ $m^* \simeq 20.7487(\phi_{\rm GCP} - \phi)$

Berthier-Jacquin-Zamponi (2011)

$$\lim_{T\to 0}\hat{\mu} \simeq 0.694315T/(\phi_{\rm GCP} - \phi)$$

$\lim_{T\to 0} p \simeq 1.92178T/(\phi_{\rm GCP} - \phi)$

Otsuki-Hayakawa (2012)

$\phi > \phi_{\rm GCP}$ $T/m^* \simeq 0.00835535(\phi - \phi_{\rm GCP})$

Berthier-Jacquin-Zamponi (2011)

$$\lim_{T\to 0}\hat{\mu} \simeq 0.1239496(\phi - \phi_{\rm GCP})$$

$\lim_{T\to 0} p \simeq 0.403001(\phi - \phi_{\rm GCP})$

Otsuki-Hayakawa (2012)

Metabasin?

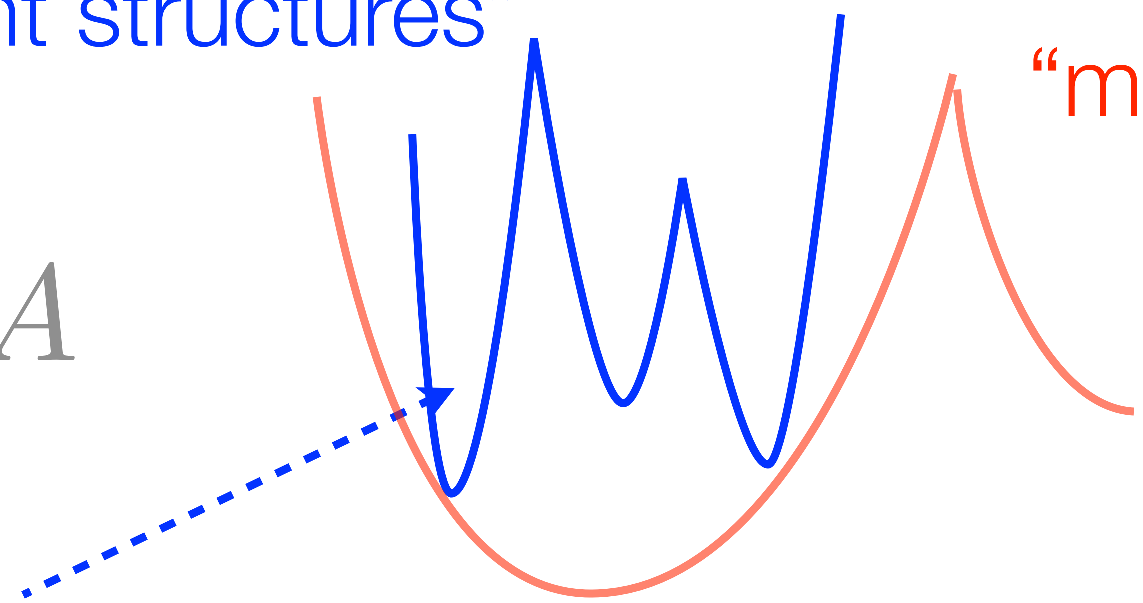
"jammed side" (soft-sphere glass)

$$\phi > \phi_{\mathrm{J}} \qquad P \propto \delta\phi$$

"inherent structures"

"meta-basins"(1RSB)

$$\mu \propto T/A$$



$$\mu_{\mathrm{harmonic}} \propto \sqrt{\delta\phi}$$ shear-modulus $$\lim_{T\to 0} \mu(\mathrm{T}) \propto \delta\phi$$

Durian, PRL 75, 4780 (1995),

O'Hern et. al. PRE E 68, 011306 (2003)

S. Okamura and H. Yoshino, arXiv:1306:2777

$$A_{\mathrm{harmonic}} \propto T/\sqrt{\delta\phi}$$ cage size $$\lim_{T\to 0} A(T) \propto T/\delta\phi$$

Brito-Wyart, JCP 131, 024504 (2009).

Ikeda-Berthier-Biroli, arXiv:1209.2814

Berthier-Jacqin-Zamponi, PR E 84, 051103 (2011).

Emulsion experiments: T. G. Mason et al, PRE 56, 3150 (1997). Guerra-Weitz (2013)

more RSB? (Gardner's transition?)

J. Kurchan, G. Parisi, P. Urbani and F. Zamponi, arXiv.1303.1028

Metabasin?

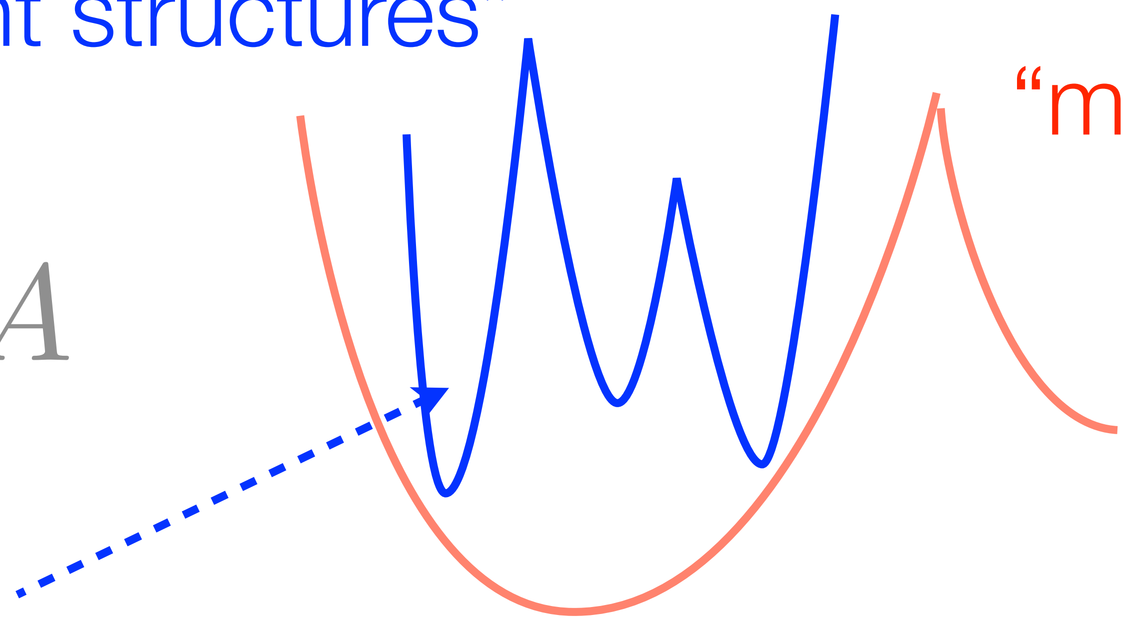
“unjammed side” (hard-sphere glass)

$\phi < \phi_{\mathrm{J}}$ $P \propto T/|\delta\phi|$

“inherent structures”

“meta-basins” (1RSB)

$\mu \propto T/A$



$\mu_{\mathrm{harmonic}} \propto T/|\delta\phi|^{3/2}$ shear-modulus $\lim_{T\to 0} \mu(T) \propto T/|\delta\phi|$

S. Okamura and H. Yoshino, arXiv:1306:2777

Brito-Wyart, EPL 76, 149 (2006).

$A_{\mathrm{harmonic}} \propto |\delta\phi|^{3/2}$ cage size $\lim_{T\to 0} A(T) \propto |\delta\phi|$

Ikeda-Berthier-Biroli, arXiv:1209.2814

Berthier-Jacqin-Zamponi, PR E 84, 051103 (2011).

Emulsion experiments: T. G. Mason et al, PRE 56, 3150 (1997). Guerra-Weitz (2013)

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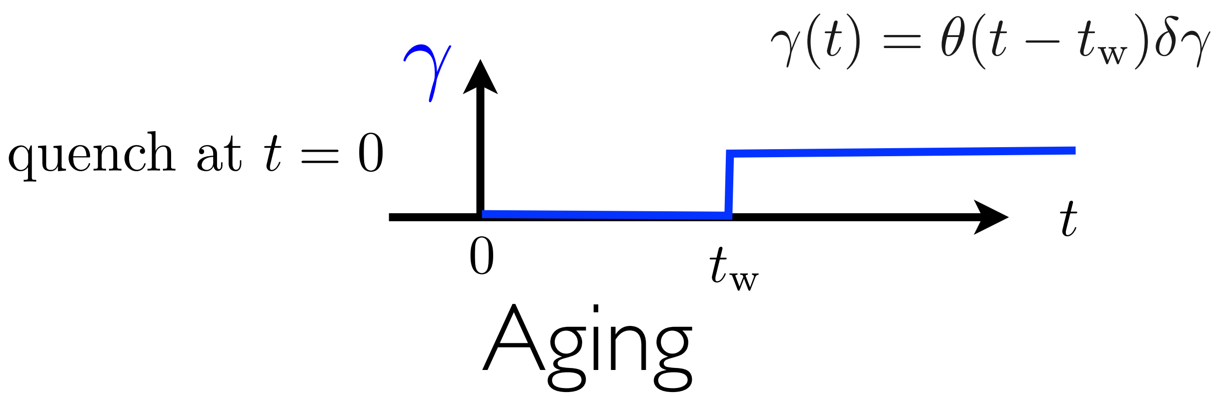
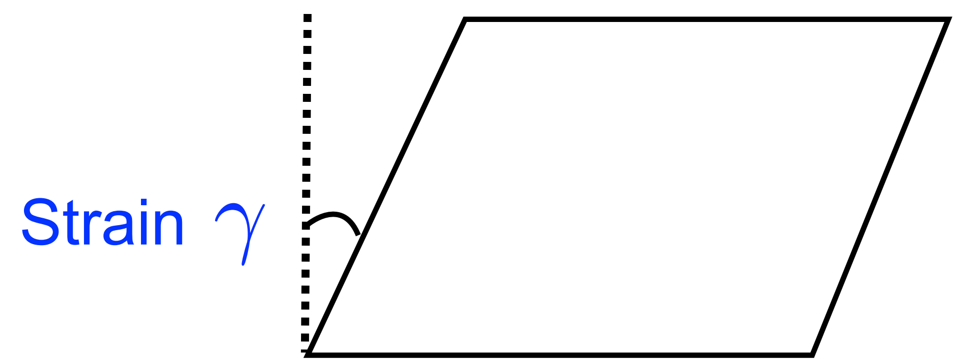
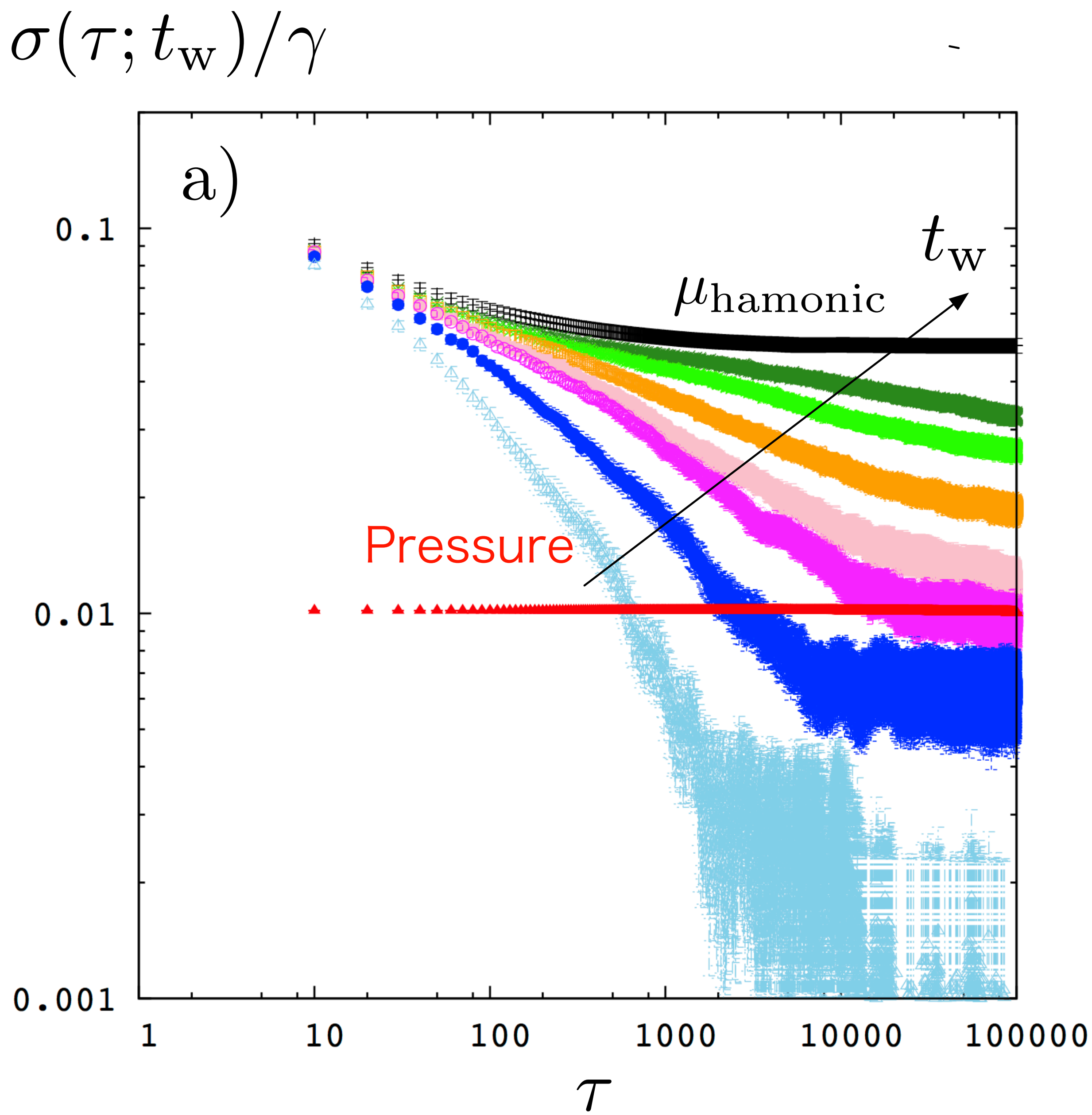
c.f. "Glass" and "jamming" transitions are disentangled in non-linear rheology
Ikeda-Berthier-Solich, PRL 109, 018301 (2012).

Shear stress relaxation : response and correlation







$\phi = 0.67 \ \ (0.65 - 0.67)$

$T/\epsilon = 10^{-5} \ \ (10^{-6}, 10^{-7})$

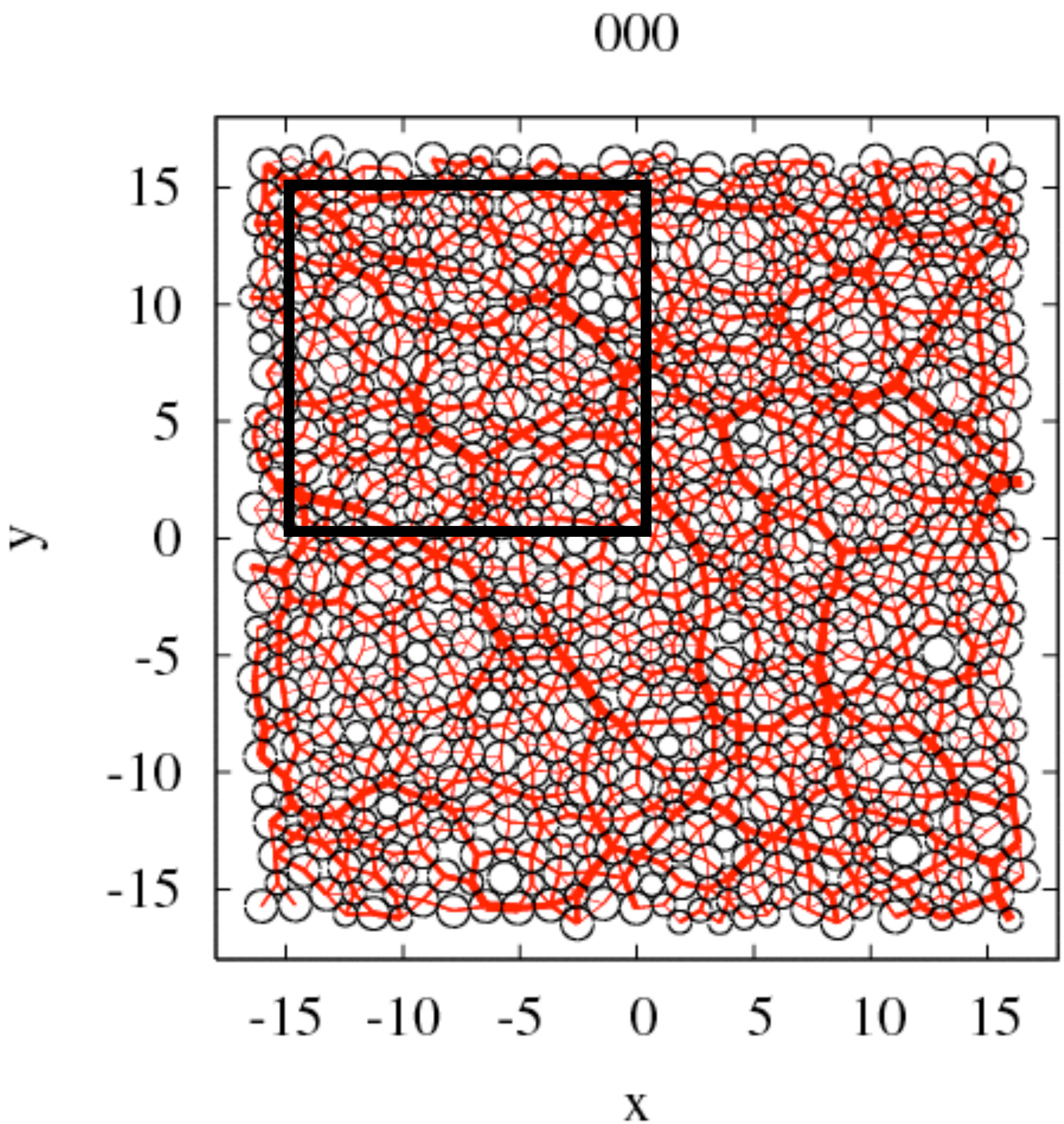
$\gamma = 0.25 \times 10^{-2} \ \ (0.25 \times 10^{-3})$

N=800 (2400)

# of samples=4096

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

Avalanche like plastic events during stress relaxation



time unit: collision time

$$\tau_{\mathrm{T}} = \sqrt{m\sigma^2/k_{\mathrm{B}}T}$$

$$N = 800$$

$$\phi = 0.85$$

$\phi_{\mathrm{J}} \sim 0.84$ (2dim)

$$T/\epsilon = 10^{-6}$$

$$\gamma = 0.05$$

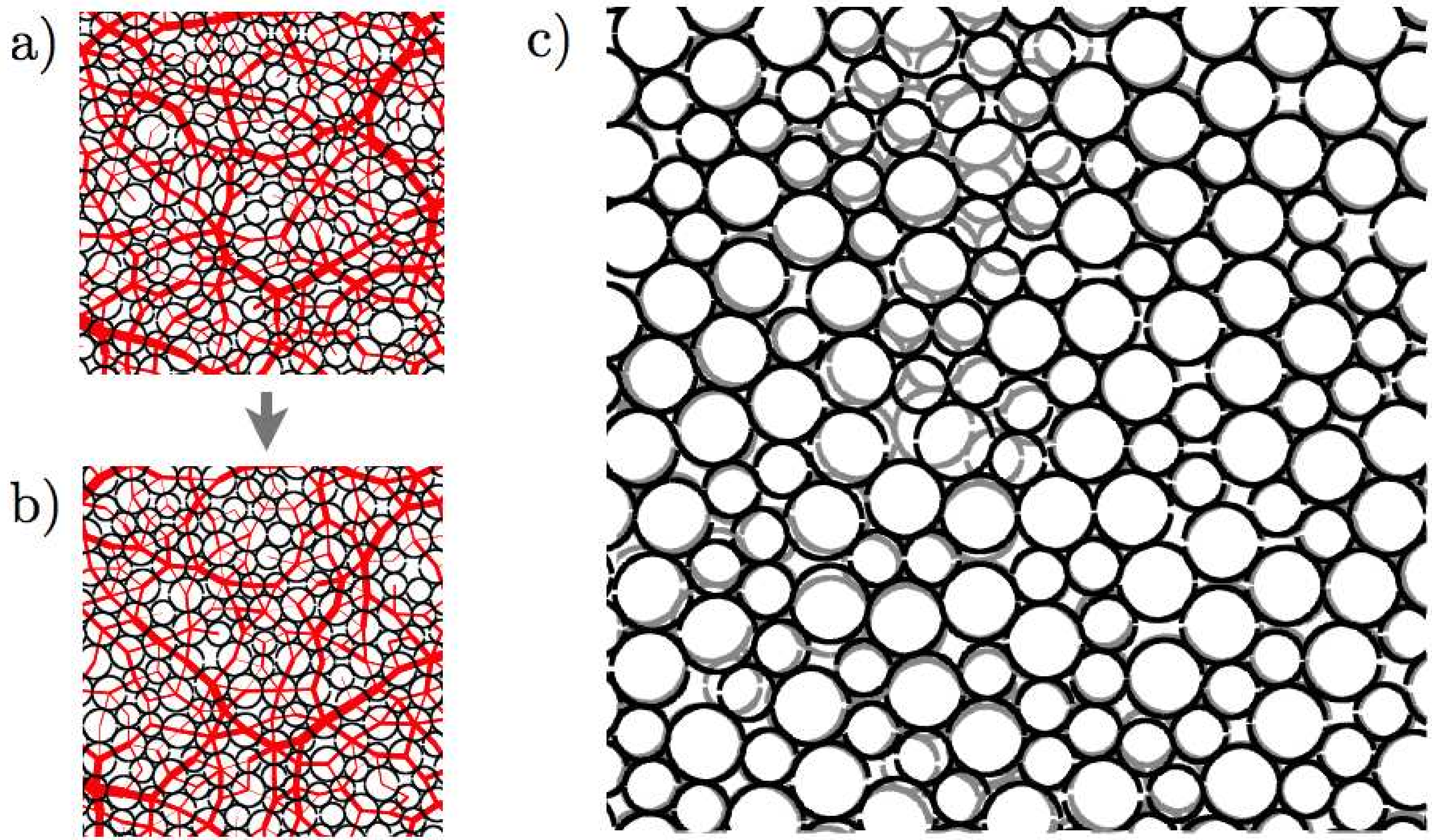


Figure 1: This figure show snaphots before/after a plastic event trigered by thermal noises. Here we used a 2-dimensional version of the model (for the purpose of a demonstration) at volume fraction $\phi = 0.85$ which is slightly above the jamming density $\phi_{\rm J} \sim 0.84$ (2-dim). The system is initially perturbed weakly by a shear-strain $\gamma = 0.05$ and let to relax at zero temperature by the conjugated gradient method which allows the system to relax using the harmonic modes. Then the thermal noise at (reduced) temperature $T = 10^{-6}$ is switched on. The configuration of particles are represented by the circles and that of the contact forces $f_{ij} = -dv_{ij}(r_{ij})/dr_{ij}$ are represented by bonds whose thickness is chosen to be proportional to f_{ij}. The panels a) and b) show the snapshots before/after a plastic event (which took about $10^4 t_{\rm micro}$ to complete). In panel c) the configuratoin of the particles before/after are overlaid : the one before the event is shown by the lighter color.

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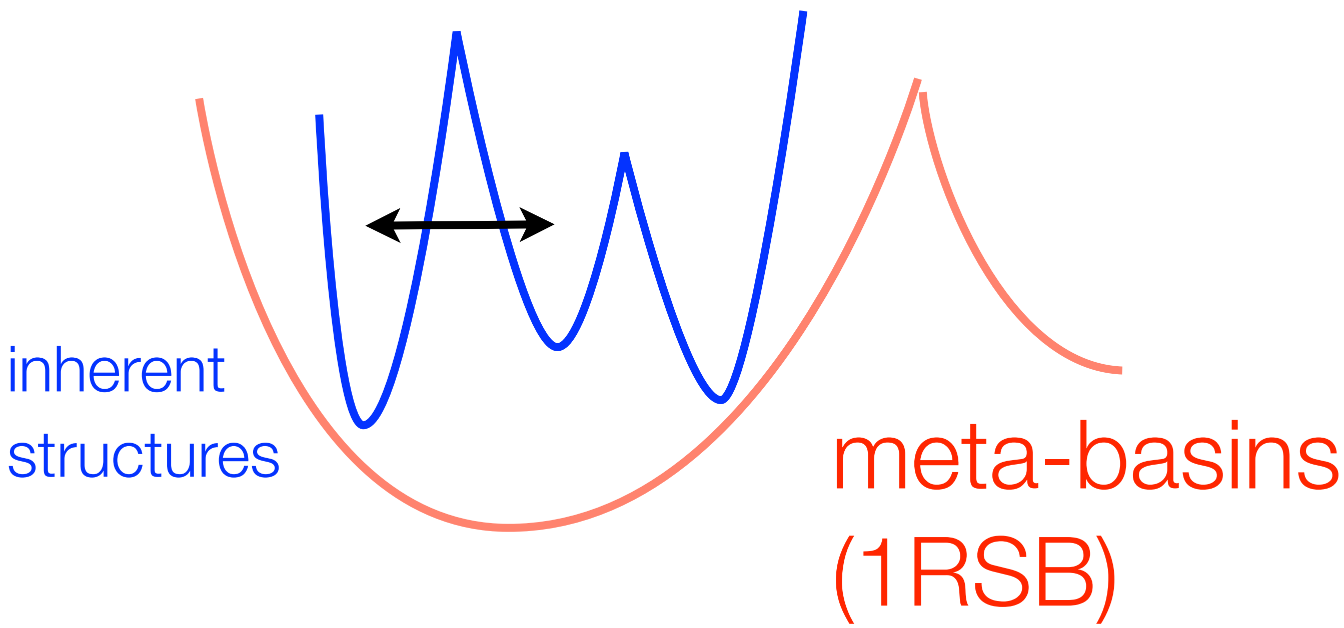
fluctuation within meta-basin: floppy modes?



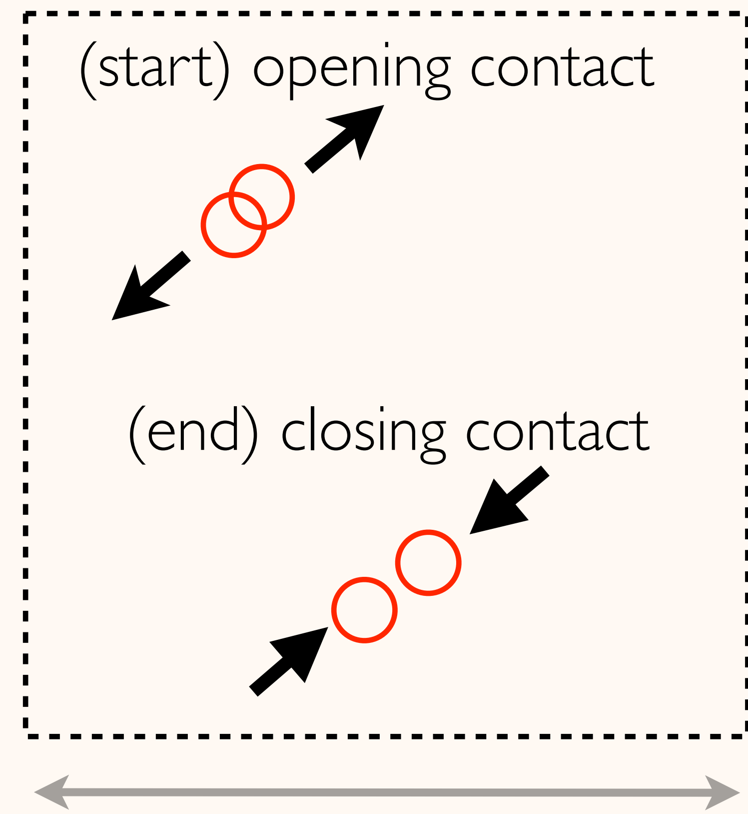
Relaxation of shear-stress via floppy modes?

$$\sigma_{xz} = \frac{1}{V}\sum_{i<j} r_{ij} f(r_{ij}) \frac{x_{ij}}{r_{ij}}\frac{z_{ij}}{r_{ij}}$$

“angular variables

Floppy mode:

$$\delta r_{ij} = |\delta R_i - \delta R_j| = 0$$



$$l_{\rm iso} \sim \delta z^{-1} \sim 1/\sqrt{\phi - \phi_{\rm J}}$$

M. Wyart, Annales de Phys, 30 (3), 1 (2005).

M. Wyart, PRL 109, 125502 (2012).

E. Lerner, G. During and M. Wyart arXiv.1302.3990

Conclusions

The rigidity of densely packed repulsive contact systems (hard-spheres, soft-particles,..) in the glassy phase at low temperatures

- Cloned liquid computation (replica+liquid theory) and MD simulation of stress-relaxation

$$\phi < \phi_{\mathrm{J}} \qquad \frac{\mu}{k_{\mathrm{B}}T} \sim \frac{p}{k_{\mathrm{B}}T} \propto \frac{1}{\phi_{\mathrm{J}} - \phi}$$

$$\phi > \phi_{\mathrm{J}} \qquad \frac{\mu}{\epsilon} \sim \frac{p}{\epsilon} \propto \phi - \phi_{\mathrm{J}}$$

- *Discussion:*

Satoshi Okamura and Hajime Yoshino, arXiv:1306:2777

  - *Breakdown of simple "harmonic solid" picture*
  - *Thermally activated floppy modes inside "meta-basins"?*
  - *AT instability ? 1+continuous RSB (Gardner's transition) ?*

J. Kurchan, G. Parisi, P. Urbani and F. Zamponi, arXiv.1303.1028