Jamming is a first-order transition with quenched disorder in the athermal quasi-static limit

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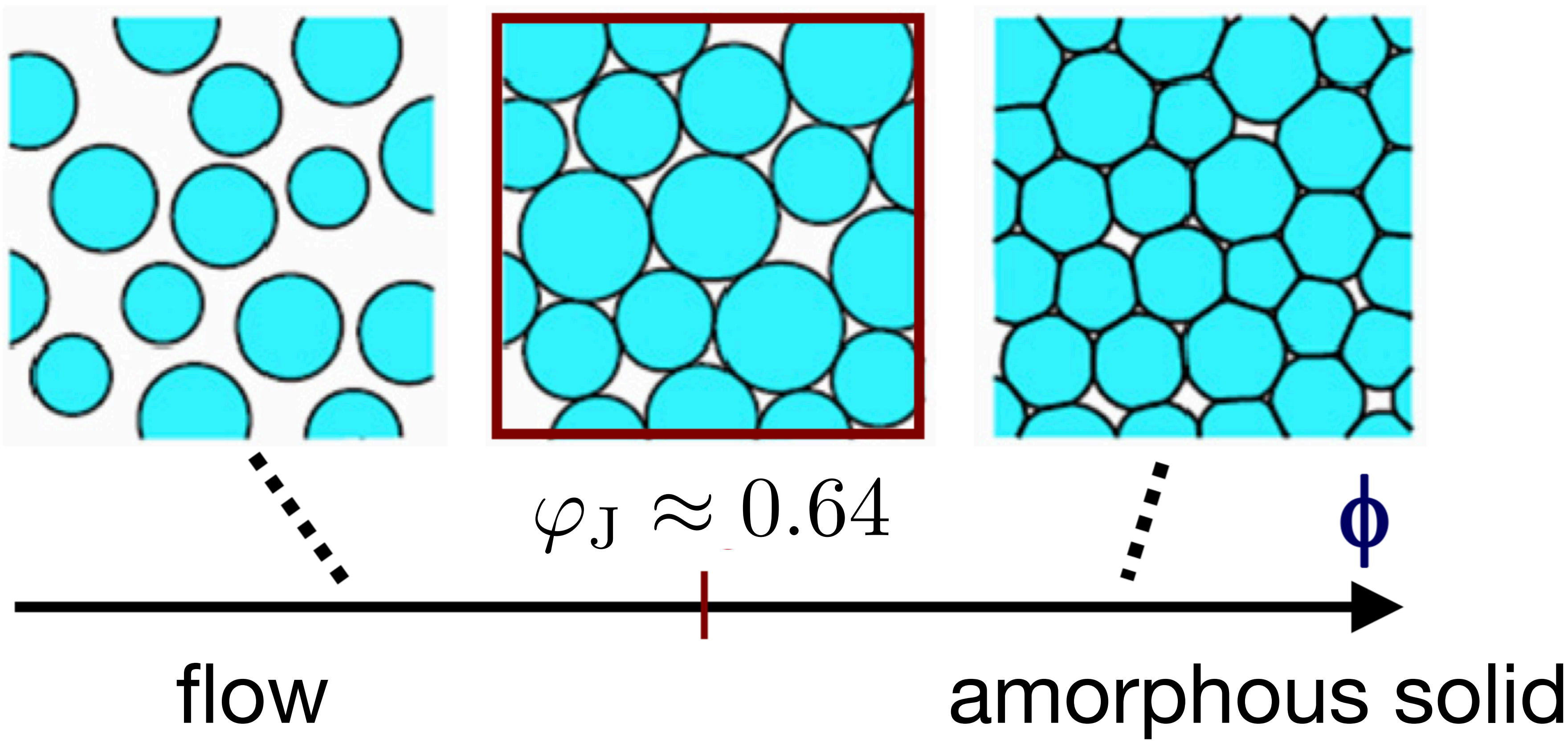
Jamming transition

Van Hecke, 2010



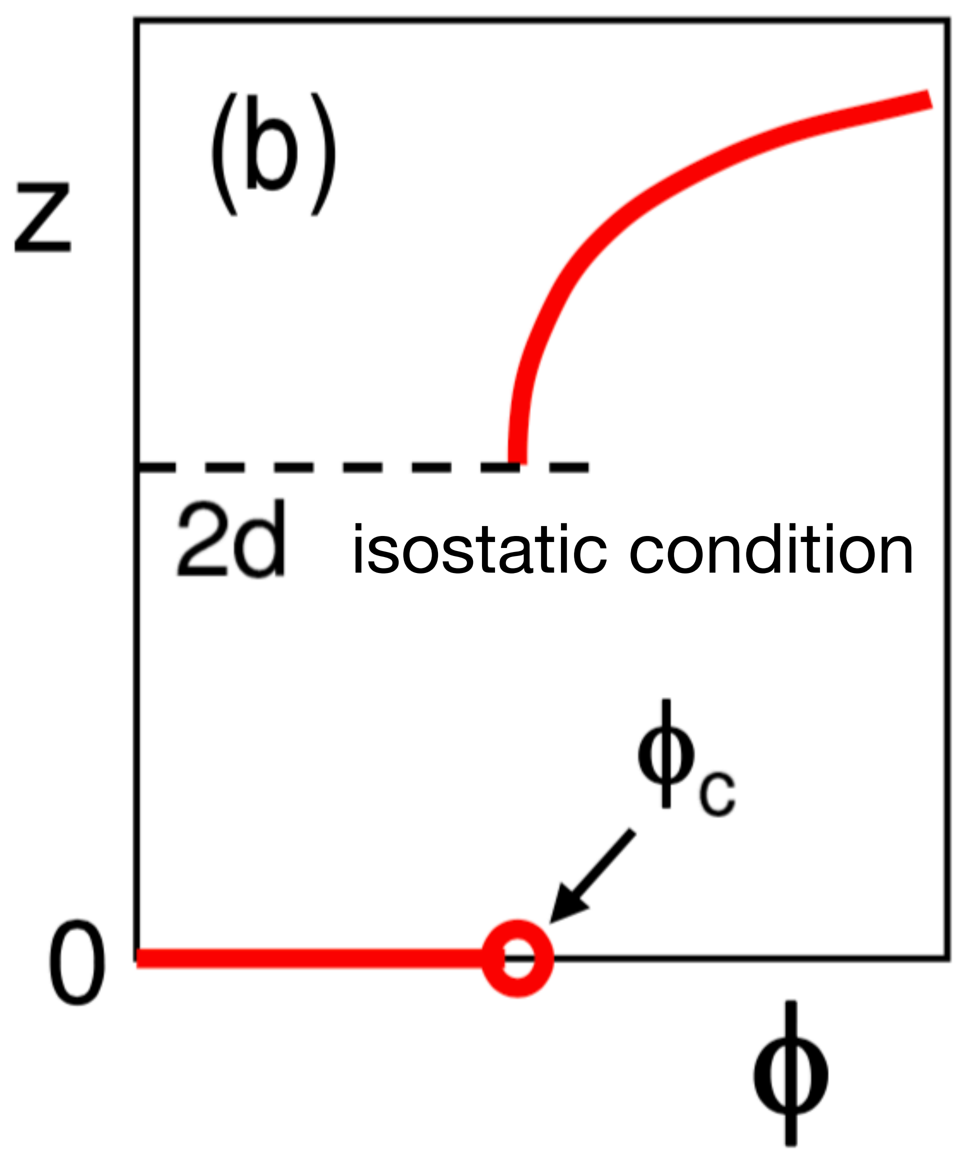
What is the nature of the jamming transition?

Is the jamming transition second-order or first-order?

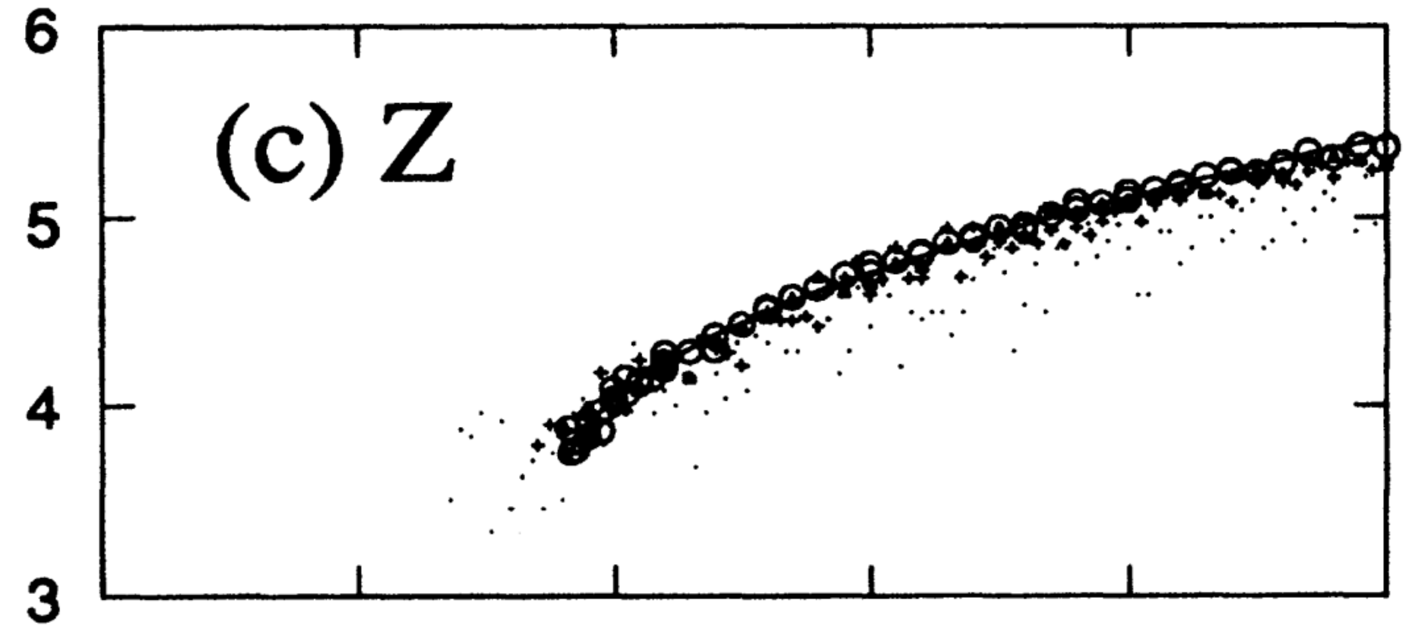
Evidence of a first-order transition

discontinuous jump of the coordination number Z (order parameter) at the jamming transition

schematic



simulation



Durian, PRL, 1997

Evidence of a second-order transition

critical scaling of shear viscosity near the jamming transition

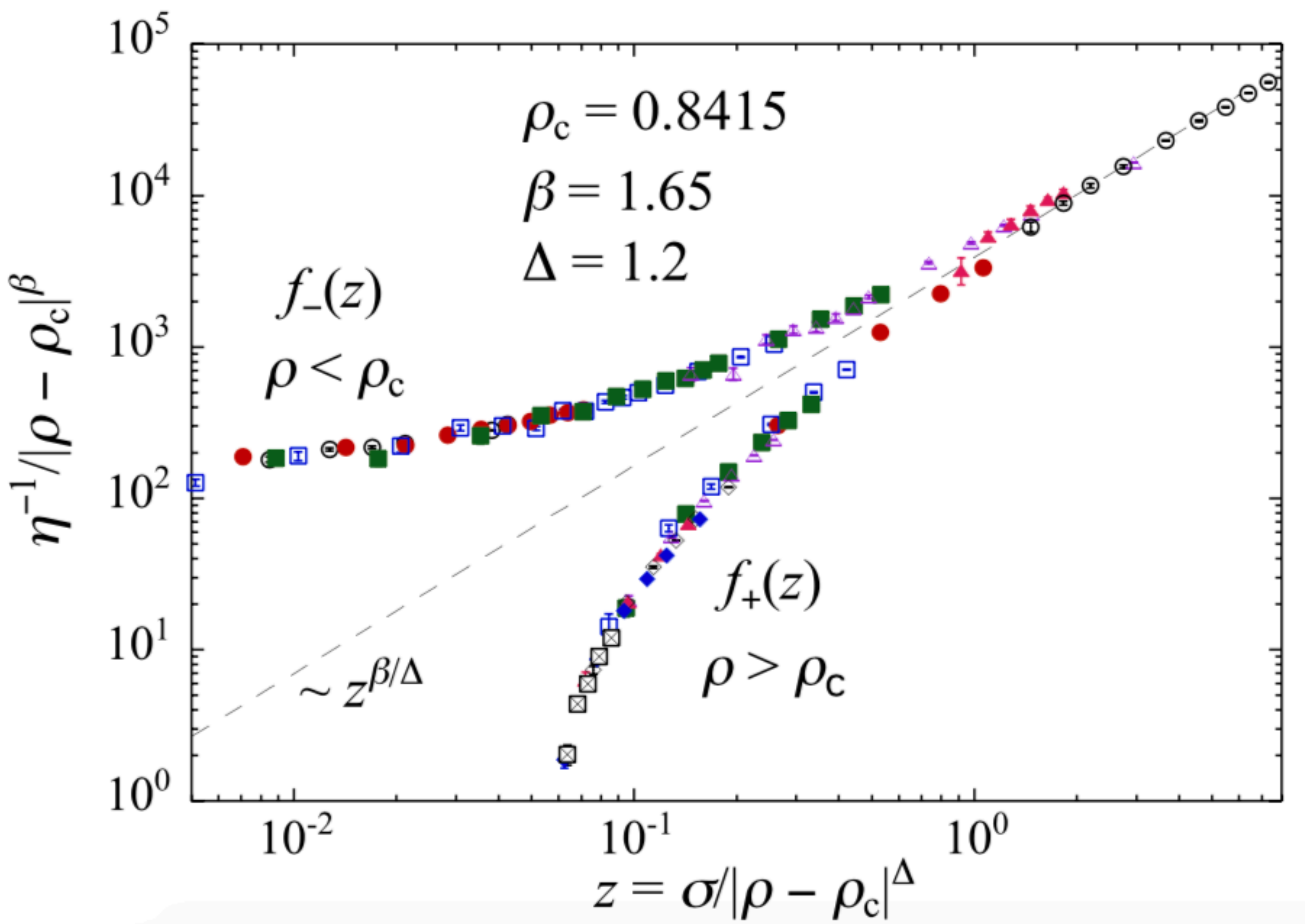
Olsson & Teitel, PRL, 2007

external field

$$\eta^{-1}(\rho, \sigma) = |\rho - \rho_c|^{\beta} f_{\pm}\left(\frac{\sigma}{|\rho - \rho_c|^{\Delta}}\right)$$

order parameter

control parameter



similar scalings are observed in models of active matter (Ning Xu et al.) and cell jamming (Lisa Manning et al.)

Mechanical marginality

diverging length scales due to mechanical marginality

- **isostatic length scale** Wyart, et al., EPL, 2005

$$l^* \sim \Delta Z^{-1} \sim (\varphi - \varphi_J)^{-1/2}$$

- **scattering length scale** Wyart, et al., Soft Matter, 2013

$$l_c \sim \Delta Z^{-1/2} \sim (\varphi - \varphi_J)^{-1/4}$$

density of vibrational states

$$l^* \sim \omega_*^{-1}$$

$$l_c \sim \omega_0^{-1/2}$$

$$D(\omega) \sim \begin{cases} \omega^{d-1} & \omega \ll \omega_0, \\ \omega^2/\omega_*^2 & \omega_0 \ll \omega \ll \omega_*, \\ \text{flat} & \omega_* \ll \omega \ll \omega_{\max}, \end{cases}$$

Power-law scalings due to marginality

- weak inter-particle force distribution

$$P(f) \sim f^{\theta}$$

- small inter-particle gap distribution

$$P(h) \sim h^{-\alpha}$$

marginal argument by Wyart:

$\theta = 1/\alpha - 2$ for extensive modes

$\theta = 1 - 2\alpha$ for localised modes

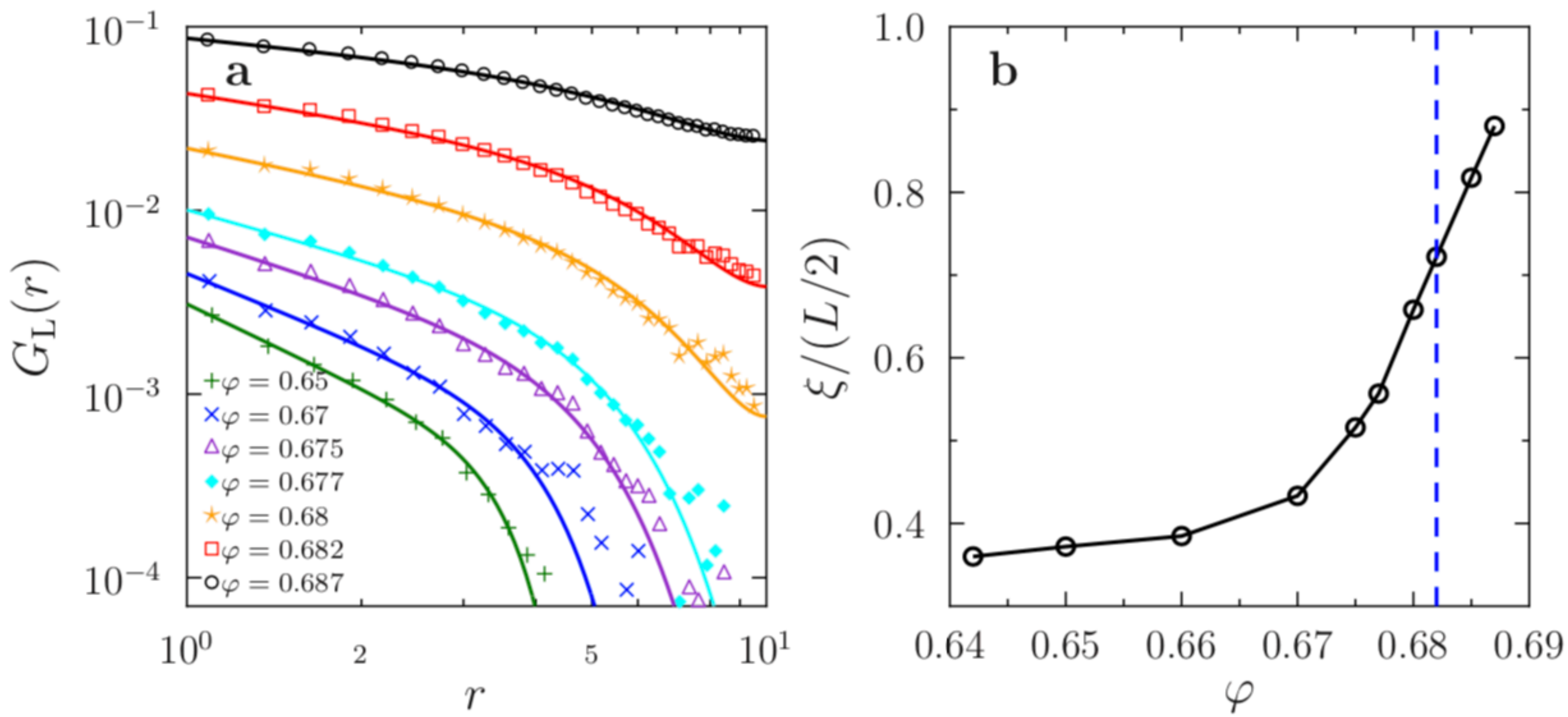
mean-field replica theory:

$\alpha = 0.41269$ and $\theta = 0.42311$ Zamponi, et al., NC, 2014

Gardner phase and landscape marginality

Zamponi, et al., NC, 2014

The entire Gardner phase, including jamming, is critical.



spatial correlation between local fluctuations of cage sizes
Berthier, et al., PNAS (2016)

infinite caging correlation length in the Gardner phase:

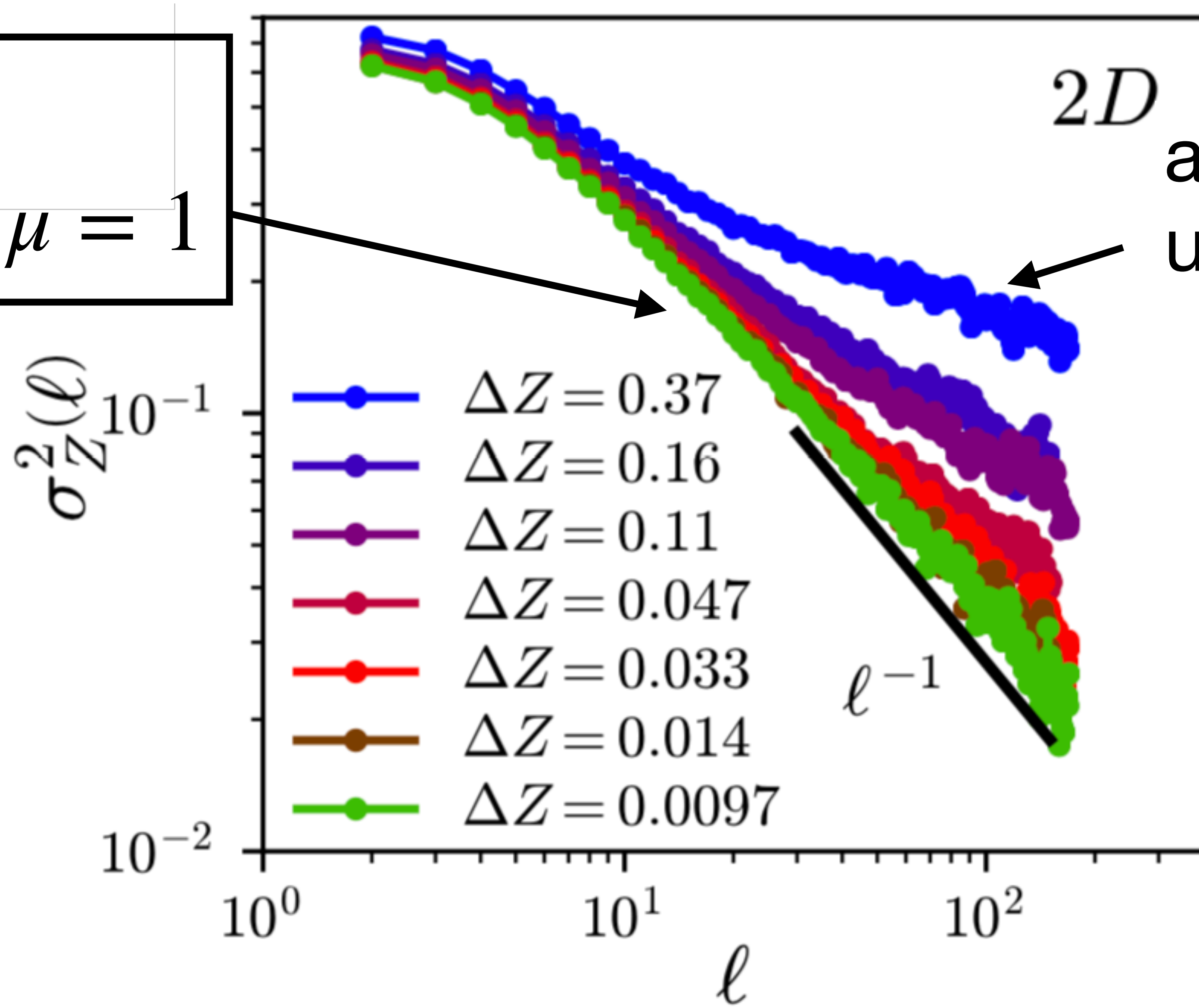
$$\xi_G \sim \infty$$

Hyperuniformity

$$\sigma_Z^2(\ell) = \frac{1}{\ell^d}\left\langle\left(\sum_{i\in\ell^d}\delta Z_i\right)^2\right\rangle$$

Hexner, et. al., 2018

hyperuniform
$\sigma_Z^2(\ell) \sim \ell^{-\mu}$ with $\mu = 1$



crossover length: $\xi_f \propto \Delta Z^{-\nu_f}$

$$\nu_f^{2d} = 1.07^{+0.1}_{-0.18} \text{ and } \nu_f^{3d} = 1.29^{+0.27}_{-0.19}$$

Many existing viewpoints

- Jamming has a mixed order: first and second?
- Jamming is critical (hyperfluctuations) and hyperuniform?

diverging lengths

1. mechanical marginality
2. hyperuniformity

above jamming

3. Gardner phase and landscape marginality

below jamming

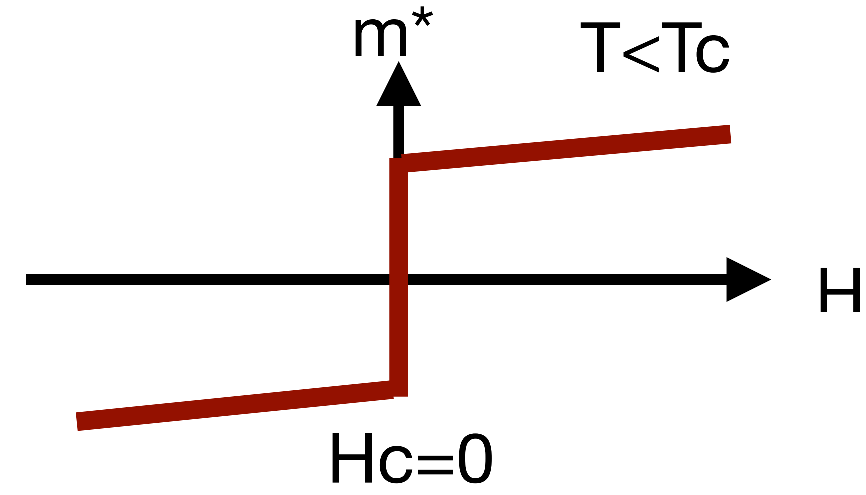
4. criticality in shear rheology
5. discontinuity in Z

both sides

Our viewpoint

Jamming is a first-order transition with quenched disorder in the athermal quasistatic limit.

First-order transition without quenched disorder



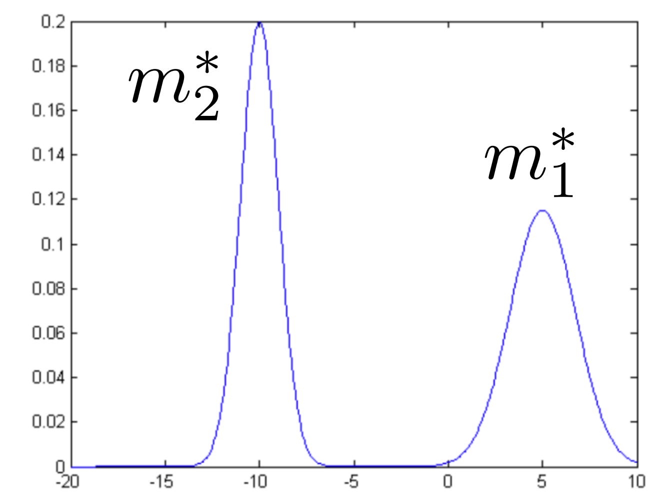
first-order transition in the Ising model

$$\mathcal{H}(\{s_i\}) = -\sum_{\langle i,j \rangle} J s_i s_j - H \sum_i s_i$$

Binder, 1987

probability distribution of the order parameter

$$p(m) \sim \underbrace{\exp\left(\frac{-N\delta f}{2k_{\mathrm{B}}T}\right)}_{F_1(H,N)} \exp\left[-\frac{(m-m_1^*)^2}{2k_B T\chi/N}\right] + \underbrace{\exp\left(\frac{N\delta f}{2k_{\mathrm{B}}T}\right)}_{F_2(H,N)} \exp\left[-\frac{(m-m_2^*)^2}{2k_B T\chi/N}\right]$$



- **fluctuation-response relation:**

$$\chi_{\mathrm{dis}} = N\left(\langle m^2 \rangle - \langle m \rangle^2\right) = \chi_{\mathrm{con}} = d\langle m \rangle / dx$$

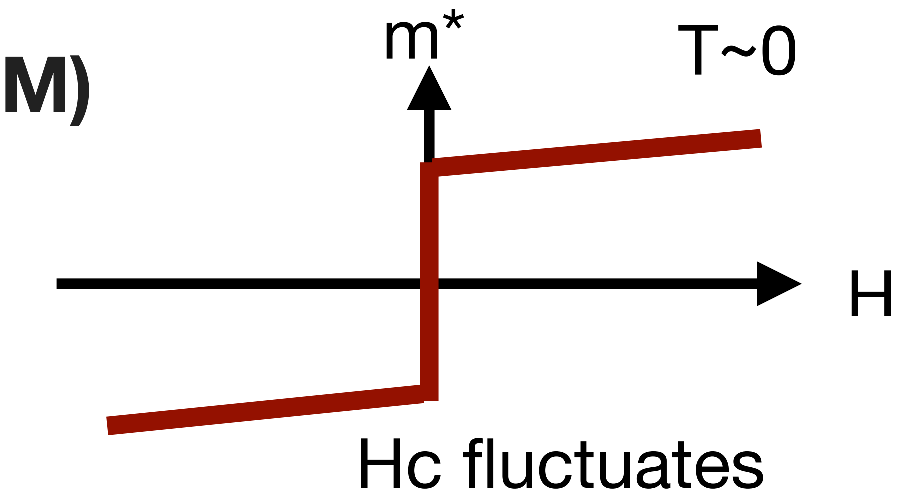
- **finite-size scaling form of the fraction of phase 1 (or 2):**

free energy difference between two phases: $\delta f \propto H - H_{\mathrm{c}}$

$$\Rightarrow \quad F_1(H,N) = \mathcal{F}_1\left[(H - H_{\mathrm{c}})N\right]$$

First-order transition with quenched disorder

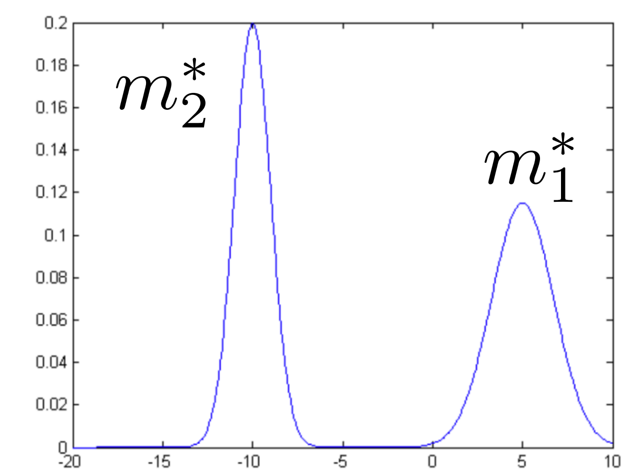
athermally driven random field Ising model (RFIM)



$$\mathcal{H}(\{s_i\}) = -\sum_{\langle i,j \rangle} J s_i s_j - \sum_i (H + h_i) s_i$$

sample-to-sample fluctuations:

$$\rho(H_\mathrm{c}) \sim \exp\left[-\frac{(H_\mathrm{c} - H_\mathrm{c}^\infty)^2}{2\sigma^2/N}\right]$$



probability distribution of the order parameter

$$p(m) = F_1\, p_1[(m - m_1^*)N^{\eta_1}] + F_2\, p_2[(m - m_2^*)N^{\eta_2}]$$

- **finite-size scaling form of the fraction of phase 1 (or 2):** $H > H_\mathrm{c}$

$$F_1(H, N) = \int_0^H \rho(H_\mathrm{c}) dH_\mathrm{c} \approx \frac{1}{2} + \frac{1}{2}\mathrm{erf}\left[(H - H_\mathrm{c}^\infty)N^{1/2}\right]$$

- **two susceptibilities:** $\chi_\mathrm{dis} = N\left(\langle m^2 \rangle - \langle m \rangle^2\right) \sim N$

$$\chi_\mathrm{con} = d\langle m \rangle / dH \sim N^{1/2}$$

$$\Rightarrow \quad \boxed{\chi_\mathrm{dis} \sim \chi_\mathrm{con}^2}$$

Comparison

- **first-order transition with quenched disorder**

distribution of transition point

$$\rho(x_{\rm c}) \sim \exp\left[-\frac{(x - x_{\rm c}^{\infty})^2}{2\sigma^2/N}\right]$$

x: control parameter
(jamming: $x = \varphi$)

phase fraction

$$F_1(x, N) = \mathscr{F}_1\left[(x - x_{\rm c}^{\infty})N^{1/2}\right]$$

susceptibilities

$$\chi_{\rm dis} \sim N\,\mathscr{X}_{\rm dis}\left[(x - x_{\rm c}^{\infty})N^{1/2}\right]$$

$$\chi_{\rm con} \sim N^{1/2}\,\mathscr{X}_{\rm con}\left[(x - x_{\rm c}^{\infty})N^{1/2}\right]$$

$$\chi_{\rm dis} \sim \chi_{\rm con}^2 \sim N$$

finite-size correction

$$|\,x_c^{\infty} - x_c^{N}| \sim N^{-1/2}$$

- **first-order transition without quenched disorder**

$$F_1(x, N) = \mathscr{F}_1\left[(x - x_{\rm c}^{\infty})N\right]$$

$$\chi_{\rm dis} = \chi_{\rm con} \sim N\,\mathscr{X}\left[(x - x_{\rm c}^{\infty})N\right]$$

- **second-order transition (without quenched disorder)**

$$F_1(x, N) = \mathscr{F}_1\left[(x - x_{\rm c}^{\infty})N^{\frac{1}{d\nu}}\right]$$

$$\chi_{\rm dis} = \chi_{\rm con} \sim N^{\frac{\gamma}{d\nu}}\,\mathscr{X}\left[(x - x_{\rm c}^{\infty})N^{\frac{1}{d\nu}}\right]$$

several first-order transitions with quenched disorder

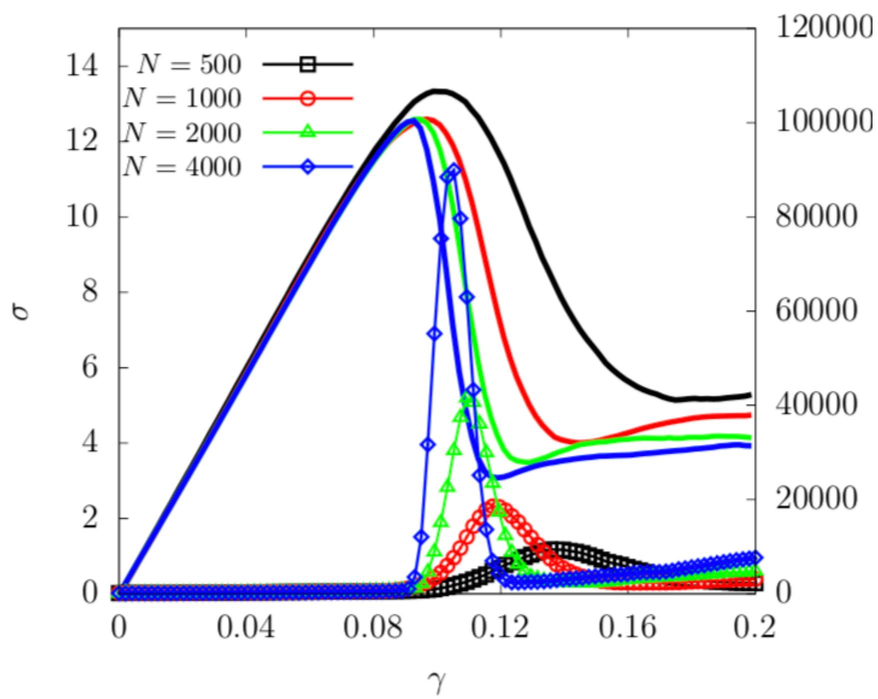
- **athermal random field Ising model driven by field**
- **yielding of stable athermal amorphous solids**

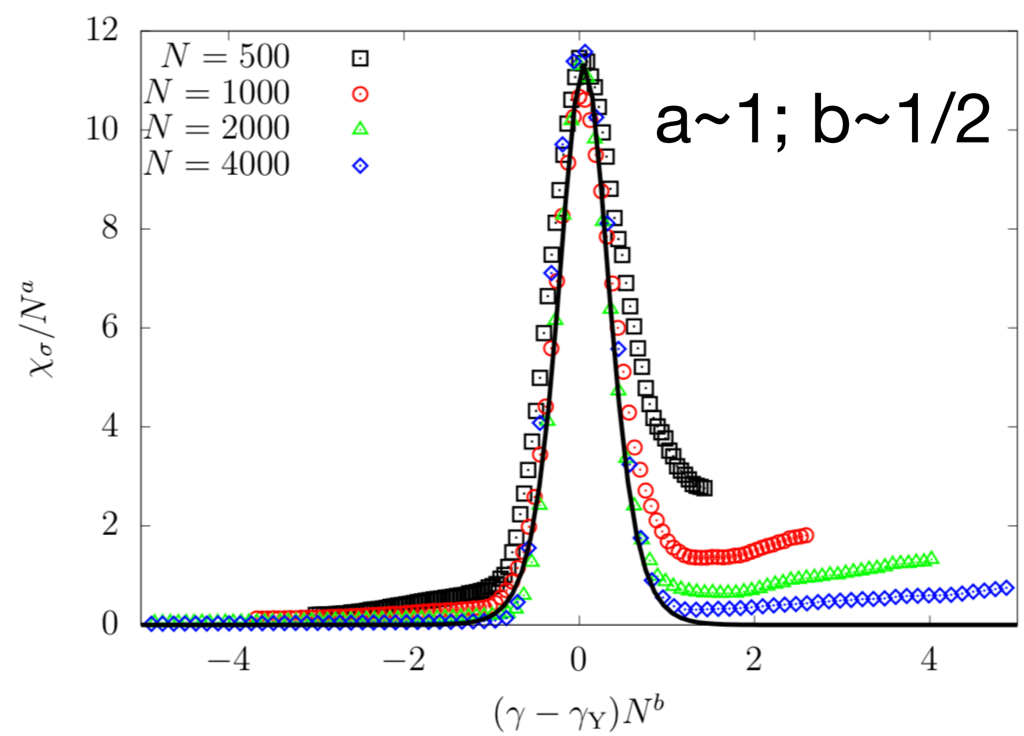
  Ozawa, et al., PNAS (2018)

- **yielding of stable hard sphere glasses**

  Jin & Yoshino (unpublished)

$$\chi_{\rm dis} \sim N \mathscr{X}_{\rm dis}\left[(x - x_c^{\infty}) N^{1/2}\right]$$





- **melting of stable hard sphere glasses**

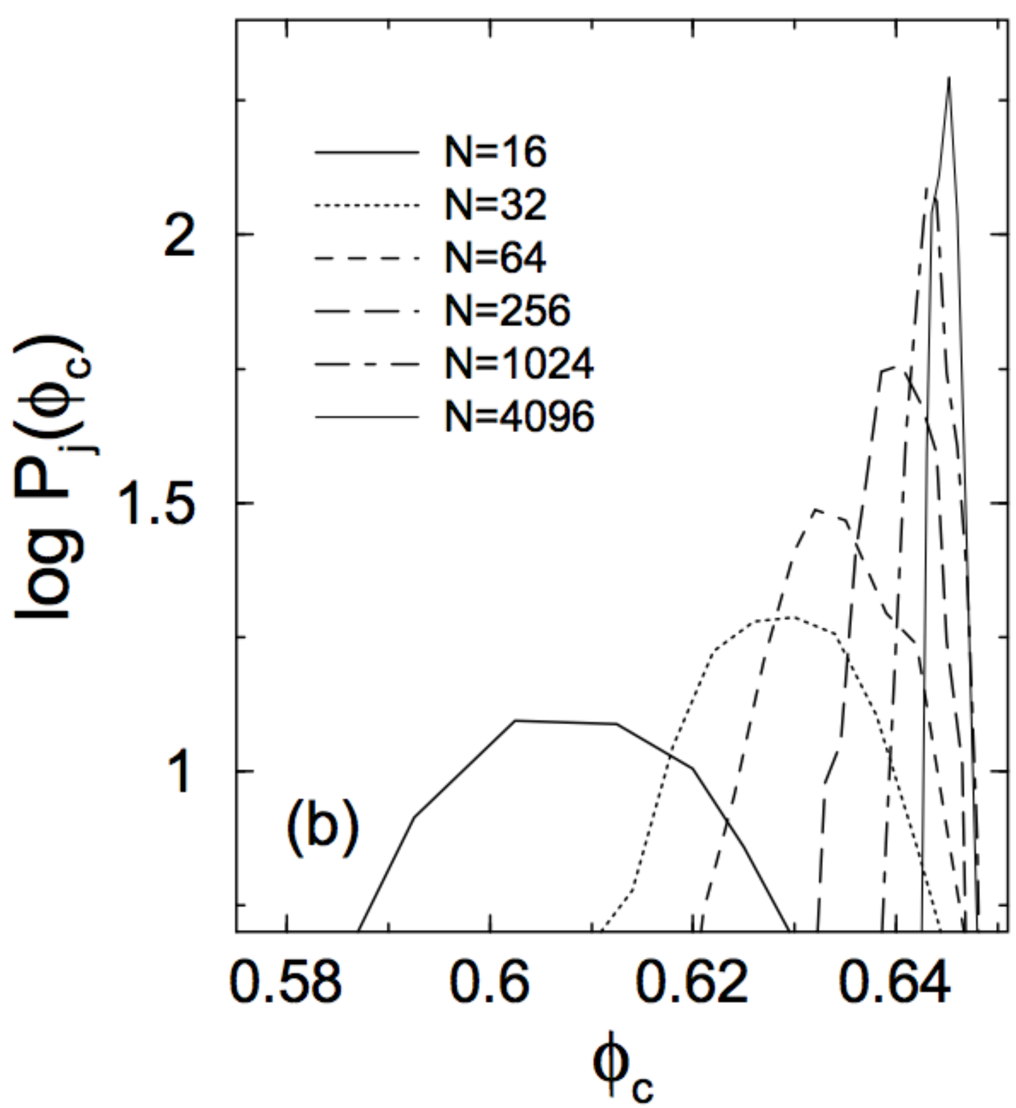
  Jin, et al., Soft Matter (2022)

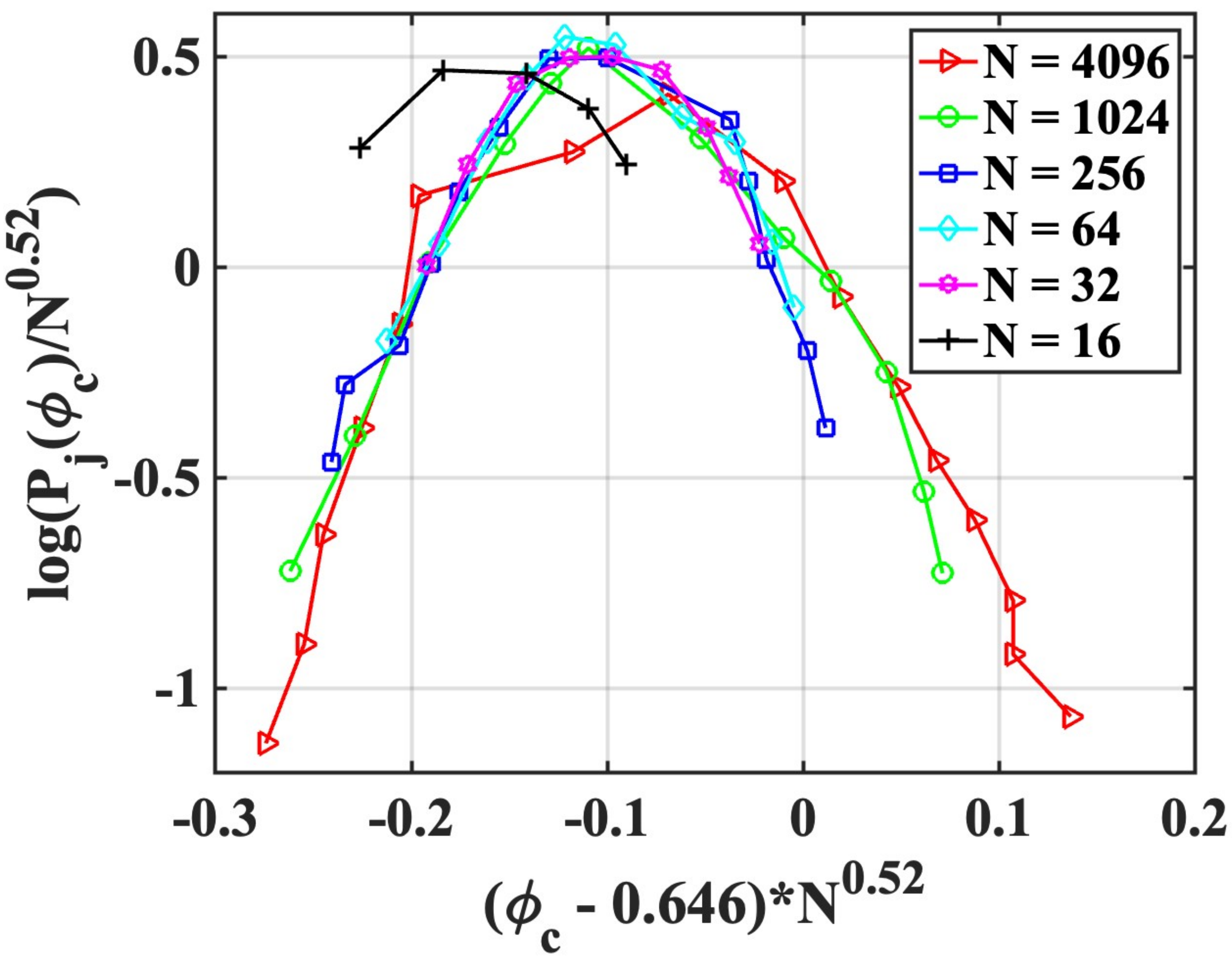
Previous finite-size results of the jamming transition

nearly Gaussian distribution of the transition point among samples

$$\rho(x_c) \sim \exp\left[-\frac{(x-x_c^\infty)^2}{2\sigma^2/N}\right]$$

rapid quench (O'Hern protocol) O'Hern, et al., PRL, 2002

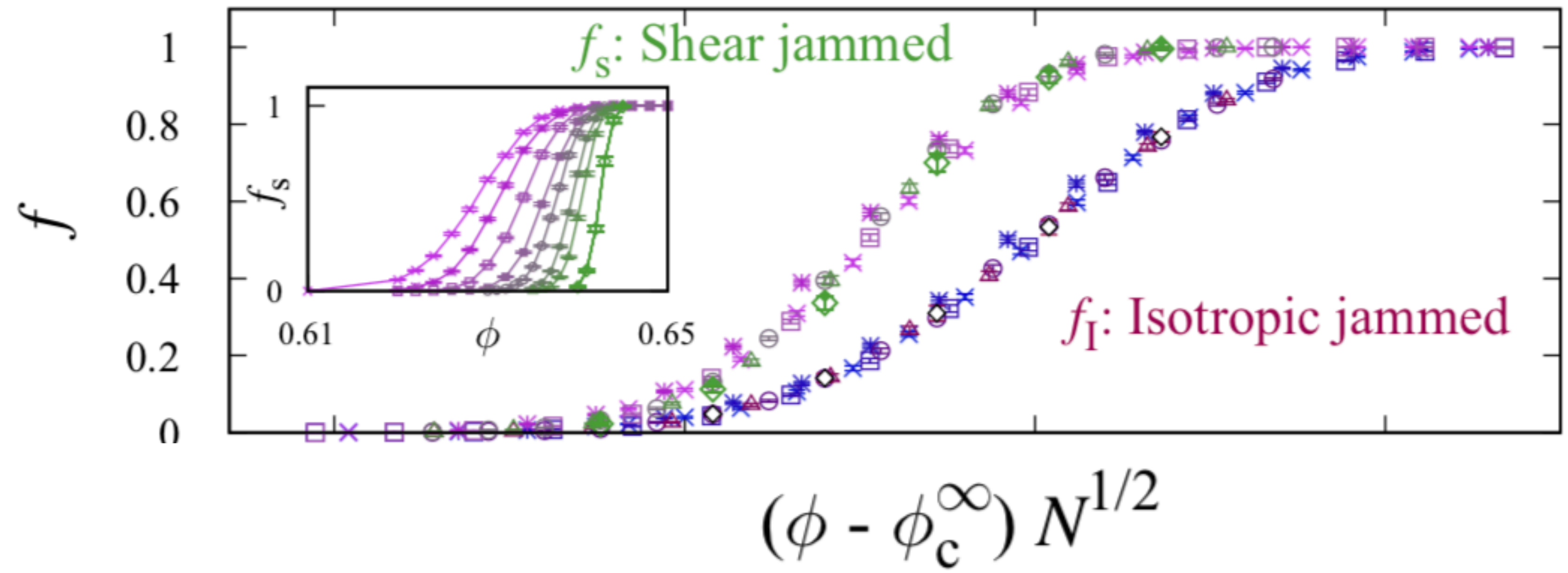




Previous finite-size results of the jamming transition

finite-size scaling of the jamming fraction $F_1(x,N) = \mathscr{F}_1\left[(x - x_c^\infty)N^{1/2}\right]$

3D:
O'Hern, et al., 2003
Baity-Jesi, et al., 2017



2D:
Teitel, et al., 2011 $f(\phi, L) = \mathcal{F}_0\left(\delta\phi L^{1/\nu}\right) + L^{-\omega}\mathcal{F}_1\left(\delta\phi L^{1/\nu}\right) \quad \nu = \omega = 1$

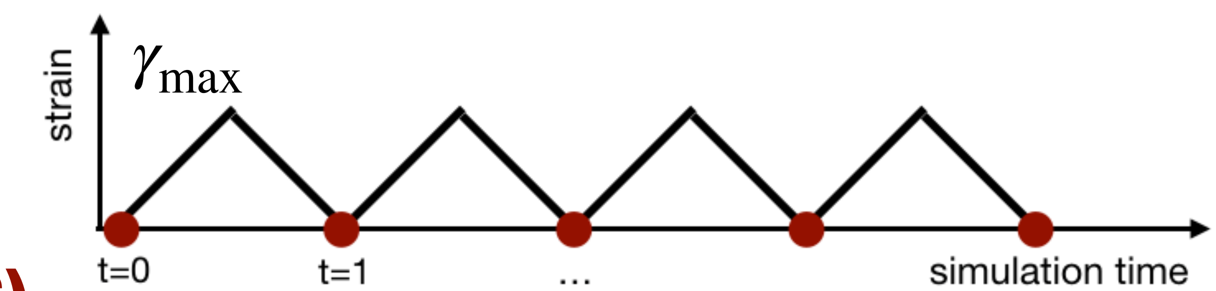
scaling independent of d: 2nd-order with an upper critical dimension d_u=2?

review by Liu & Nagle (2010)

There appears to be another diverging length scale whose connection to the length scales introduced above is not understood. The finite-size shift of the position of the jamming transition, ϕ_c, yields a length scale that apparently diverges as $|\phi - \phi_c|^{-0.7}$ in both two and three dimensions (10). The same exponent shows up in simulations in which a hard disk is pushed through a sphere packing below ϕ_c (23). Finally, the same exponent has been observed for correlations of the transverse velocity in athermal, slowly sheared sphere packings near the jamming transition (24), but only for certain models of the dynamics (25). It is not known whether the exponent is really different from 1/2.

Models and methods

- **frictionless**
- **athermal: T = 0**
- **Harmonic repulsion:** $U(r_{ij}) = \frac{\epsilon}{2}\left(1 - \frac{r_{ij}}{\sigma_{ij}}\right)^2 \Theta\left(1 - \frac{r_{ij}}{\sigma_{ij}}\right)$
- **bidisperse:** diameter ratio 1.4:1; number ratio 1:1
- **two and three dimensions**

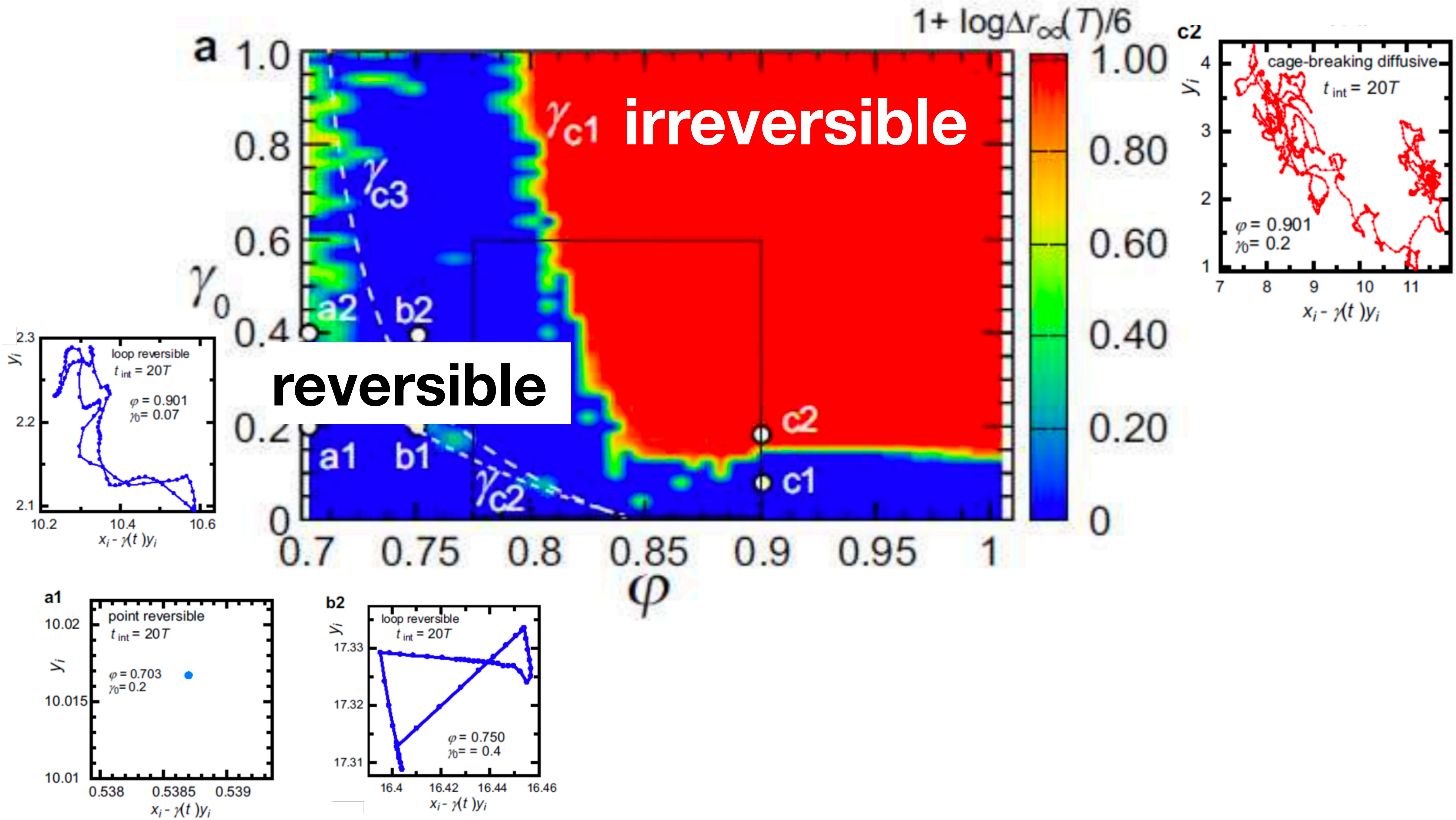


- **athermal quasi-static shear (AQS)**
- **energy minimisation by the FIRE algorithm** PRL (2006)
- **constant volume (control parameter of the transition)**
- **cyclic shear: well-controlled sampling of states**

Reversible and irreversible states under cyclic athermal quasi-static shear

maximum strain - density phase diagram in 2D

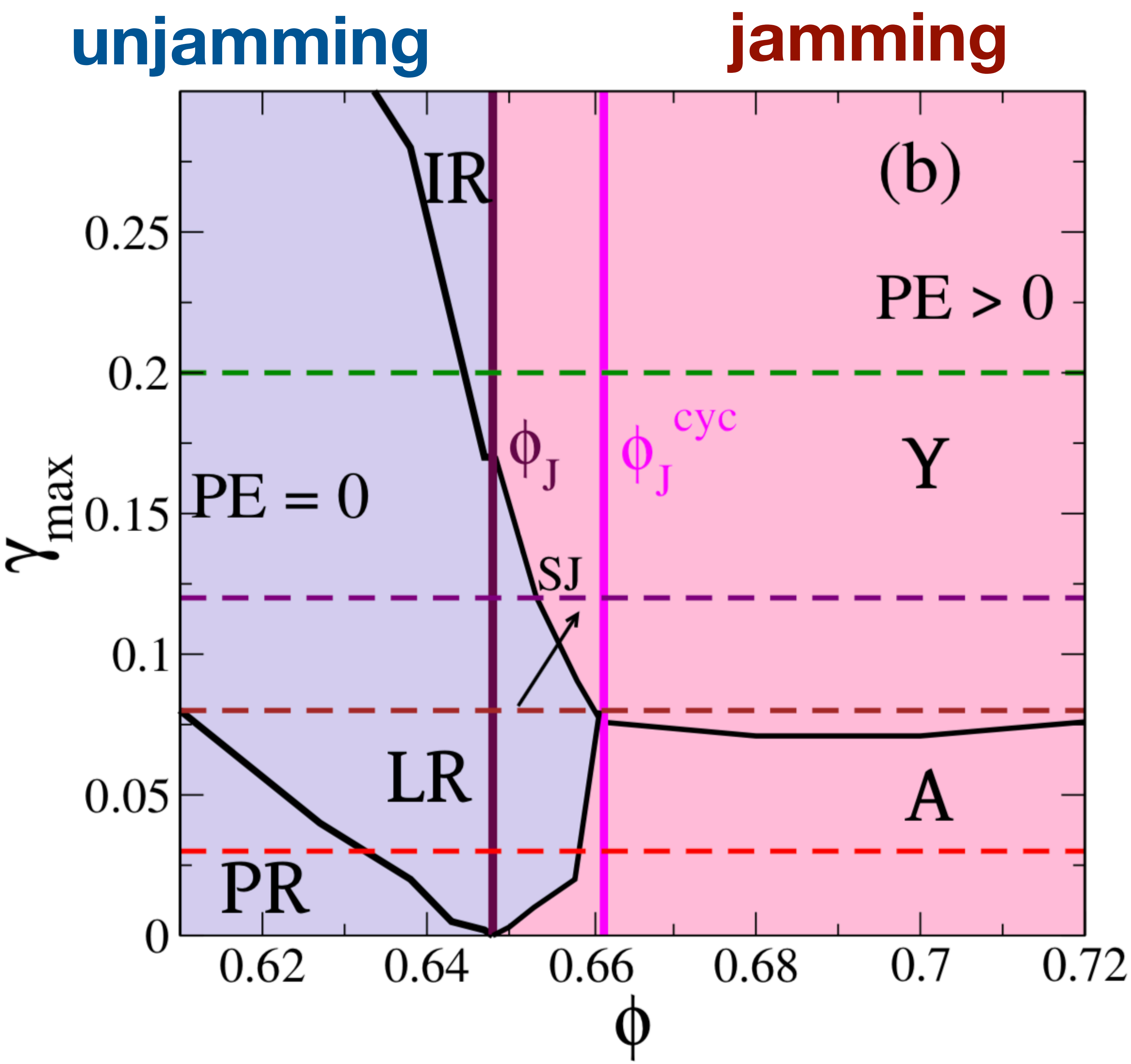
Nagasawa, Miyazaki & Kawasaki, 2019



Reversible and irreversible states under cyclic athermal quasi-static shear

maximum strain - density phase diagram in 3D

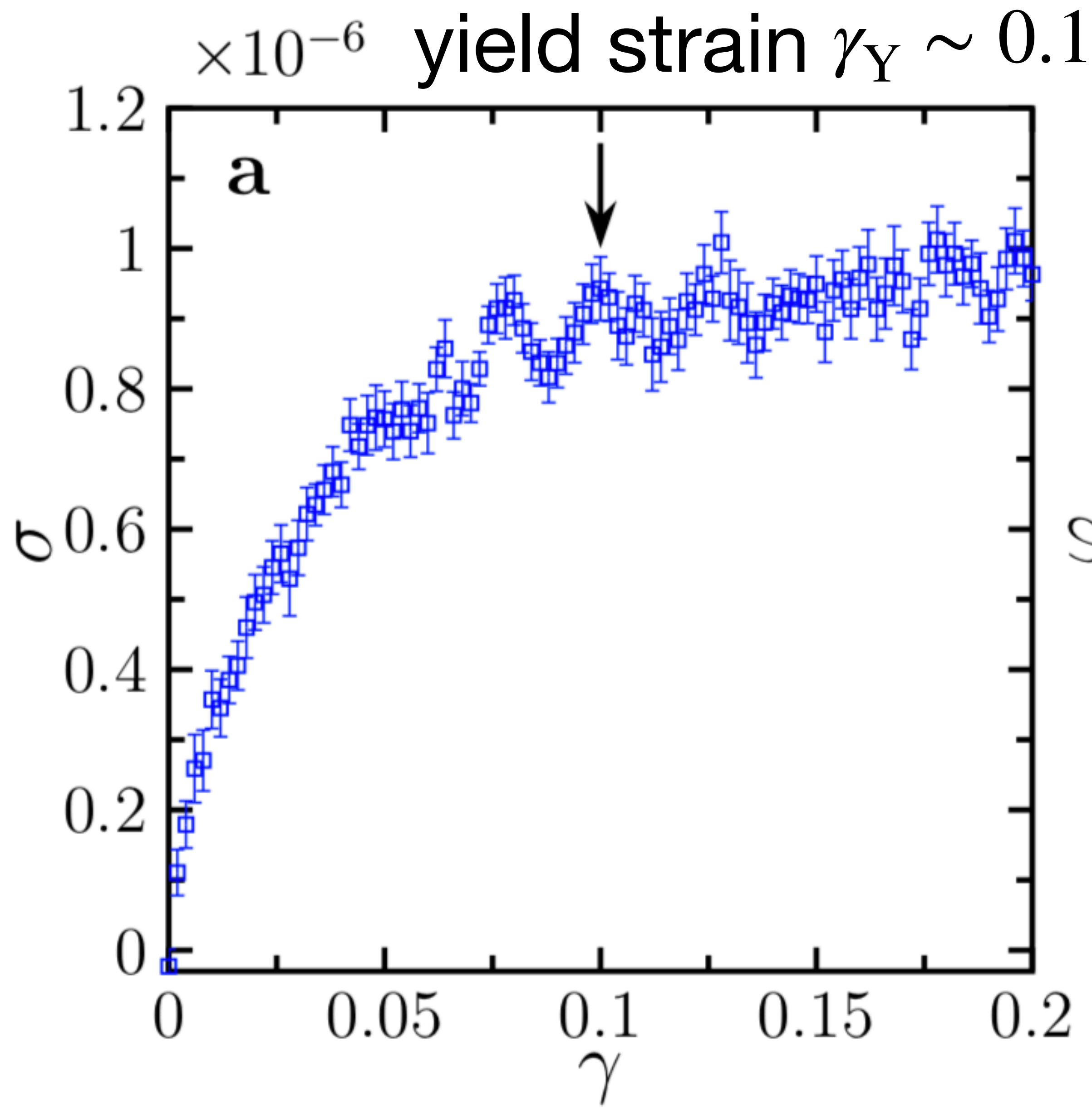
Das, Vinutha & Sastry, 2020



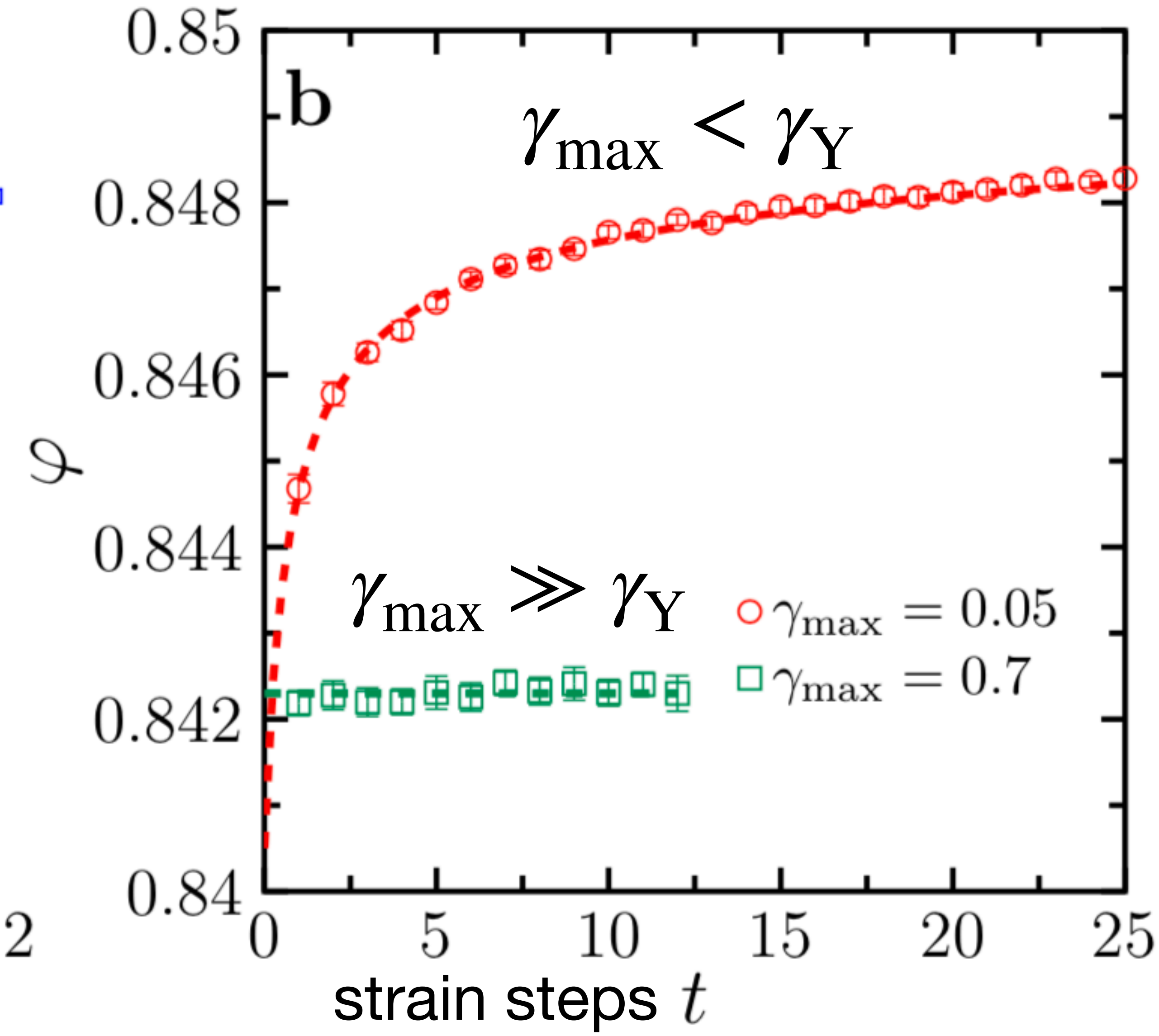
Small and large strain amplitude

constant pressure shear

simple shear



cyclic shear



t=1: one cycle

in this study: $\gamma_{max} \gg \gamma_Y$

History independence in steady states

constant volume shear:

$$\varphi \sim \varphi_{\rm J}$$

initial condition:

- rapid quench

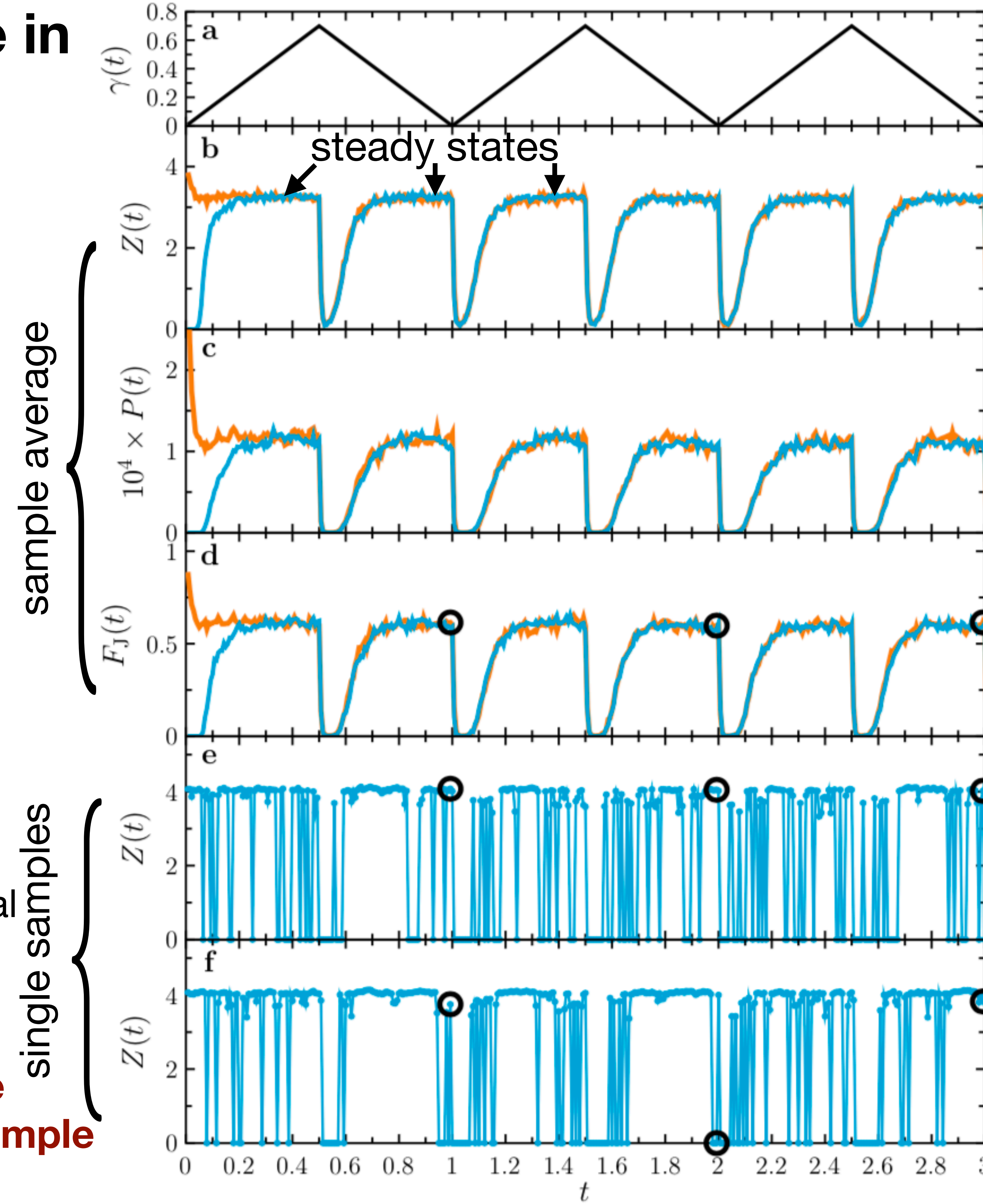
$$\varphi_{\rm j} = \varphi_{\rm J} \approx 0.843$$

- mechanically annealed

$$\varphi_{\rm j} \approx 0.848$$

Ensemble of states:

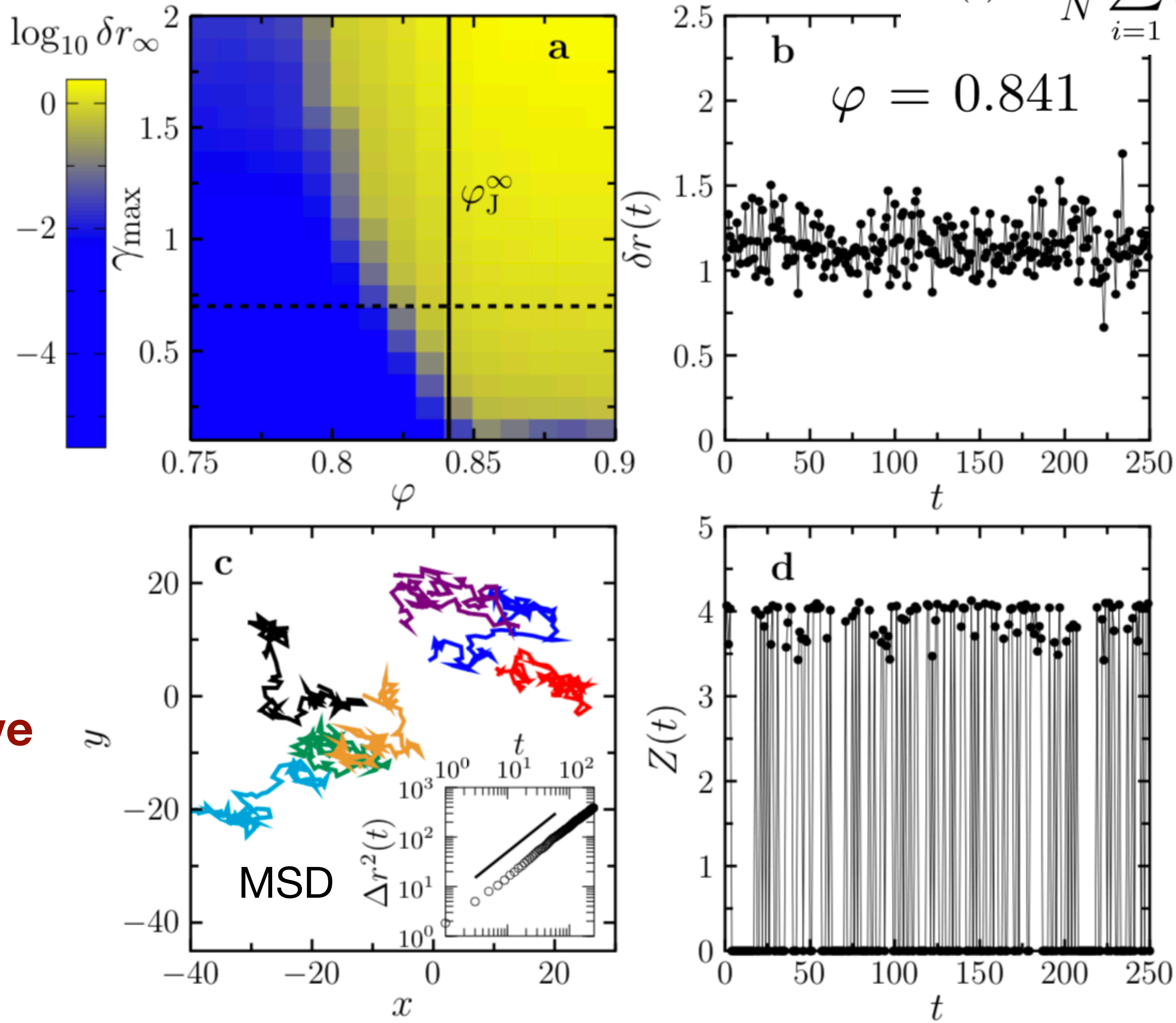
collected $\gamma = 0$ at before reversal



jamming/unjamming states are sampled through sample-to-sample fluctuations

States at the zero strain

$$\delta r(t) = \frac{1}{N}\sum_{i=1}^{N}|\mathbf{r}_i(t+1) - \mathbf{r}_i(t)|$$



irreversible

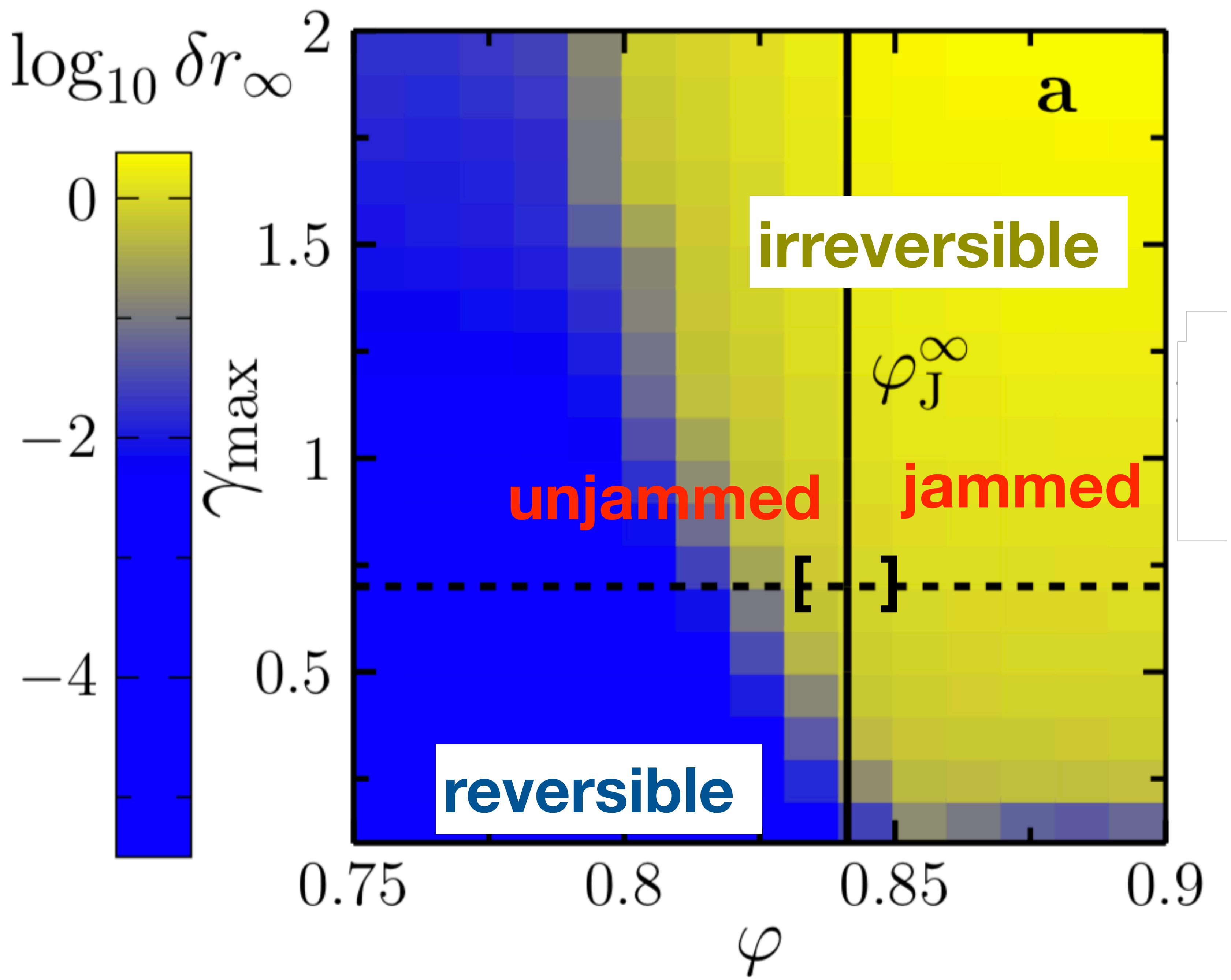
jamming

diffusive

unjamming

Jamming transition within the irreversible phase

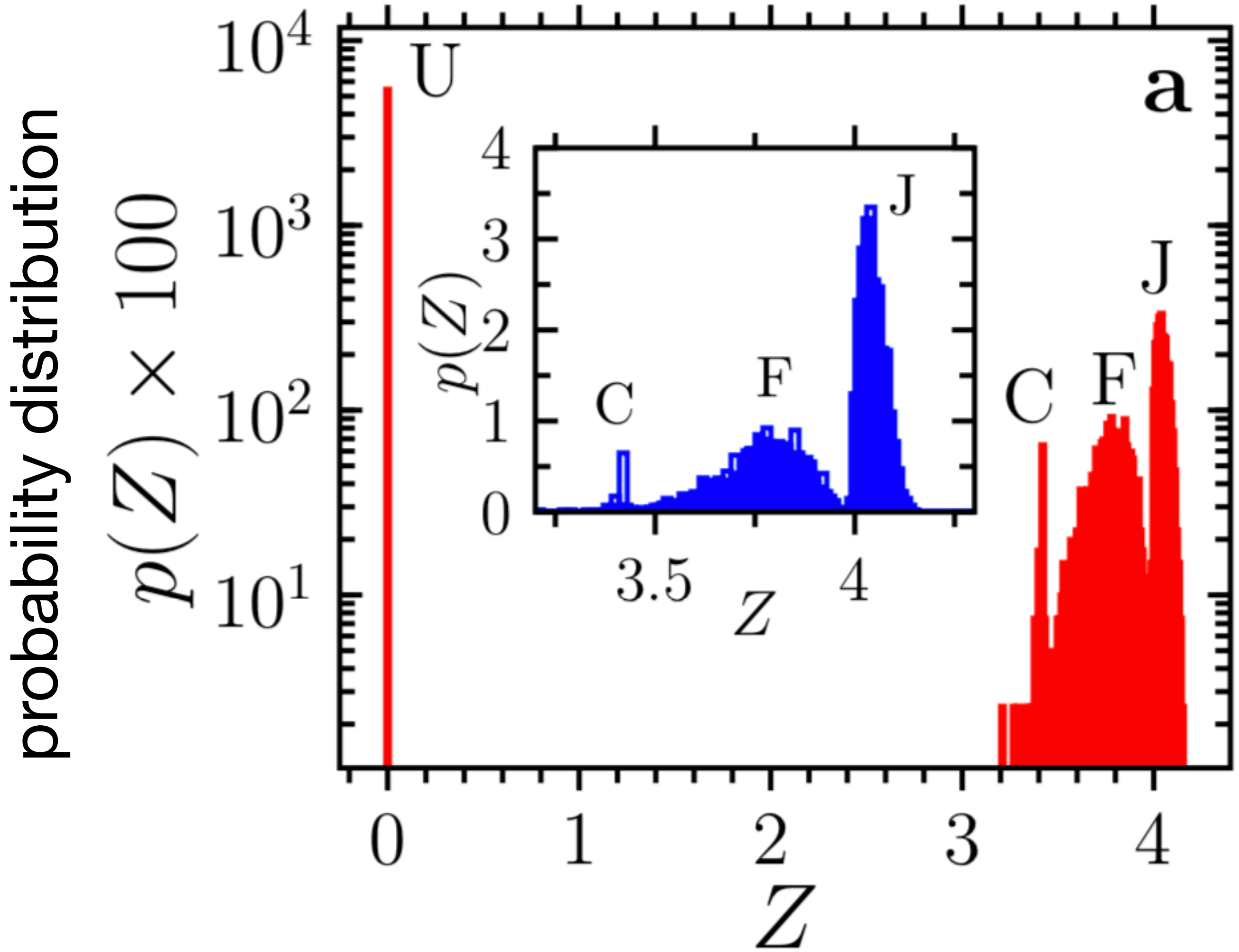
maximum strain - density phase diagram



the ensemble of states are collected:

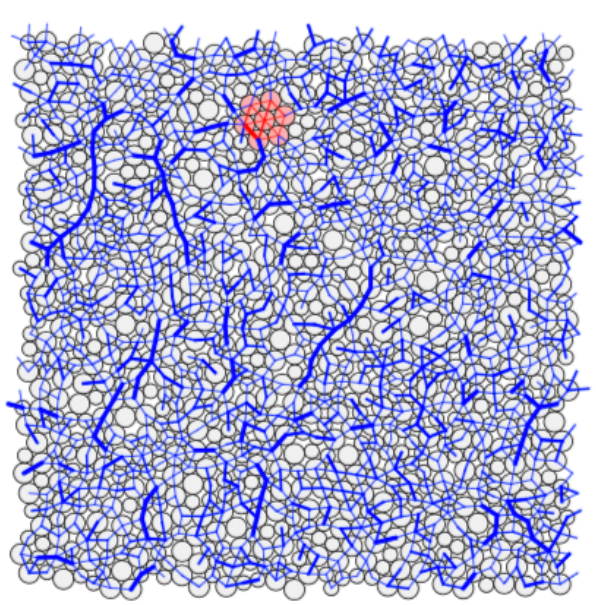
1. with $\gamma_{\max} = 0.7$ and 1.0
2. at a few φ in the irreversible phase, where the jamming transition occurs
3. at the zero strain

Four states in the ensemble: unjammed, partially crystallized, fragile and jammed

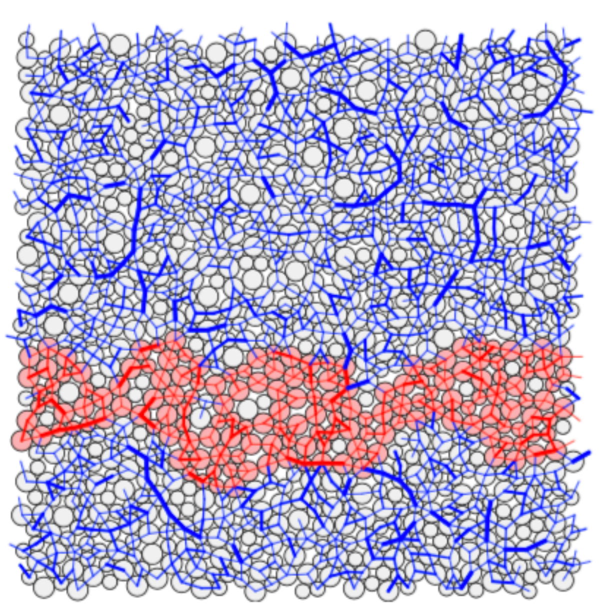


Z: order parameter

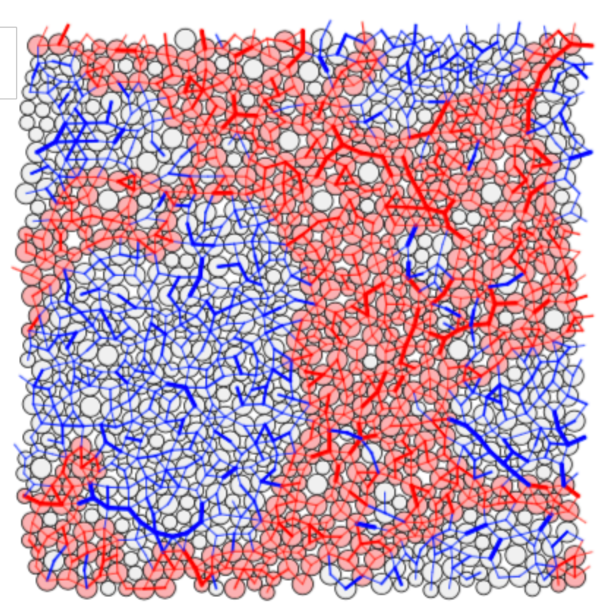
partially crystallized



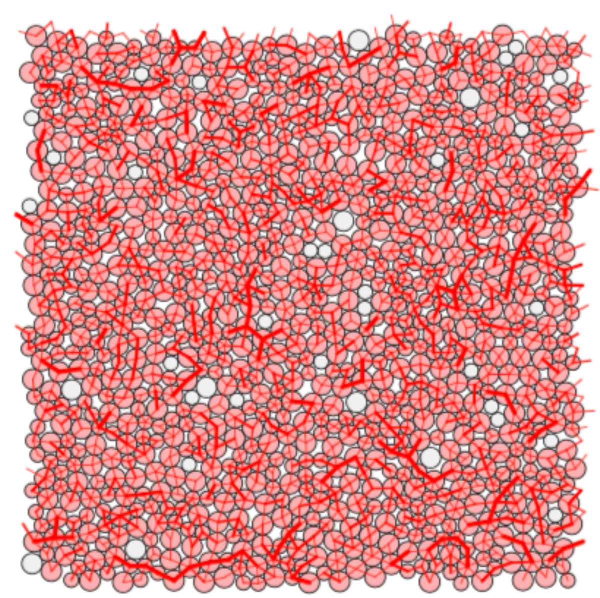
fragile I



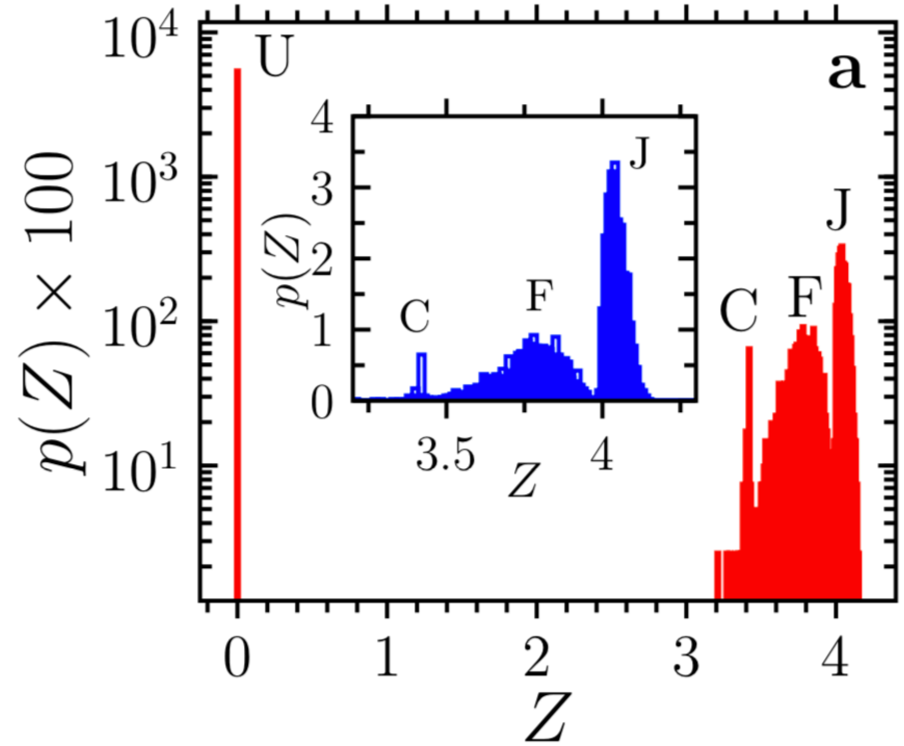
fragile II



jammed

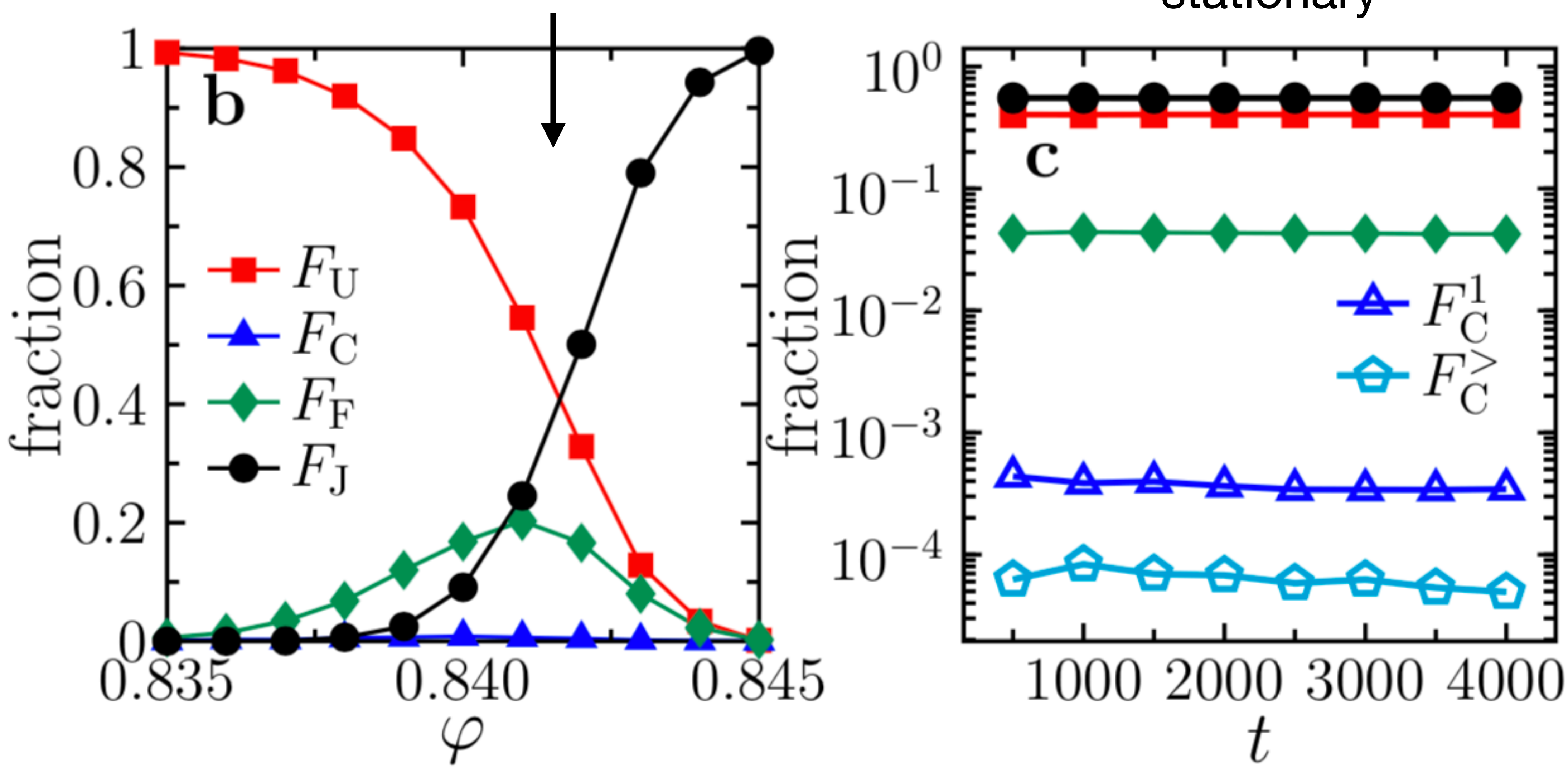


Dependence on the density and time



jamming transition

stationary

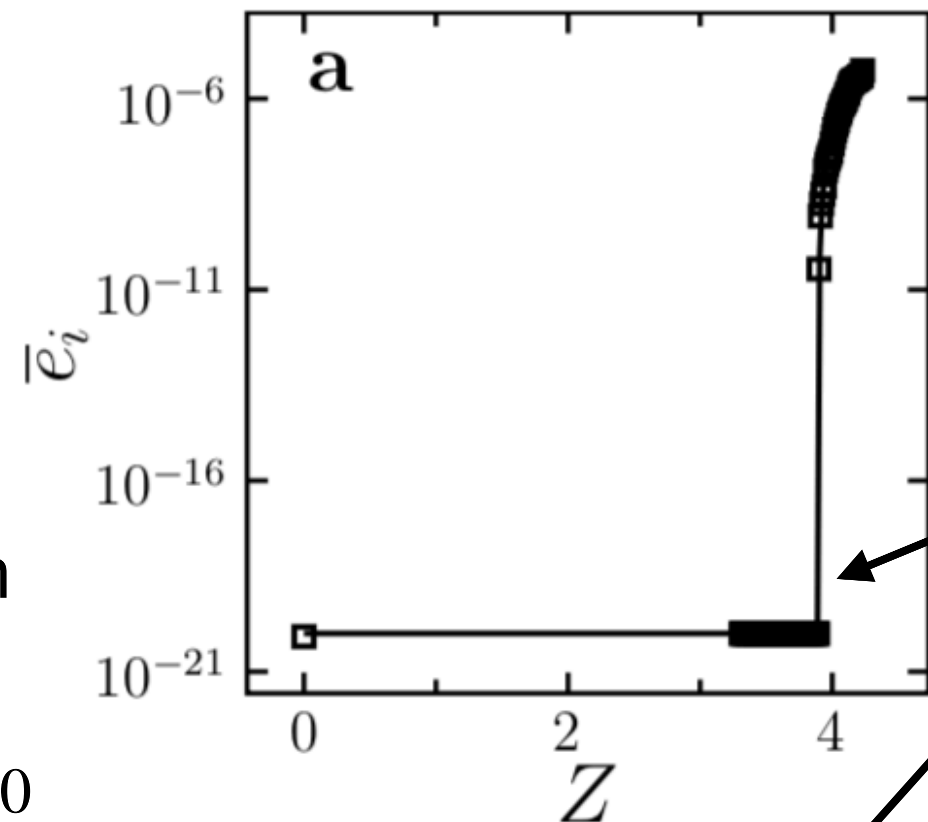


single crystal unit cell

multi crystal unit cell

Nature of fragile states

fragile states are not strictly force balanced



fragile states (0<Z<4):

- zero energy
- non-zero net force

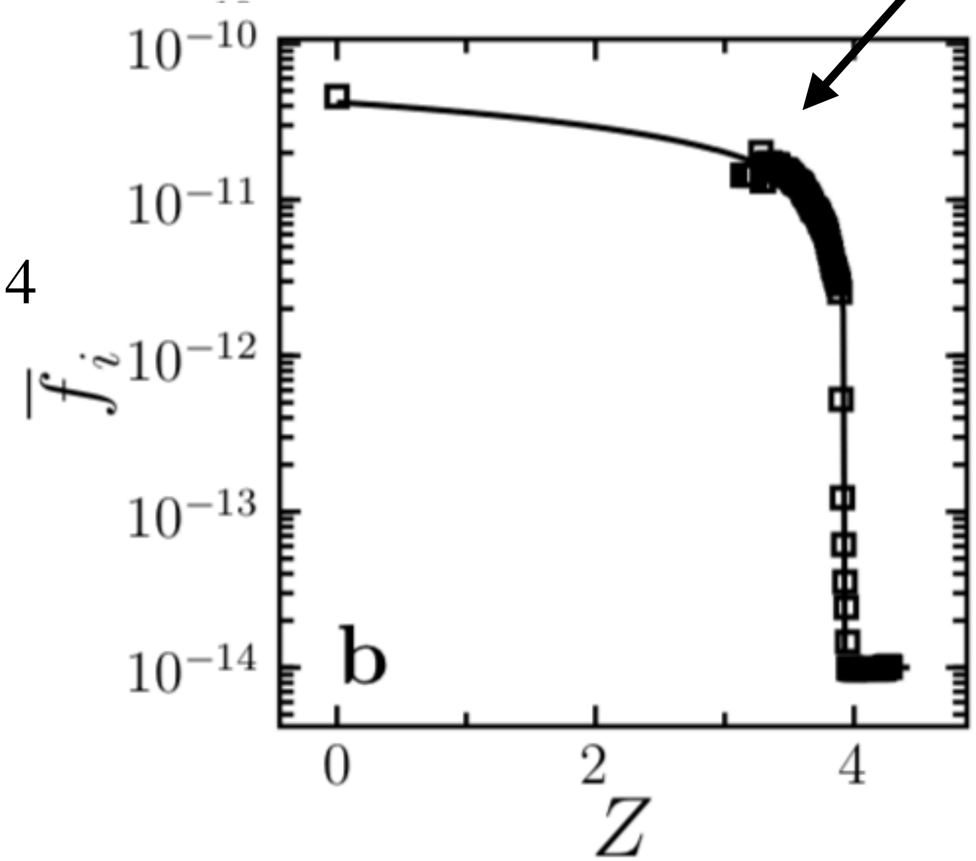
stopping criterion

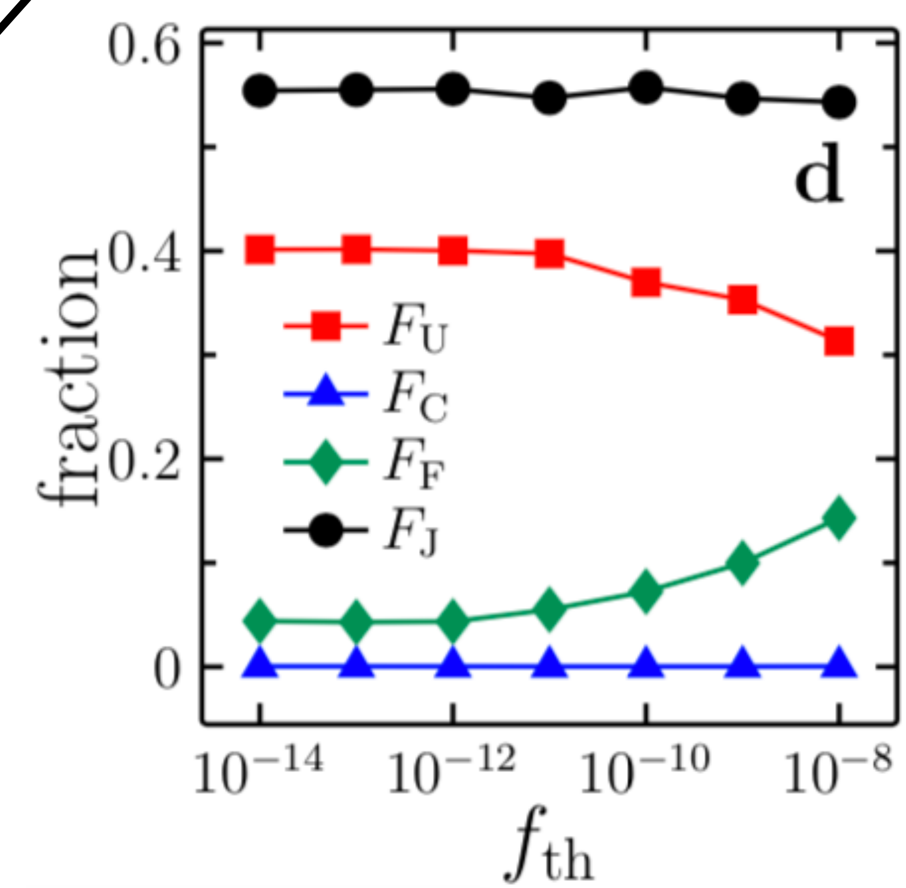
1. energy:

$$\overline{e}_i < e_{\mathrm{th}} = 10^{-20}$$

2. net force :

$$\bar{f}_i < f_{\mathrm{th}} = 10^{-14}$$





In the quasi-static limit, we should count fragile as unjammed states!

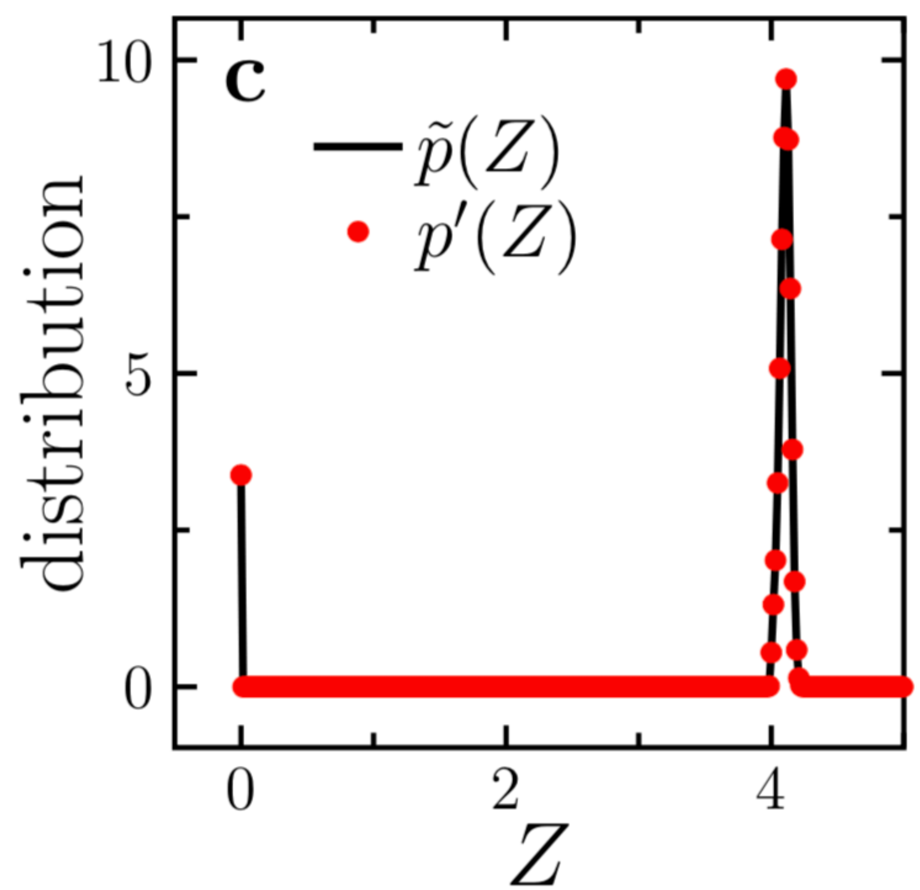
Nature of fragile states

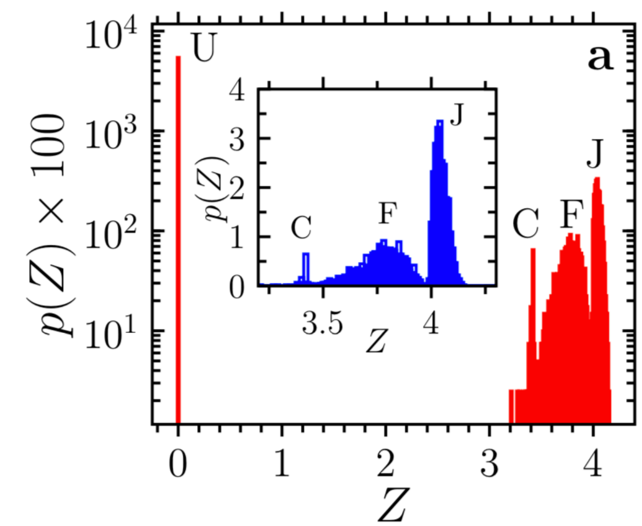
- **Fragile states are unstable to mechanical perturbations:**

after a cycle of compression-decompression, all fragile states become unjammed

$$\varphi \rightarrow \varphi + \delta\varphi \rightarrow \varphi$$

$$\delta\varphi = 10^{-8}$$



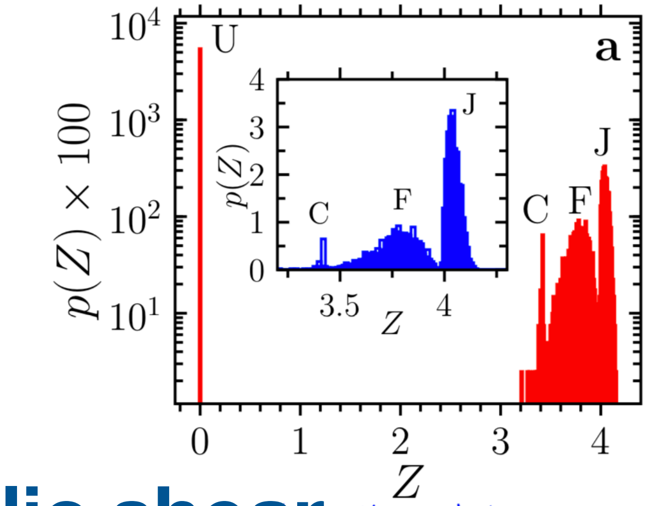


- In the following analysis, fragile and partially crystallized states are counted as unjammed.

- Only two states remain in the ensemble: unjammed (Z=0), jammed (Z>2d).

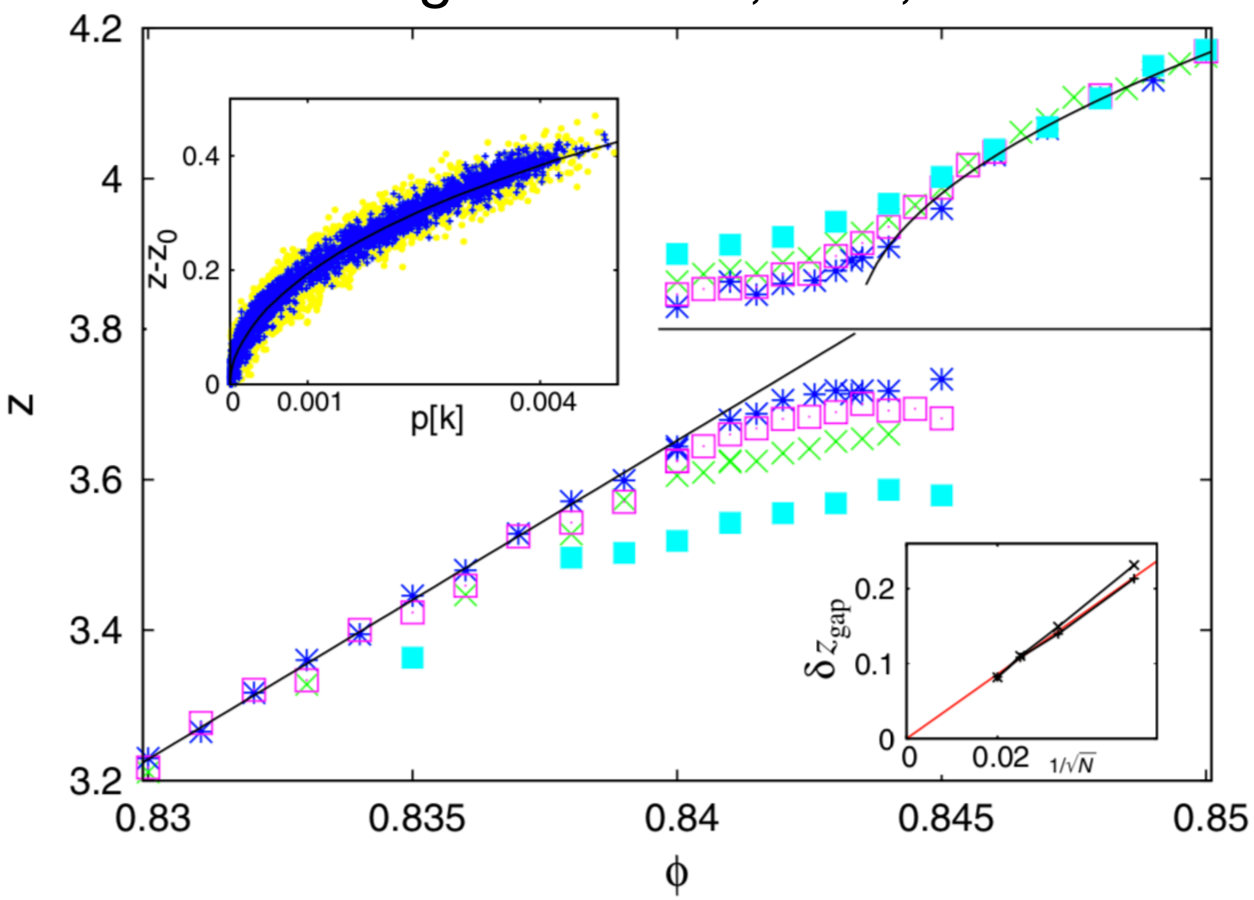
- **First-order:** P(Z) is always double-peaked.

Influence of fragile states

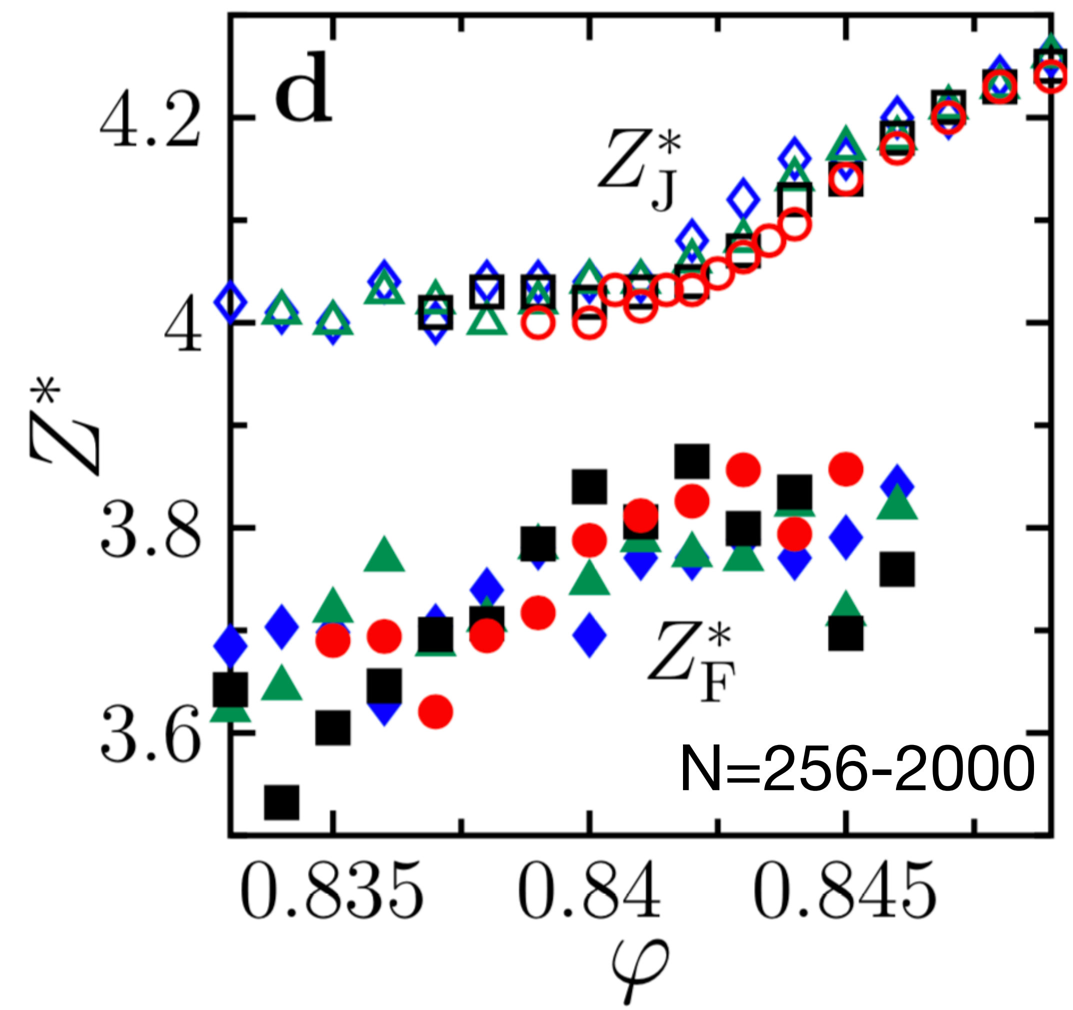


uniform shear

Heussinger & Barrat, PRL, 2009

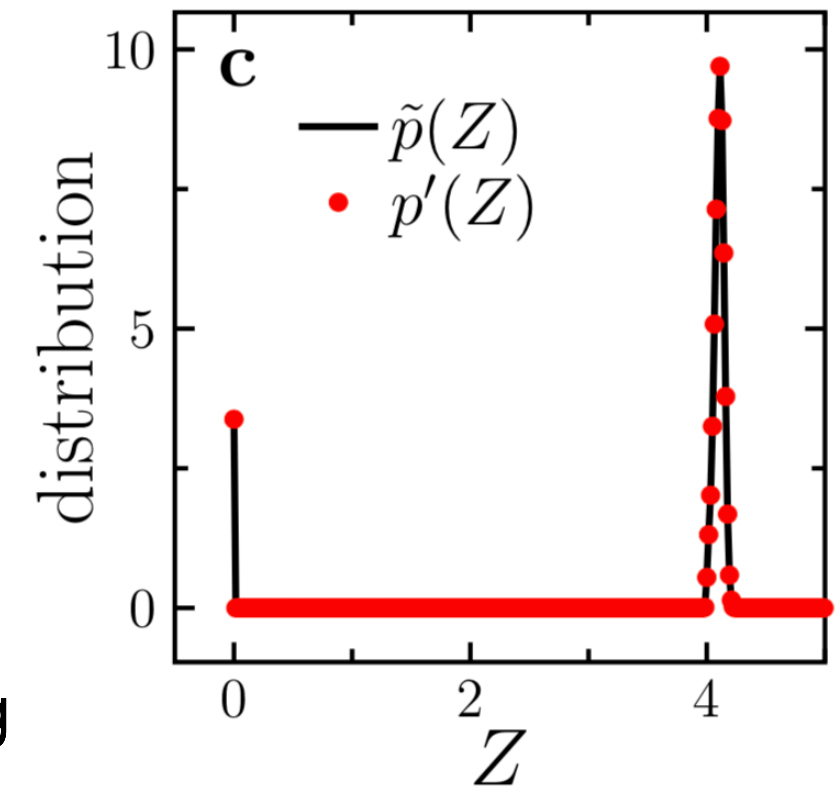


cyclic shear



- in the real quasi-static limit: fragile states should all disappear
- if fragile states are not removed, the jump in Z diminishes, and jamming might be continuous
- if fragile states are not removed, the unjamming fraction F_u is altered

Scaling form of p(Z)



fraction of jamming

$$p(Z) = (1 - F_{\rm J})\delta(Z) + F_{\rm J}\, p_{\rm J}\left[(Z - Z_{\rm J}^{*})N^{\eta}\right]$$

unjammed peak

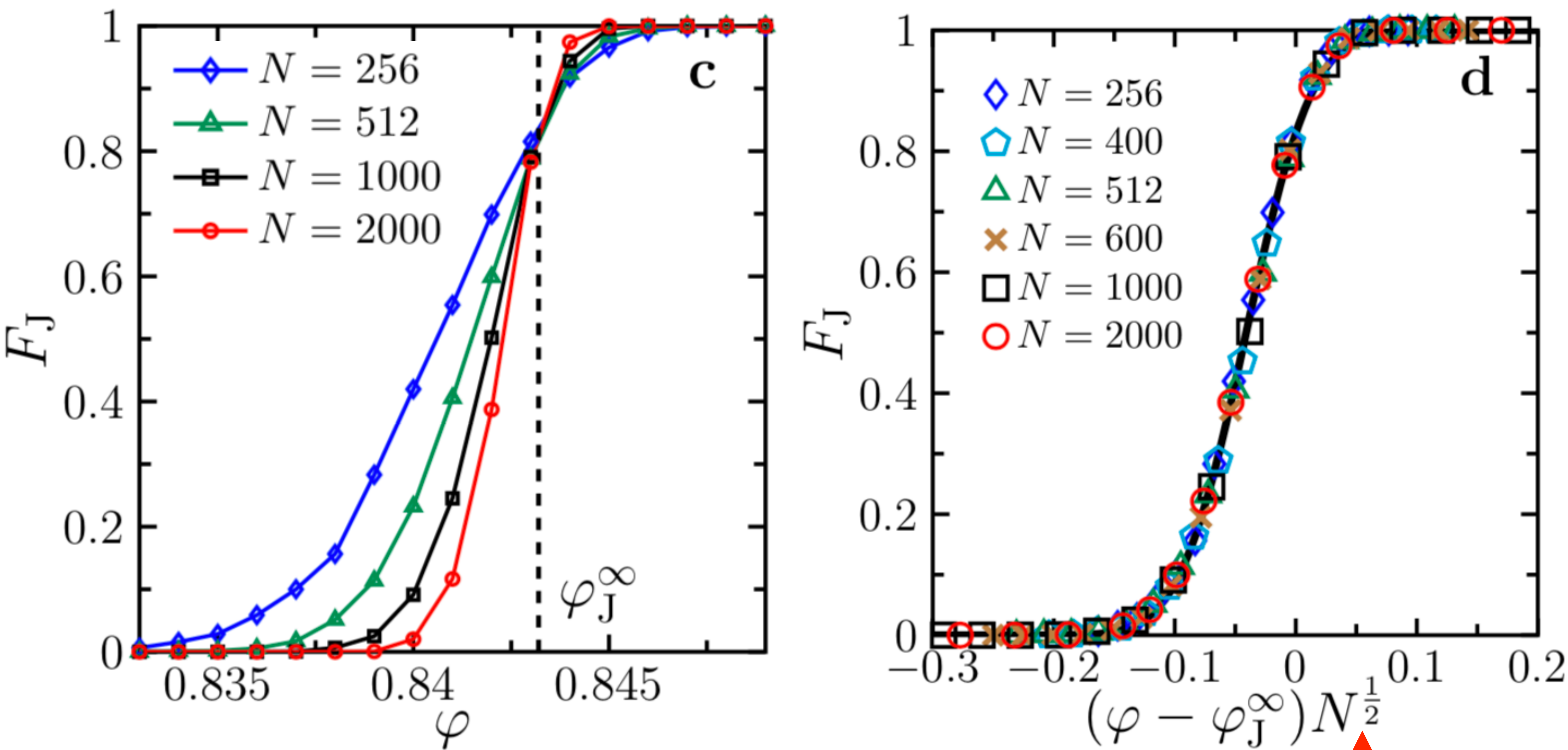
jammed peak

if jamming were a standard 1st-order transition

$$F_{\rm J}(\varphi, N) = \mathcal{F}_{\rm J}\left[(\varphi - \varphi_{\rm J}^{\infty})N\right]$$

$\lambda = 1$

Finite-size scaling of the jamming fraction



$$\varphi_J^\infty = 0.8432$$

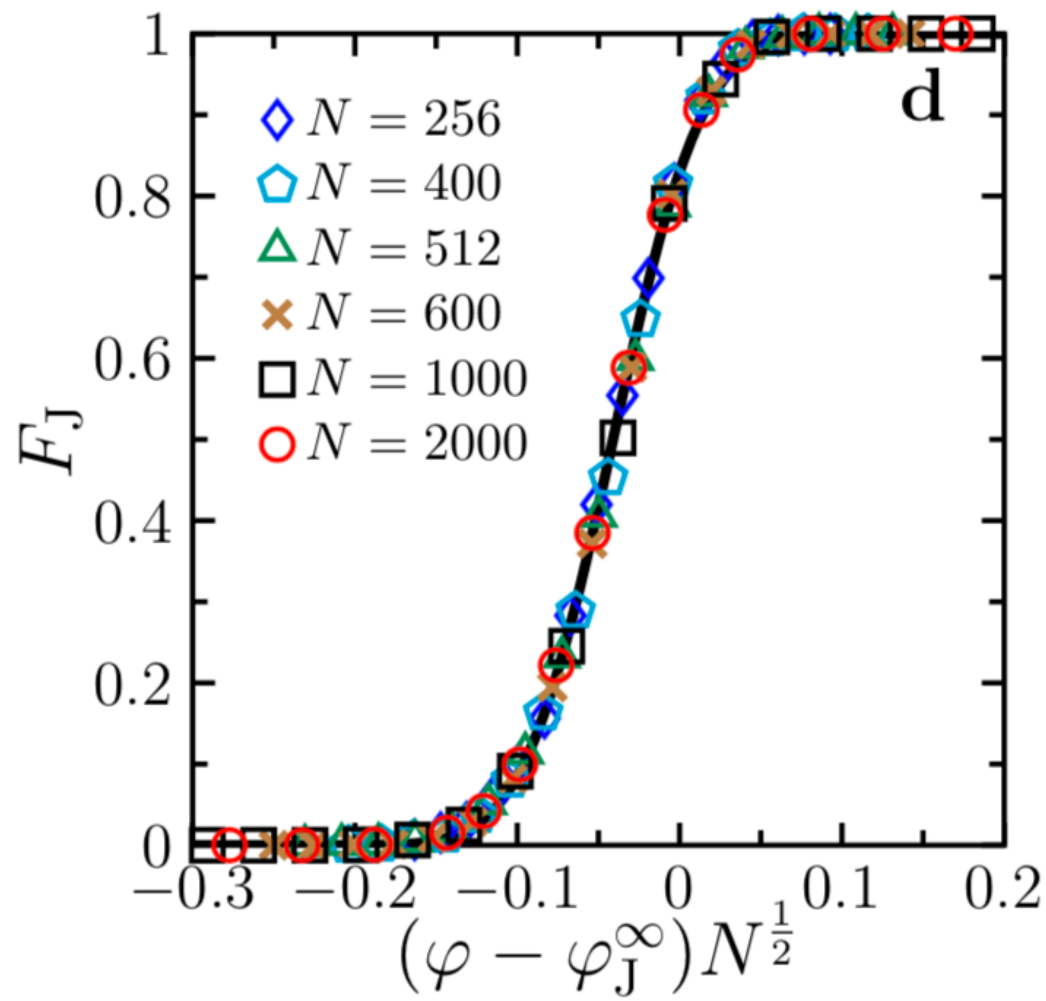
$$\lambda = 1/2$$

two dimensions

Fluctuation of the jamming transition density in finite-sized systems

$$\rho(\varphi_J^N) \sim \exp\left[-\frac{(\delta\hat{\varphi}_J + u)^2}{2\sigma_\varphi^2}\right], \quad \boxed{\delta\hat{\varphi}_J = (\varphi_J^N - \varphi_J^\infty)N^{1/2}}$$

$$F_J(\varphi, N) = \int_0^\varphi \rho(\varphi_J^N)\, d\varphi_J^N \approx \frac{1}{2} + \frac{1}{2}\mathrm{erf}\left[\frac{\delta\hat{\varphi} + u}{\sqrt{2}\sigma_\varphi}\right]$$

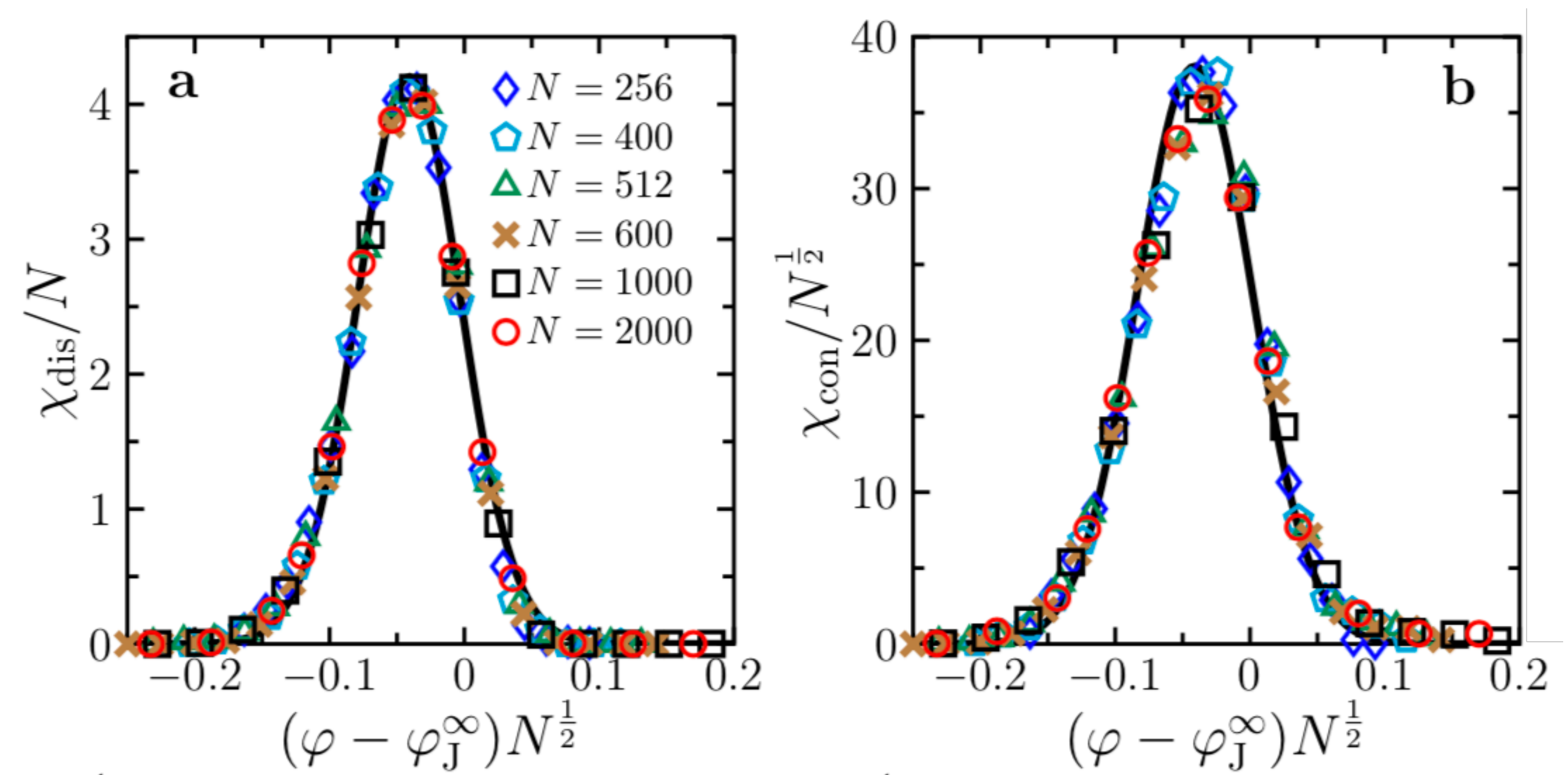


Two susceptibilities

- disconnected: $\chi_{\mathrm{dis}} \equiv N\sigma_Z^2 = N\langle(Z - \langle Z\rangle)^2\rangle$
- connected: $\chi_{\mathrm{con}} = d\langle Z\rangle/d\varphi$

$$\frac{\chi_{\mathrm{dis}}(\varphi, N)}{N} \approx (Z_{\mathrm{J}}^*)^2[1 - F_{\mathrm{J}}(\varphi, N)]F_{\mathrm{J}}(\varphi, N)$$

$$\frac{\chi_{\mathrm{con}}(\varphi, N)}{N^{1/2}} \approx \frac{Z_{\mathrm{J}}^*}{\sigma_\varphi\sqrt{2\pi}} \exp\left[-\left(\frac{\delta\hat{\varphi} + u}{\sqrt{2}\sigma_\varphi}\right)^2\right]$$

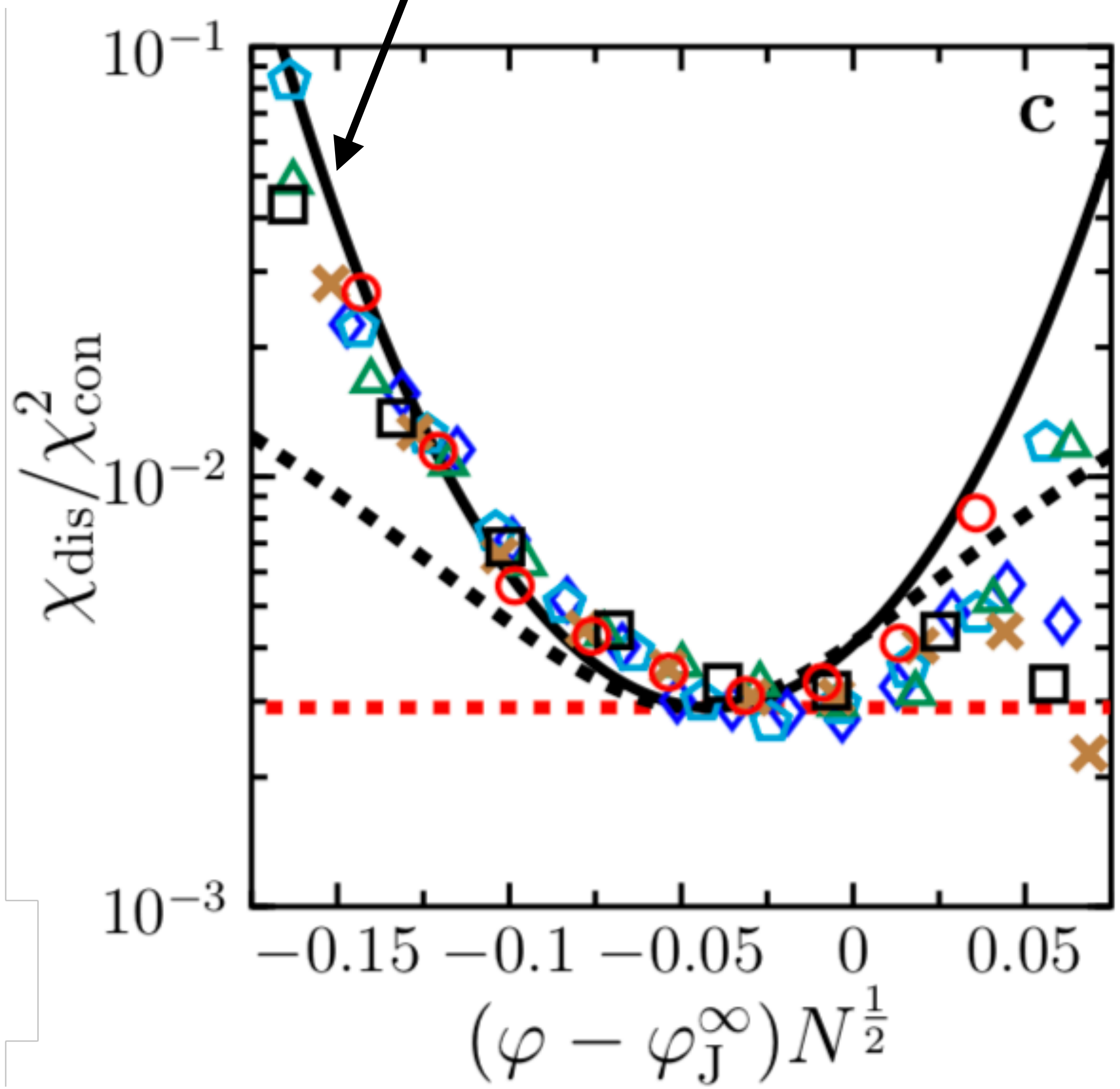


$\chi_{\mathrm{dis}} \sim N\mathscr{X}_{\mathrm{dis}}\left[(x - x_{\mathrm{c}}^{\infty})N^{1/2}\right]$ $\chi_{\mathrm{con}} \sim N^{1/2}\mathscr{X}_{\mathrm{con}}\left[(x - x_{\mathrm{c}}^{\infty})N^{1/2}\right]$

Relation between two susceptibilities

without expansion

expansion around the transition



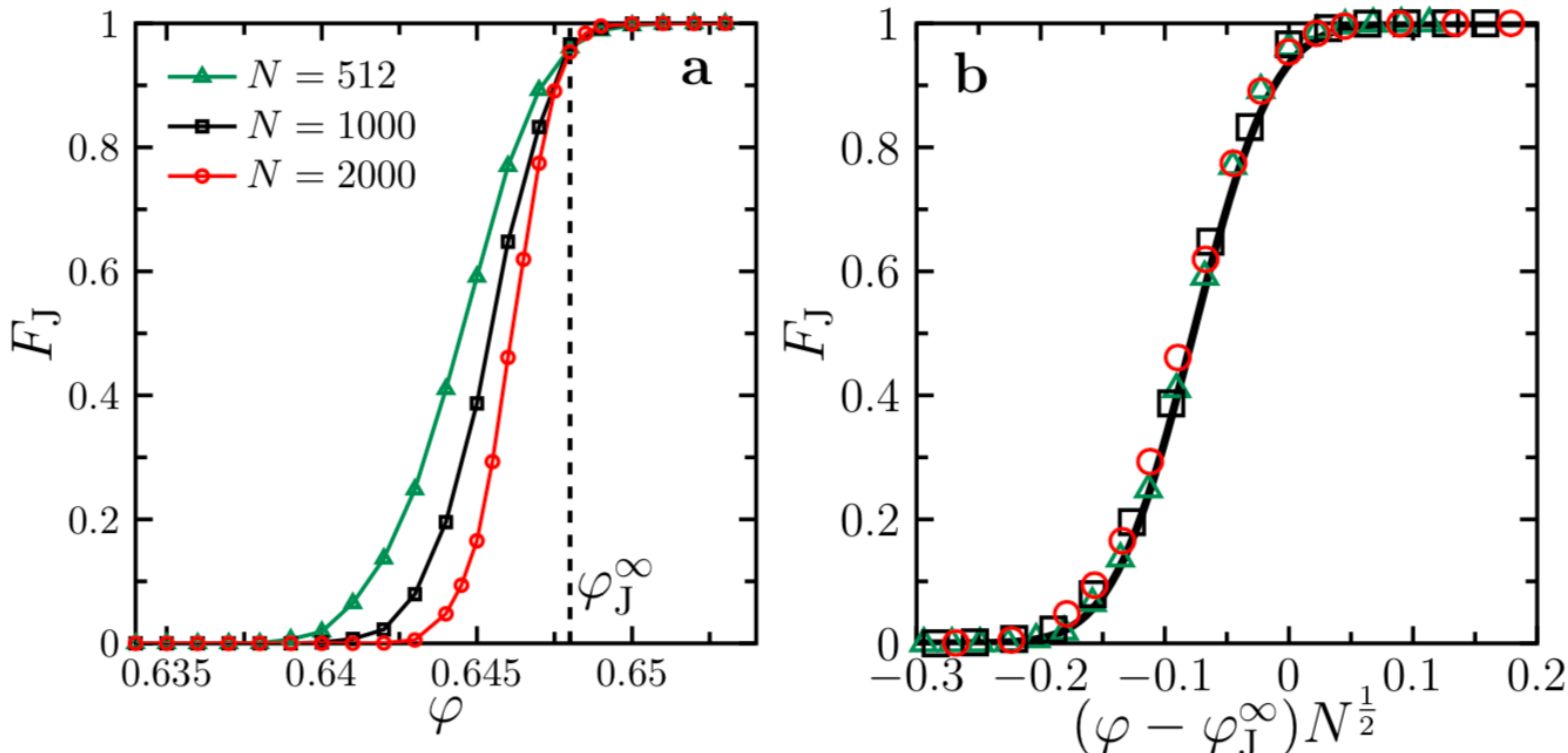
second order

$$\frac{\chi_{\rm dis}}{\chi^2_{\rm con}} \approx \frac{\pi\sigma_\varphi^2}{2}\left[1 + \left(2 - \frac{4}{\pi}\right)\left(\frac{\delta\hat{\varphi} + u}{\sqrt{2}\sigma_\varphi}\right)^2\right]$$

first order

$$\chi_{\rm dis} \sim \chi^2_{\rm con}$$

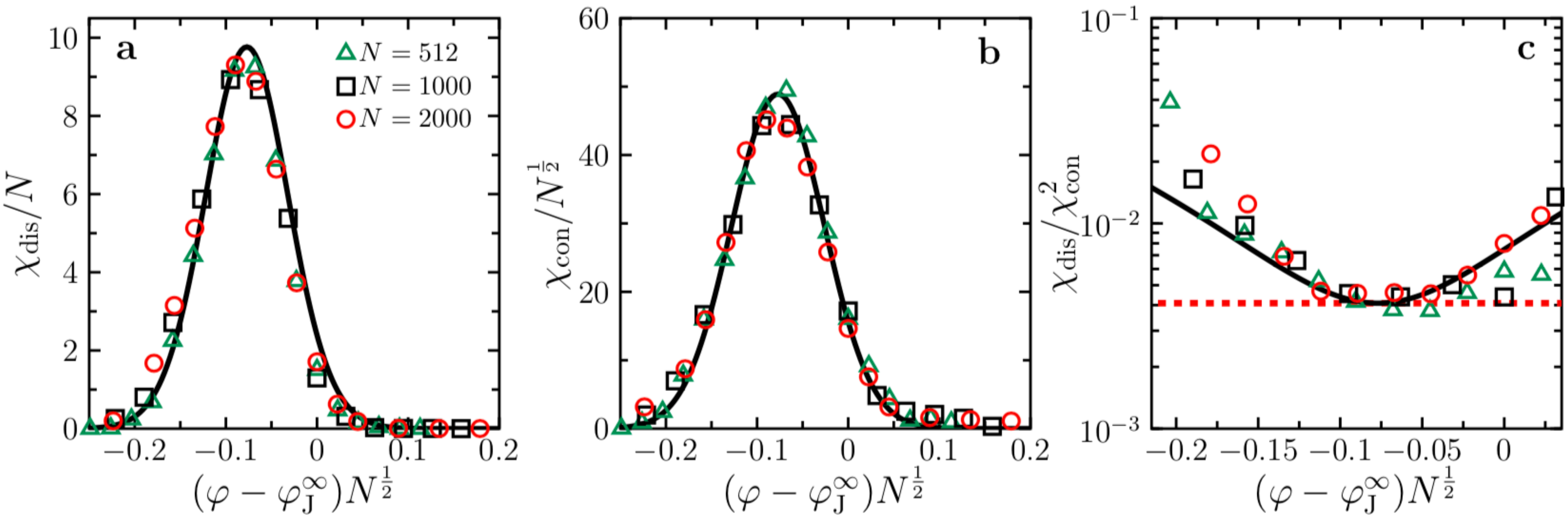
Finite-size scaling of the jamming fraction in 3D



$$\varphi_J^\infty = 0.648$$

$$\lambda = 1/2$$

Susceptibility data in 3D



$$\frac{\chi_{\rm dis}(\varphi, N)}{N} \approx (Z_{\rm J}^*)^2[1 - F_{\rm J}(\varphi, N)]F_{\rm J}(\varphi, N)$$

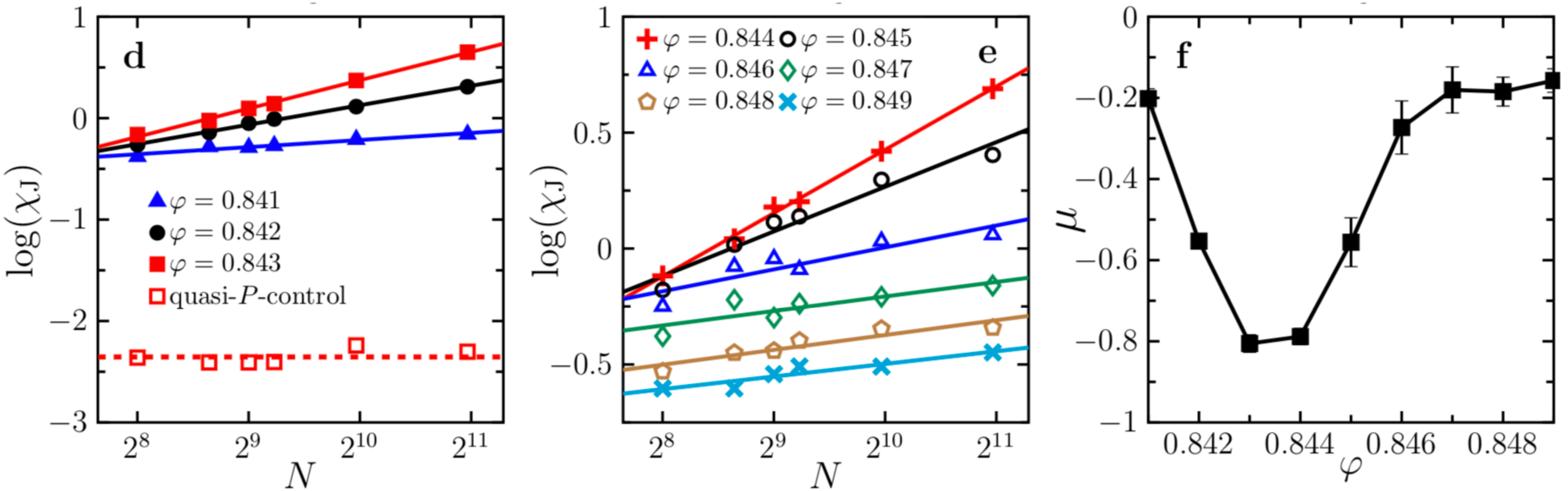
$$\frac{\chi_{\rm con}(\varphi, N)}{N^{1/2}} \approx \frac{Z_{\rm J}^*}{\sigma_\varphi\sqrt{2\pi}} \exp\left[-\left(\frac{\delta\hat{\varphi} + u}{\sqrt{2}\sigma_\varphi}\right)^2\right]$$

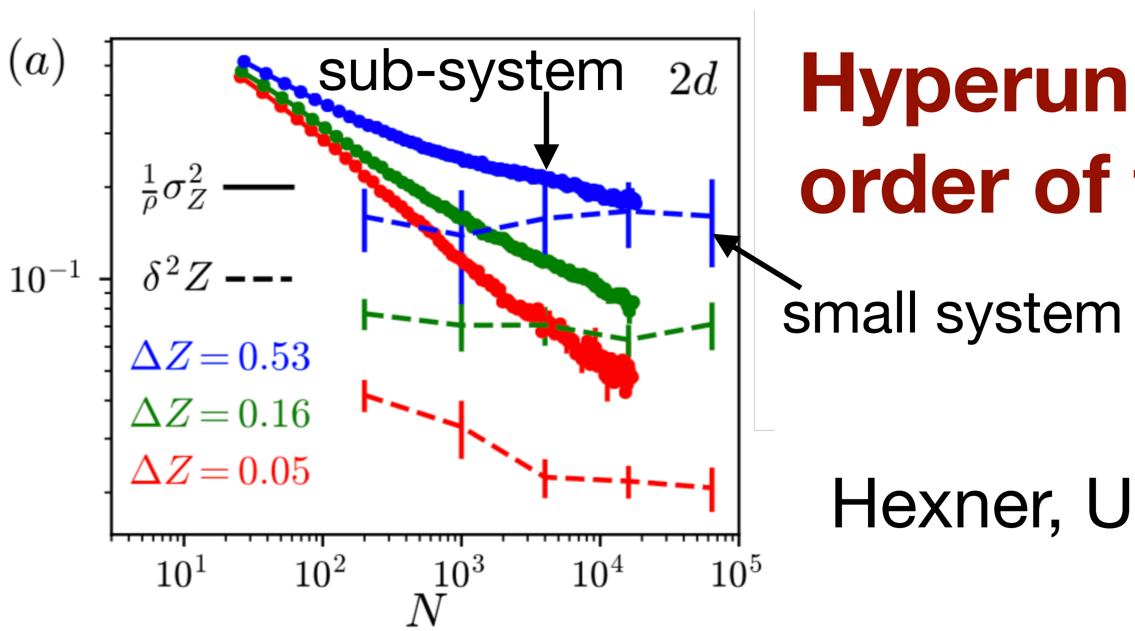
Susceptibility of jammed states

$$\chi_J \equiv N\sigma_J^2 = N\langle (Z - Z_J^*)^2 \rangle_J$$

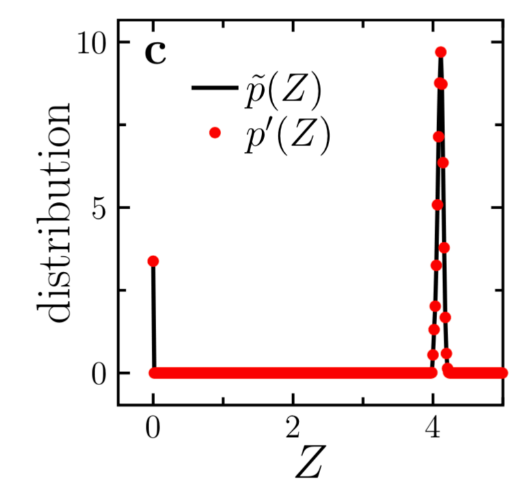
$$\chi_J \sim N^{-\mu/d}$$

(i) $\mu = 0$: uniformity
(ii) $\mu > 0$: hyperuniformity
(iii) $\mu < 0$: hyperfluctuations





Hyperuniformity is irrelevant to the order of the jamming transition.



Hexner, Urbani & Zamponi, 2019

Conclusions

Jamming is a first-order transition with quenched disorder.

conditions:

- **athermal limit:**

sample-to-sample fluctuations due to disorder >> thermal fluctuations

- **quasi-static limit:** no fragile states

The properties of the jammed (isostatic/mechanically marginal) and unjammed (Gardner) phases are irrelevant to the order of the jamming transition.

Open questions

- **In the quasi-static limit: jamming is first-order**

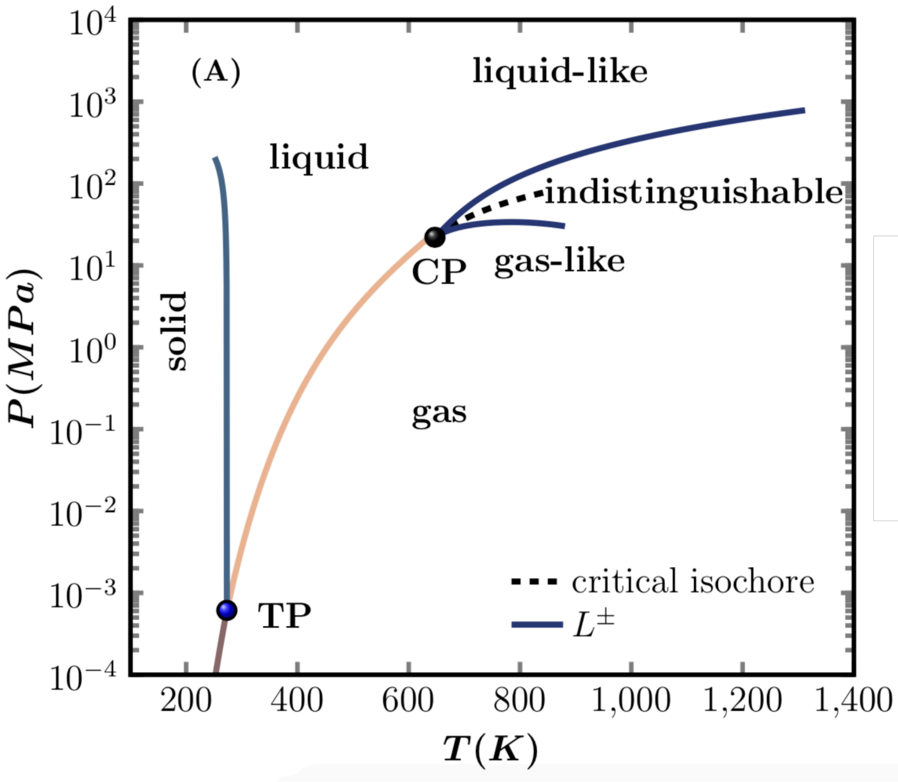
this work: arXiv:2403.01834

- **Under finite shear rates: jamming is second-order**

Olsson & Teitel, PRL, 2007

Fragile (transient) states plays a crucial role?

Unify first- and second-order jamming transitions?



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Thank you for your time and attention!