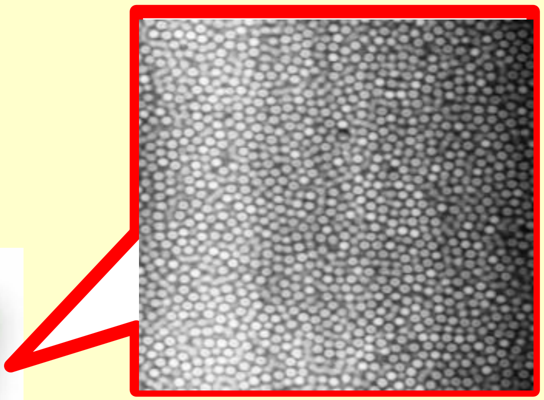
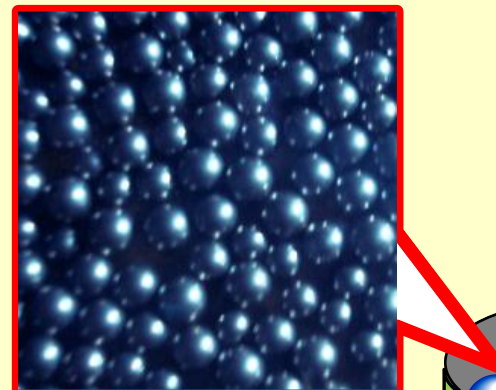
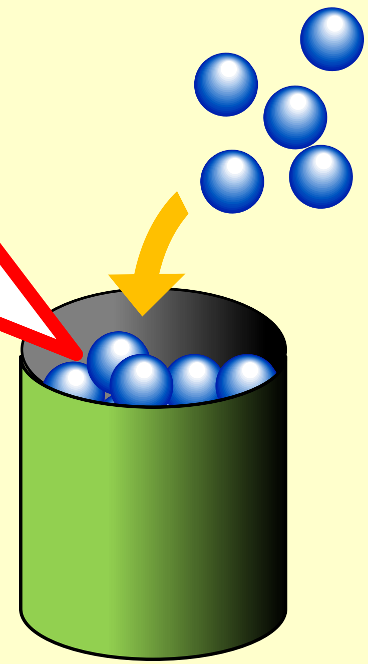
Unified Picture of Glass and Jamming Transitions







Kunimasa Miyazaki

See also arXiv:1207.6925

(Kyoto meeting 08/02/2012)

ACKNOWLEDGEMENTS

Misaki Ozawa
Takeshi Kuroiwa
Atsushi Ikeda

Funded by

2006 - 2010
NEQ SOFT
Non-equilibrium soft matter physics

筑波大学
University of Tsukuba

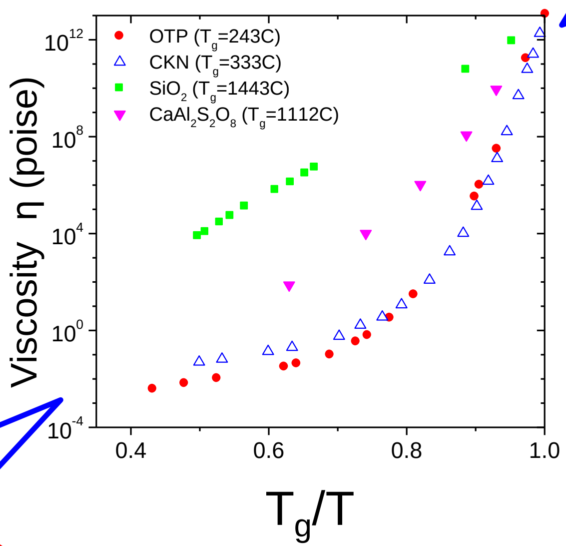
OVERVIEW

- *Introduction*
- *Mean Field Scenario of the Glass Transition*
  - *Glass Transition in Higher Dimensions*
  - *Glass Transition of Long-Ranged Systems*
- *Jamming Transition versus Glass Transition*
- *Conclusions*

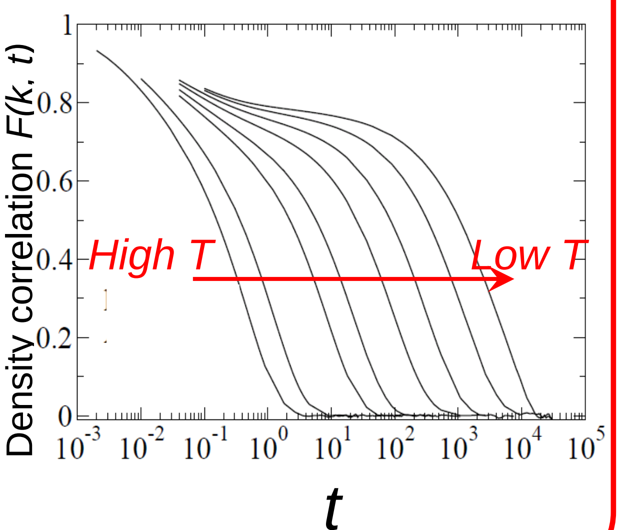
INTRODUCTION

What is the Glass Transition?

Macroscopic dynamics



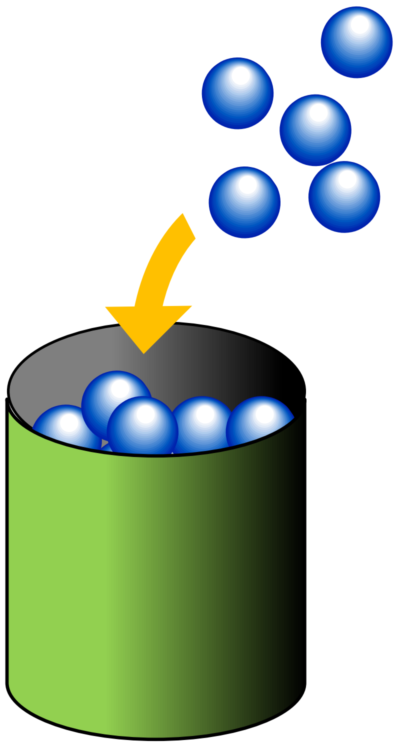
Microscopic dynamics



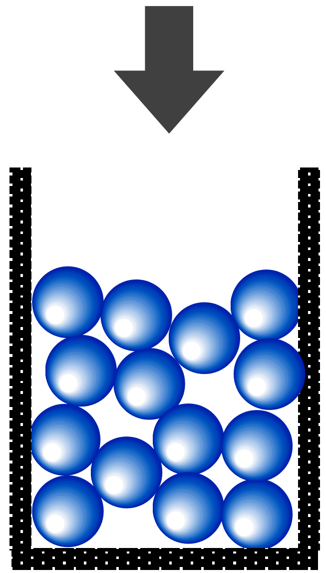
Drastic slow down of dynamics of supercooled liquids at low temperatures or at high densities

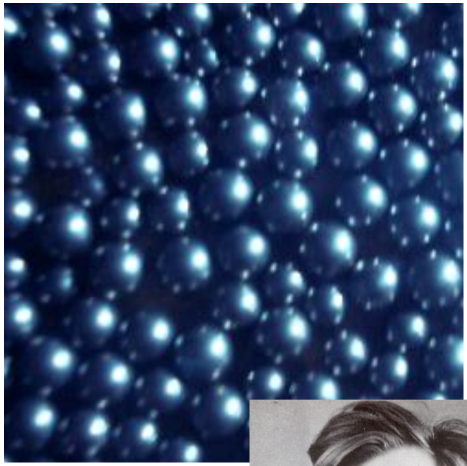
INTRODUCTION

What is the Jamming Transition?

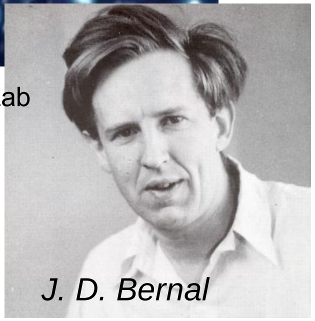


g or P





From HP Tanaka 's Lab

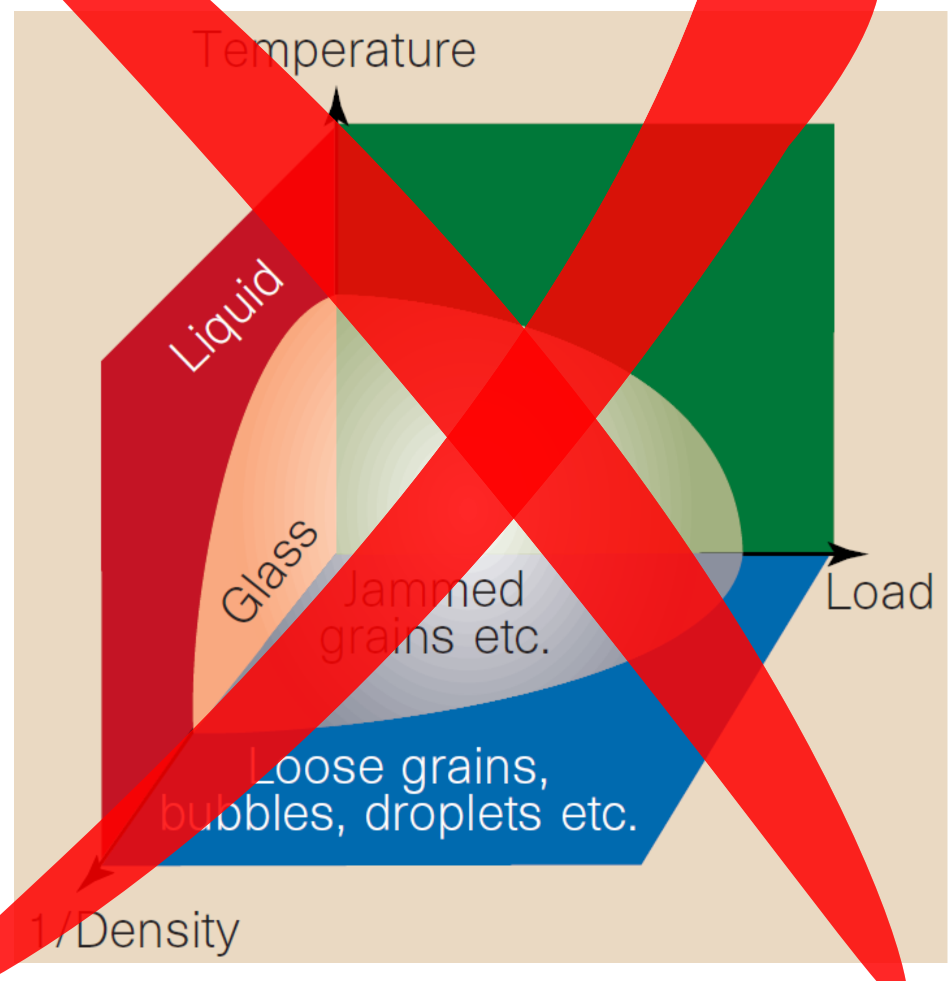


J. D. Bernal

- *The volume fraction (density) of the hard balls poured into a jar randomly is always about* $\varphi_{\mathrm{J}} \approx 64\%$ *! !*
- *It flows under external stresses (such as the shear force)*

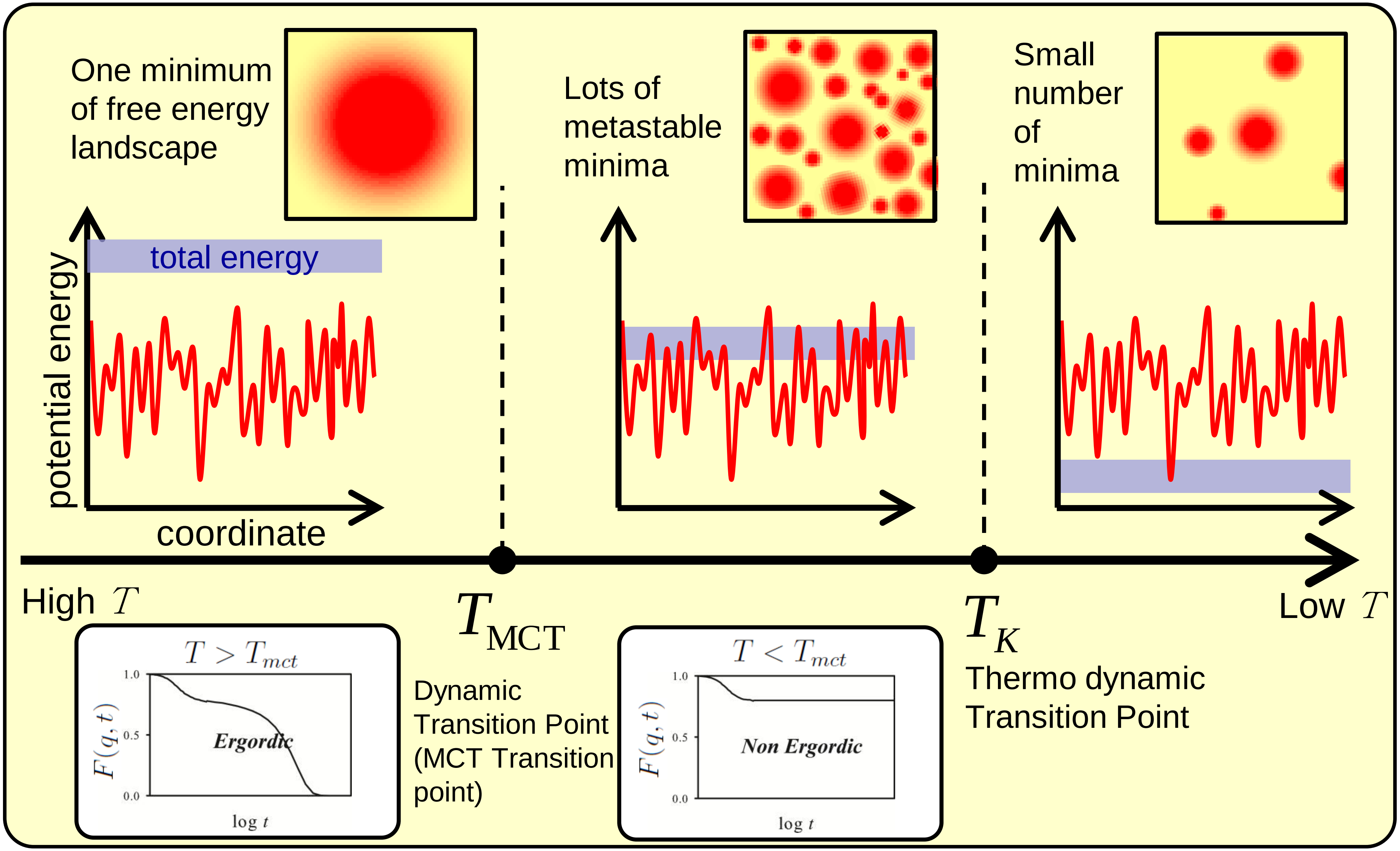
INTRODUCTION

What is the relation btwn Glass and Jamming Transition?

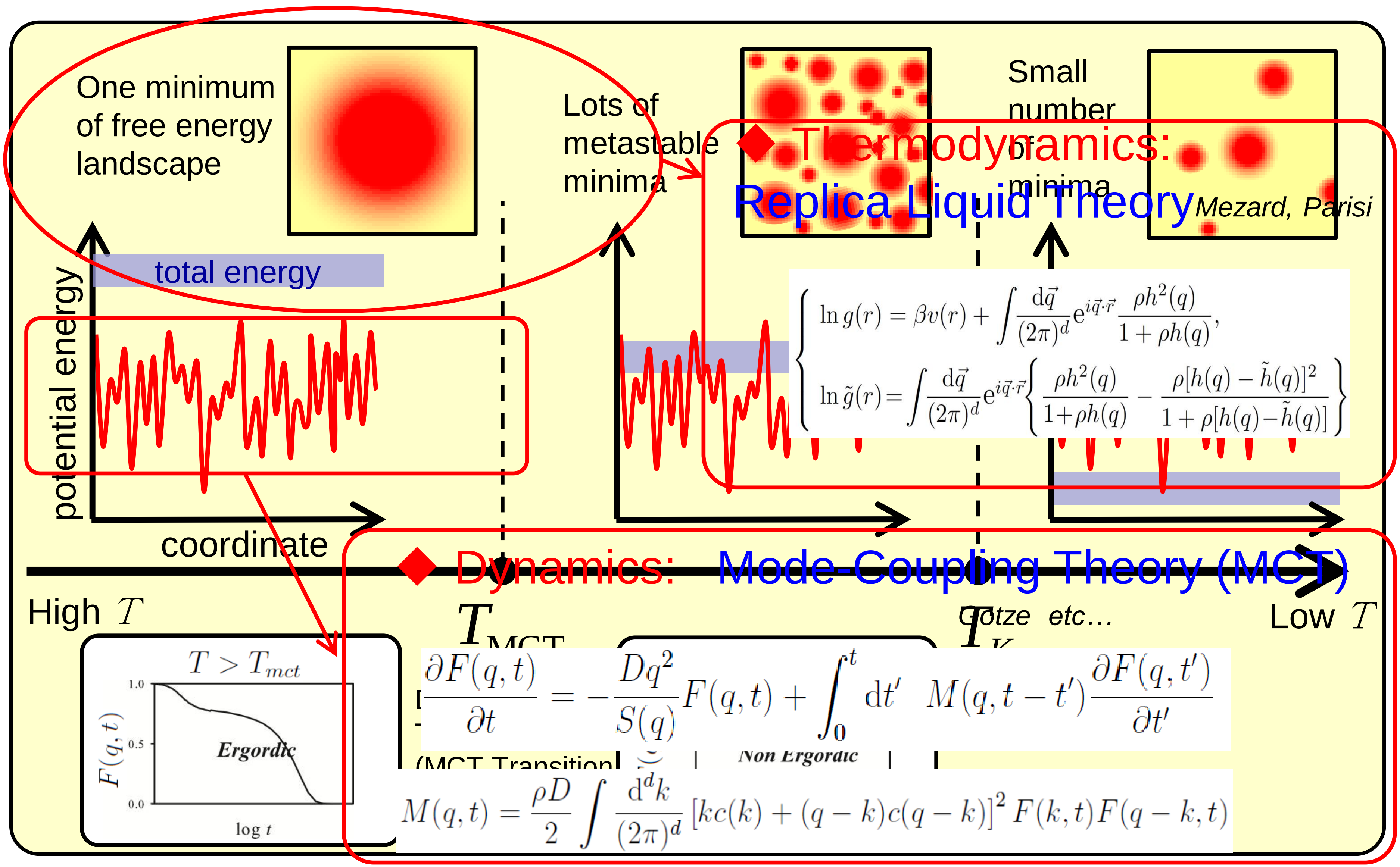


Liu and Nagel, Nature 1998

Mean Field Scenario of the Glass transition



Mean Field "Theory" of the Glass transition



◆ Thermodynamics: Replica Liquid Theory *Mezard, Parisi*

$$\begin{cases} \ln g(r) = \beta v(r) + \int \frac{d\vec{q}}{(2\pi)^d} e^{i\vec{q}\cdot\vec{r}} \frac{\rho h^2(q)}{1+\rho h(q)}, \\ \ln \tilde{g}(r) = \int \frac{d\vec{q}}{(2\pi)^d} e^{i\vec{q}\cdot\vec{r}} \left\{ \frac{\rho h^2(q)}{1+\rho h(q)} - \frac{\rho[h(q)-\tilde{h}(q)]^2}{1+\rho[h(q)-\tilde{h}(q)]} \right\} \end{cases}$$

◆ Dynamics: Mode-Coupling Theory (MCT) *Götze etc…*

$$\frac{\partial F(q,t)}{\partial t} = -\frac{Dq^2}{S(q)} F(q,t) + \int_0^t dt' \; M(q,t-t') \frac{\partial F(q,t')}{\partial t'}$$

$$M(q,t) = \frac{\rho D}{2} \int \frac{d^d k}{(2\pi)^d} \left[kc(k) + (q-k)c(q-k)\right]^2 F(k,t) F(q-k,t)$$

Mean Field Scenario of the Glass transition

If this mean field scenario is correct,

- *MCT should work better in Higher Dimensions*

- *MCT should work better for Long-Ranged Systems*

- *Dynamic (MCT) transition point should mark the qualitative change of the free energy landscape (inherent structures)*

Mean Field Scenario of the Glass transition

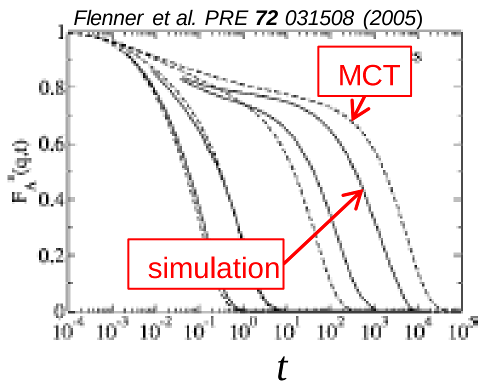
MD vs MCT for hard sphere glasses at d=4

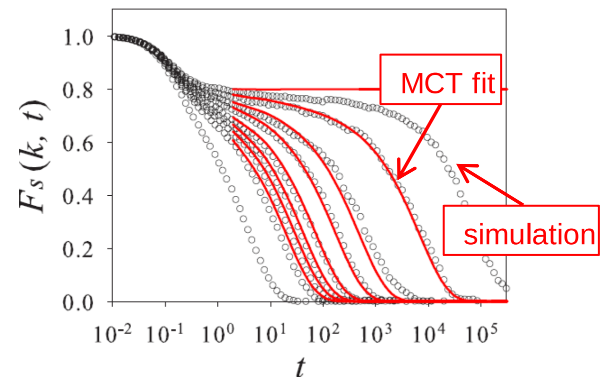
P. Charbonneau, A. Ikeda, J. A. van Meel, and KM, PRE (2010)

d=3

d=4

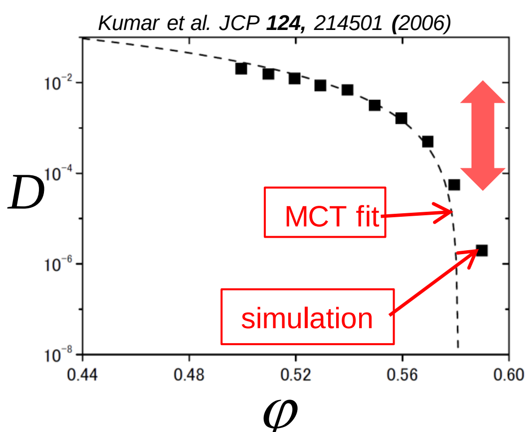
Density correlation

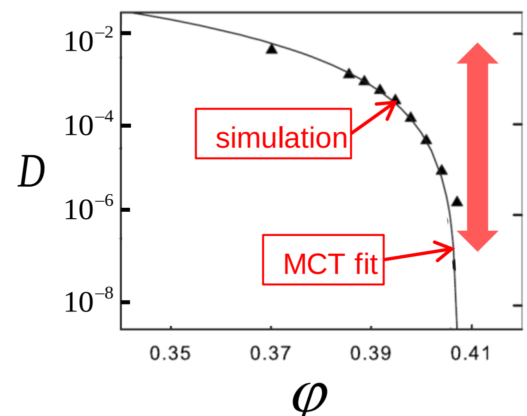




Diffusion constant

$$D \propto |\varphi - \varphi_{mct}|^{\gamma}$$





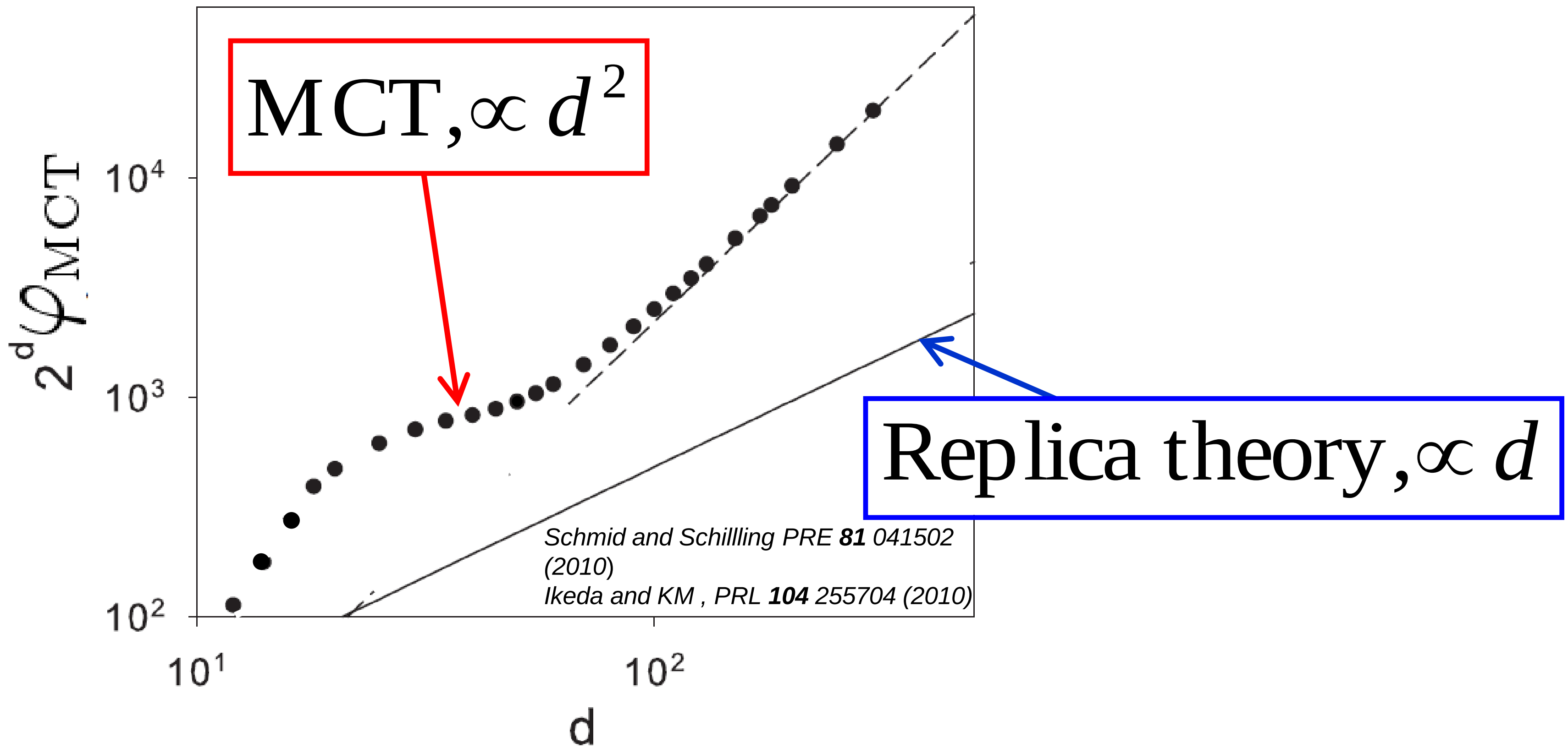
MCT's critical scaling works better at higher dimensions!

Mean Field Scenario of the Glass transition

But, not at VERY high dimensions…

MCT becomes less quantitative as *d* increases

*A. Ikeda and KM , PRL **104** 255704 (2010)*



See also Charbonneau, Ikeda, Parisi, and Zamponi, PRL **107** (2011) 185702

Mean Field Scenario of the Glass transition

If this mean field scenario is correct,

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???

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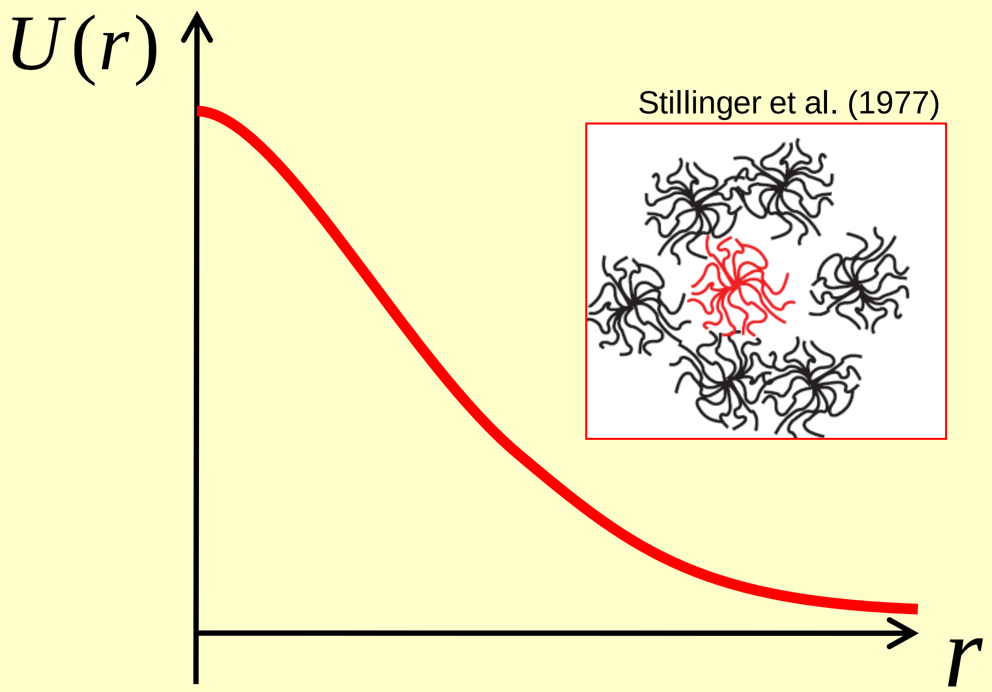
Mean Field Scenario of the Glass transition

Glass Transition of Long-Ranged Systems

Long-ranged Potential = Dense Ultra-Soft Potential

Gaussian Core Model (GCM)

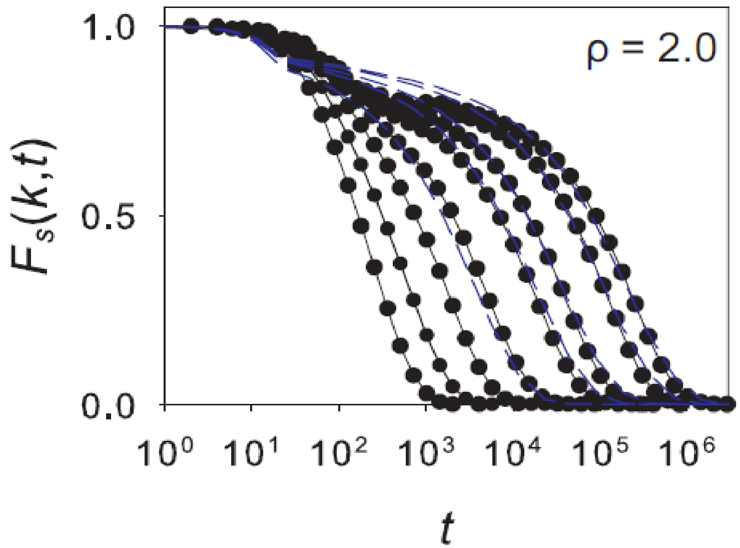


$$U(r) = \varepsilon \exp\left[-\frac{r^2}{\sigma^2}\right]$$

Mean Field Scenario of the Glass transition

Glass Transition of Long-Ranged Systems

MCT works unprecedentedly well!!



	KA LJ	GCM (ρ = 1.5)	GCM (ρ = 2.0)
T_{mct} (simulation+fitting)	0.435	0.202×10^{-5}	0.266×10^{-6}
T_{mct} (theory)	0.922	0.266×10^{-5}	0.340×10^{-6}
Deviations	112 %	33 %	28 %

INTRODUCTION

If this mean field scenario is correct,

- *MCT should work better in Higher Dimensions*

???

- *MCT should work better for Long-Ranged Systems*

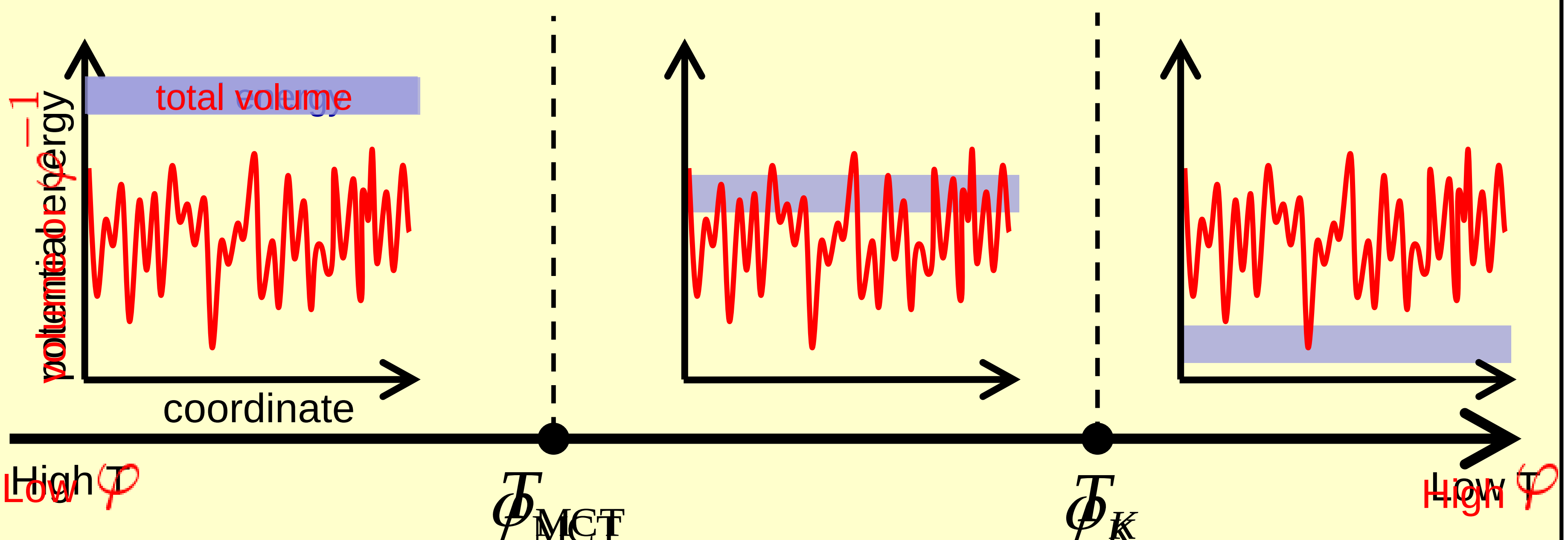
- *Dynamic (MCT) transition point should mark the qualitative change of the free energy landscape (inherent structures)*

Jamming Transition versus Glass Transition

Free energy landscape (inherent structures) for hard sphere fluids

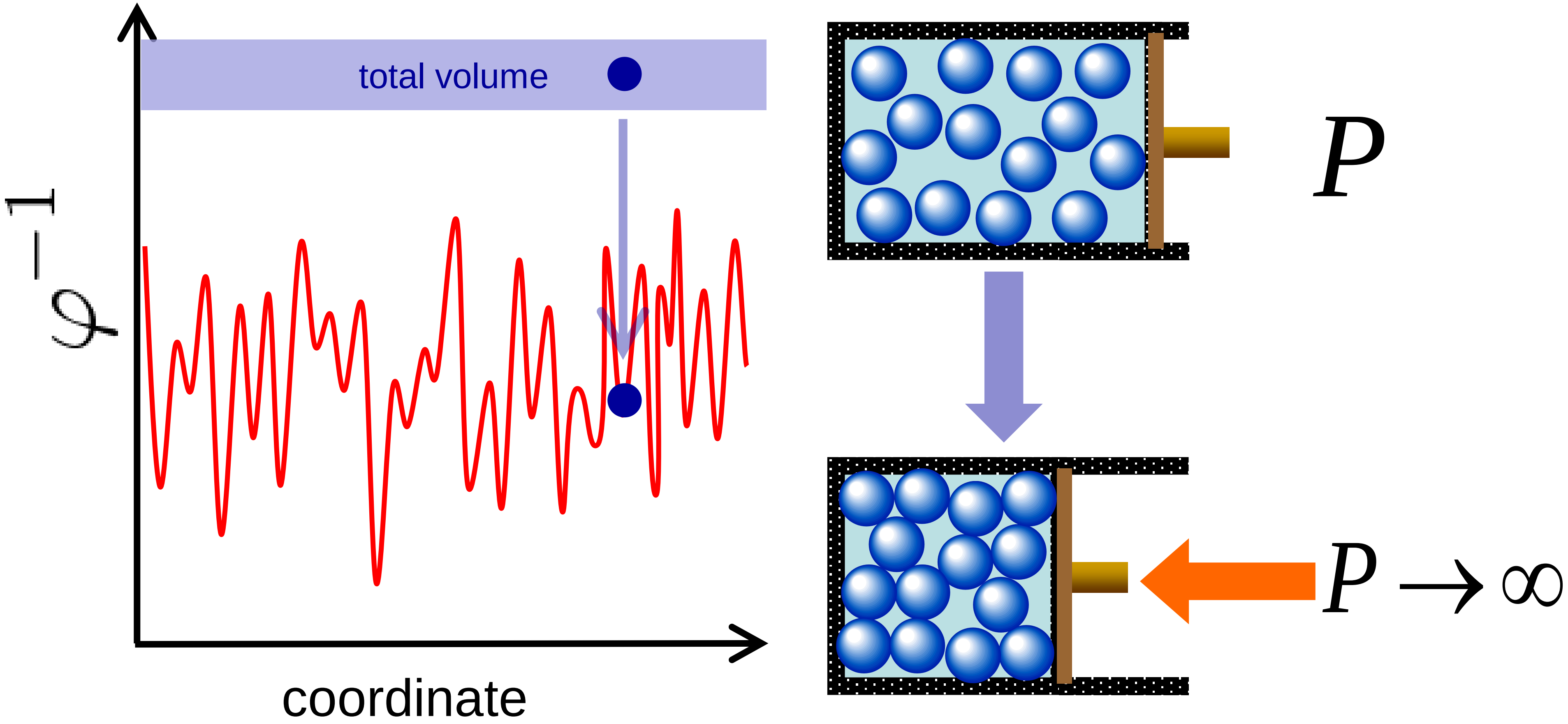
If we use (P,V) *or* (P,φ) *instead of* (T,E)

density



Jamming Transition versus Glass Transition

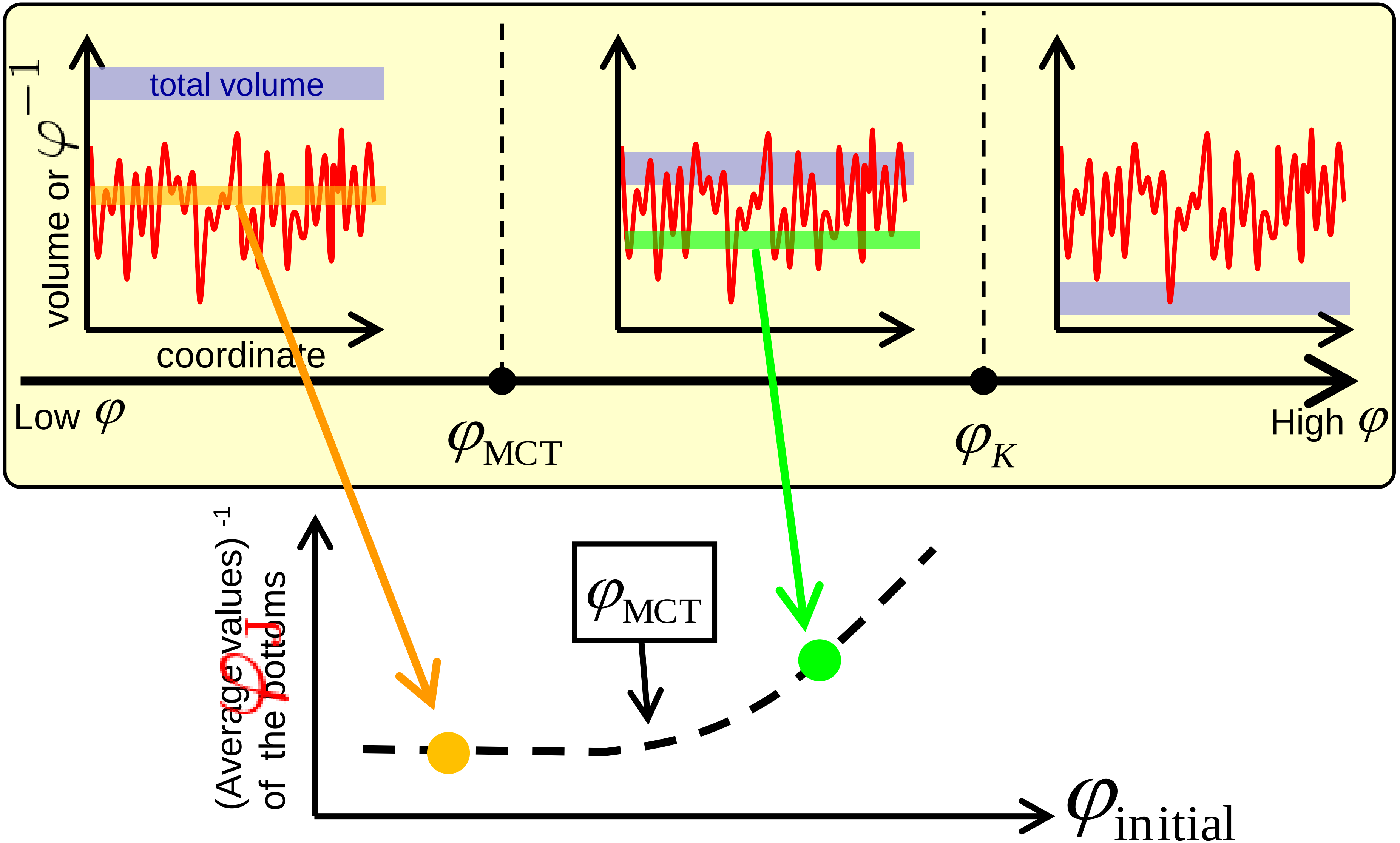
Visualize the "Energy" Landscape



This is nothing but the Jamming transition

Jamming Transition versus Glass Transition

The average will be lowered as density increases



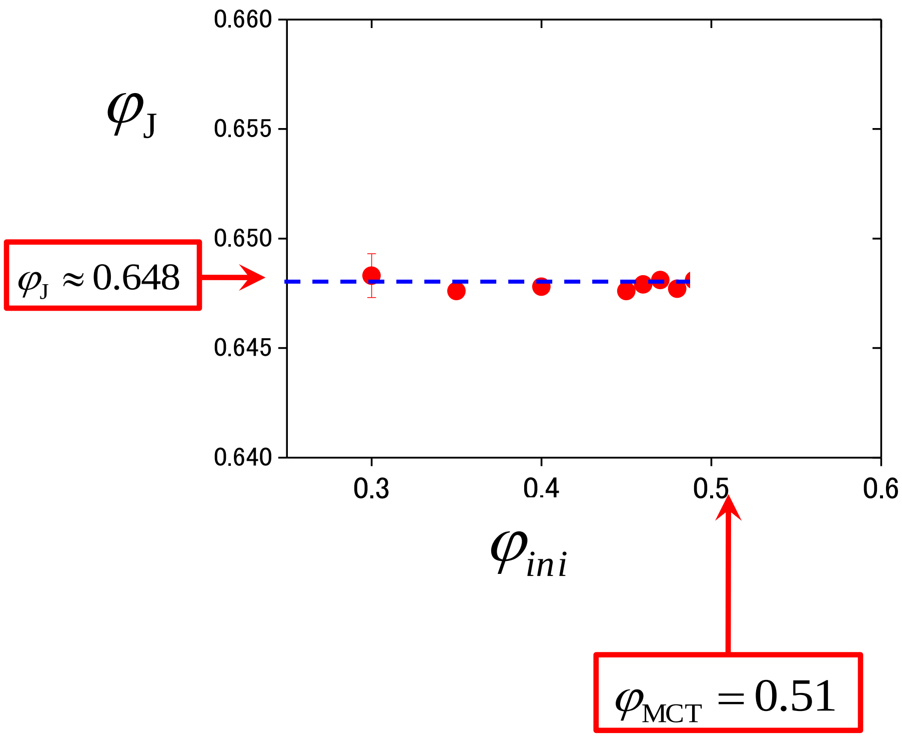
Jamming Transition versus Glass Transition

Initial density dependence of jamming transition points

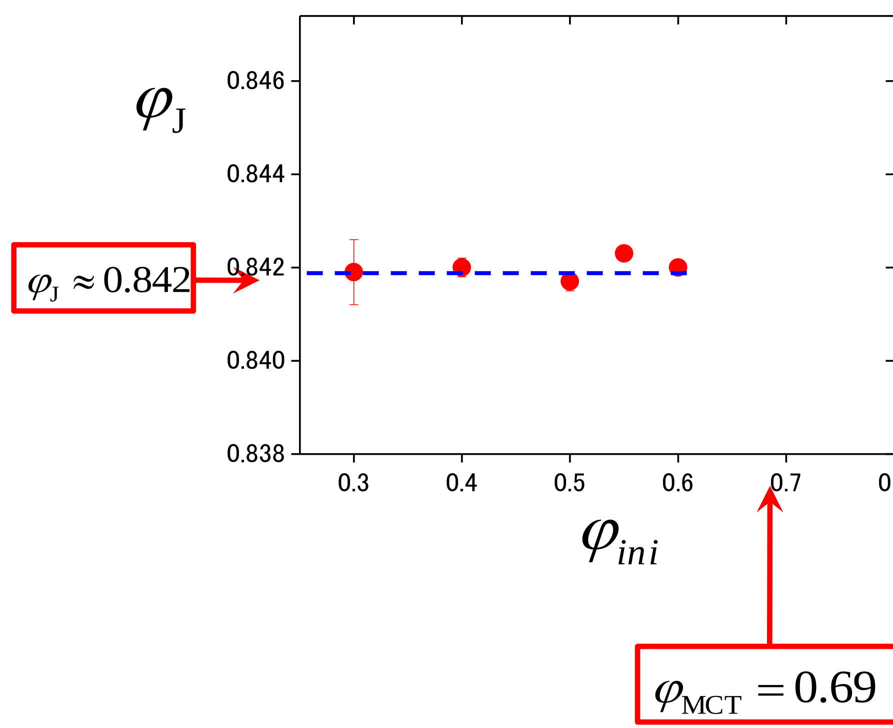
Ozawa, Kuroiwa, Ikeda, and KM [arXiv:1207.6925]

Binary Hard Spheres with size ratio 1.4 and composition ratio 0.5:0.5

d=3



d=2



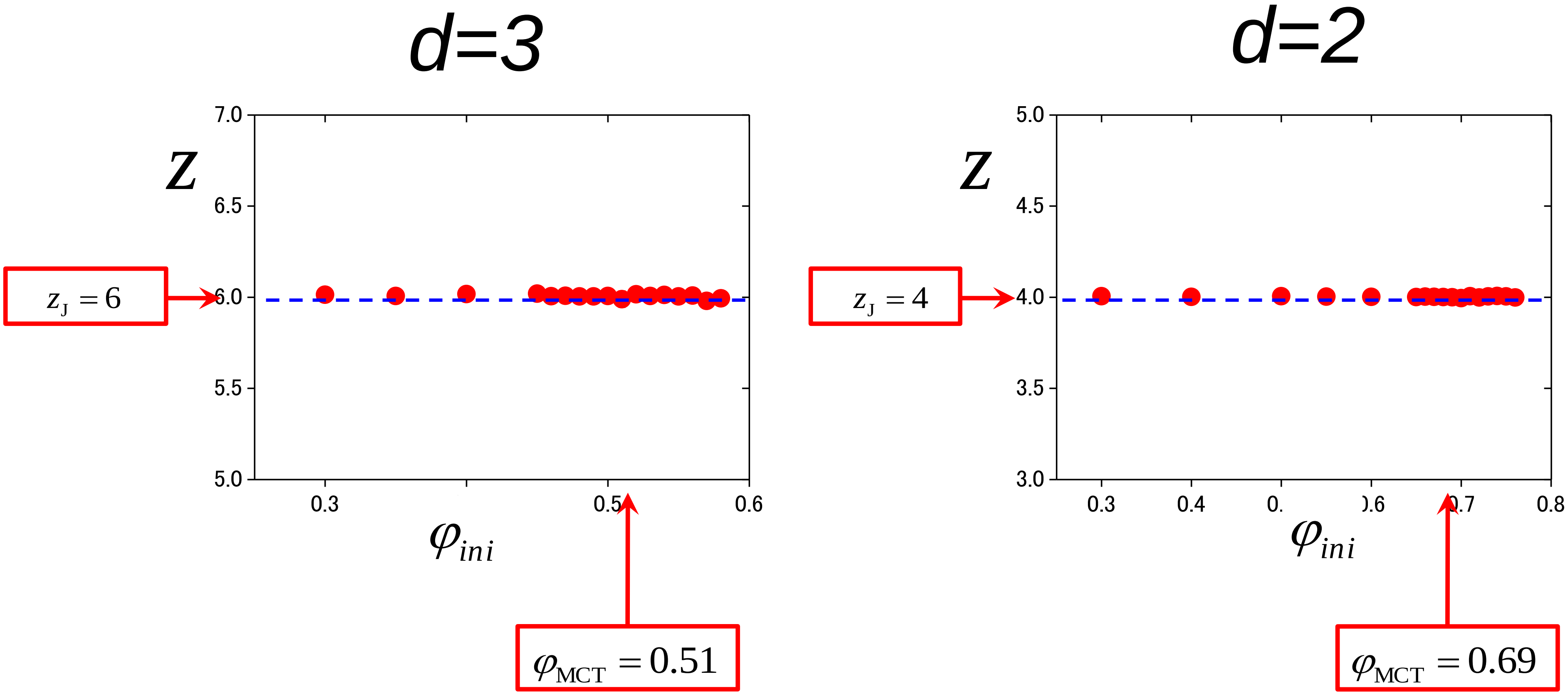
See also Chaudhuri, Berthier, Sastry, PRL **104** (2010) 165701

Jamming Transition versus Glass Transition

Contact Numbers

Ozawa, Kuroiwa, Ikeda, and KM arXiv:1207.6925

Remain Isostatic! $z_J = 2d$



Strong evidence that the system remains still amorphous!

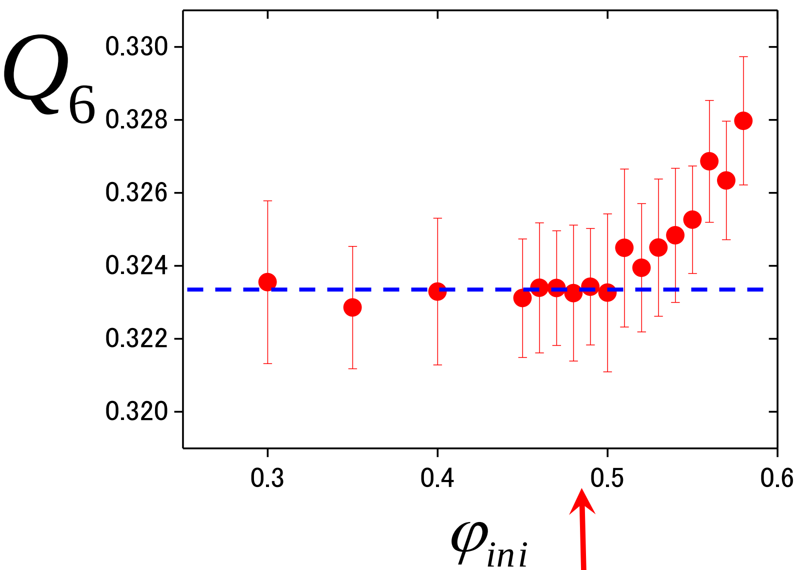
Jamming Transition versus Glass Transition

Orientational Order Parameters

Ozawa, Kuroiwa, Ikeda, and KM arXiv:1207.6925

d=3

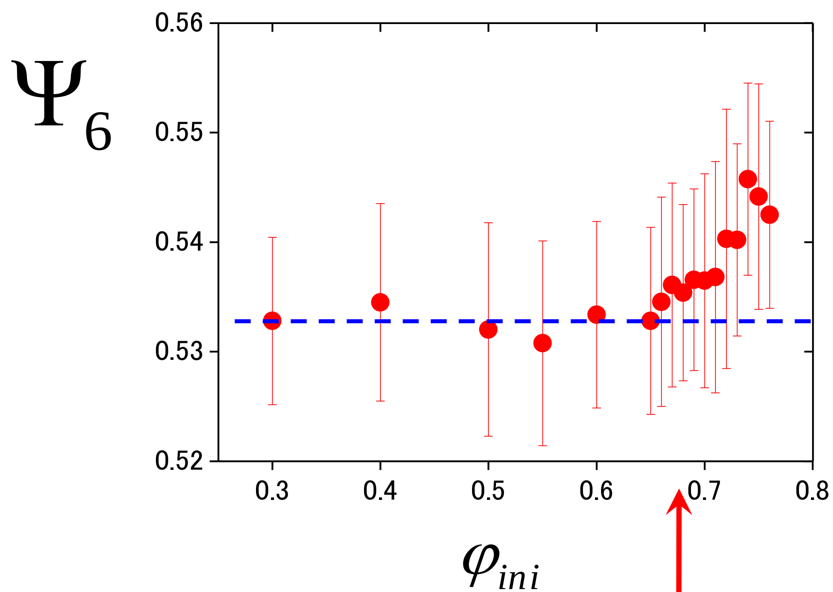
$$Q_6 = \sqrt{\sum_{m=6}^{6}\left|\frac{1}{N_b}\sum Y_6^m(\theta,\phi)\right|^2}$$



$\boxed{\varphi_{\mathrm{MCT}} = 0.51}$

d=2

$$\Psi_6 = \left|\frac{1}{N_b}\sum \exp\left[6i\theta_{ij}\right]\right|$$

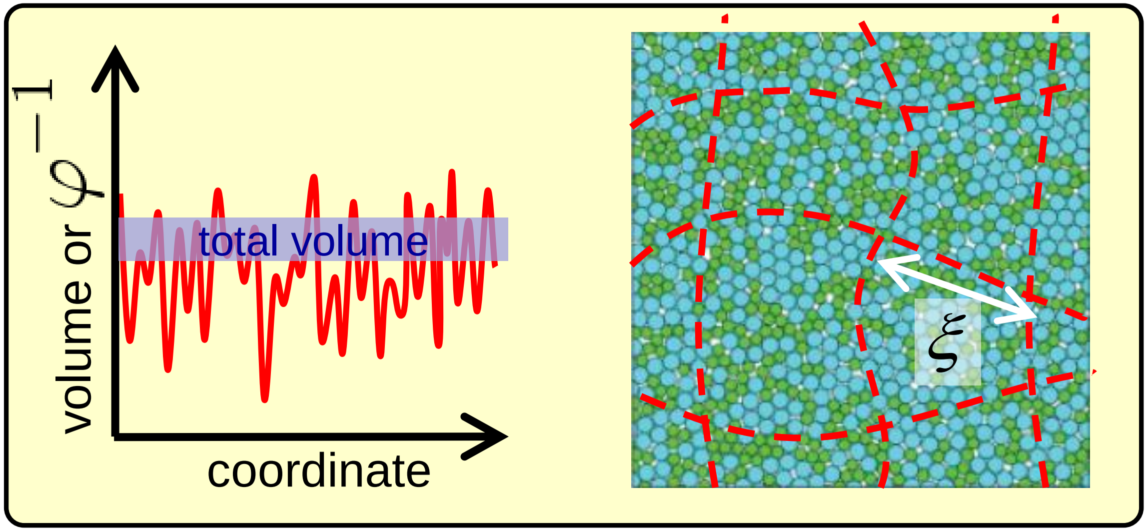


$\boxed{\varphi_{\mathrm{MCT}} = 0.69}$

See also Schreck, O'Hern, Silbert, PRE 84 (2011) 011305

Jamming Transition versus Glass Transition

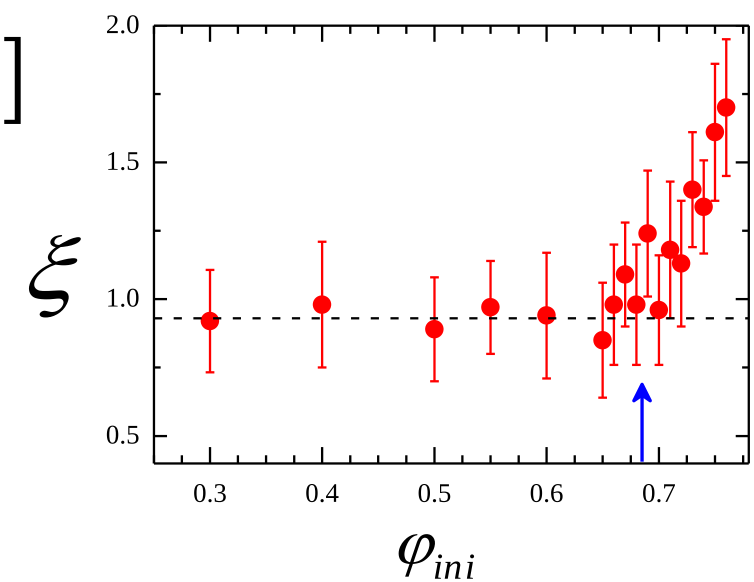
Order hidden in Disorder?



Being in a rugged landscape means that many amorphous *states* or "*mosaics*" coexist.

$$g_6(r) = \langle \delta\Psi_6(r)\delta\Psi_6(0) \rangle = \exp[-r/\xi]$$

d=2



Ozawa, Kuroiwa, Ikeda, and KM arXiv:1207.6925

CONCLUSIONS

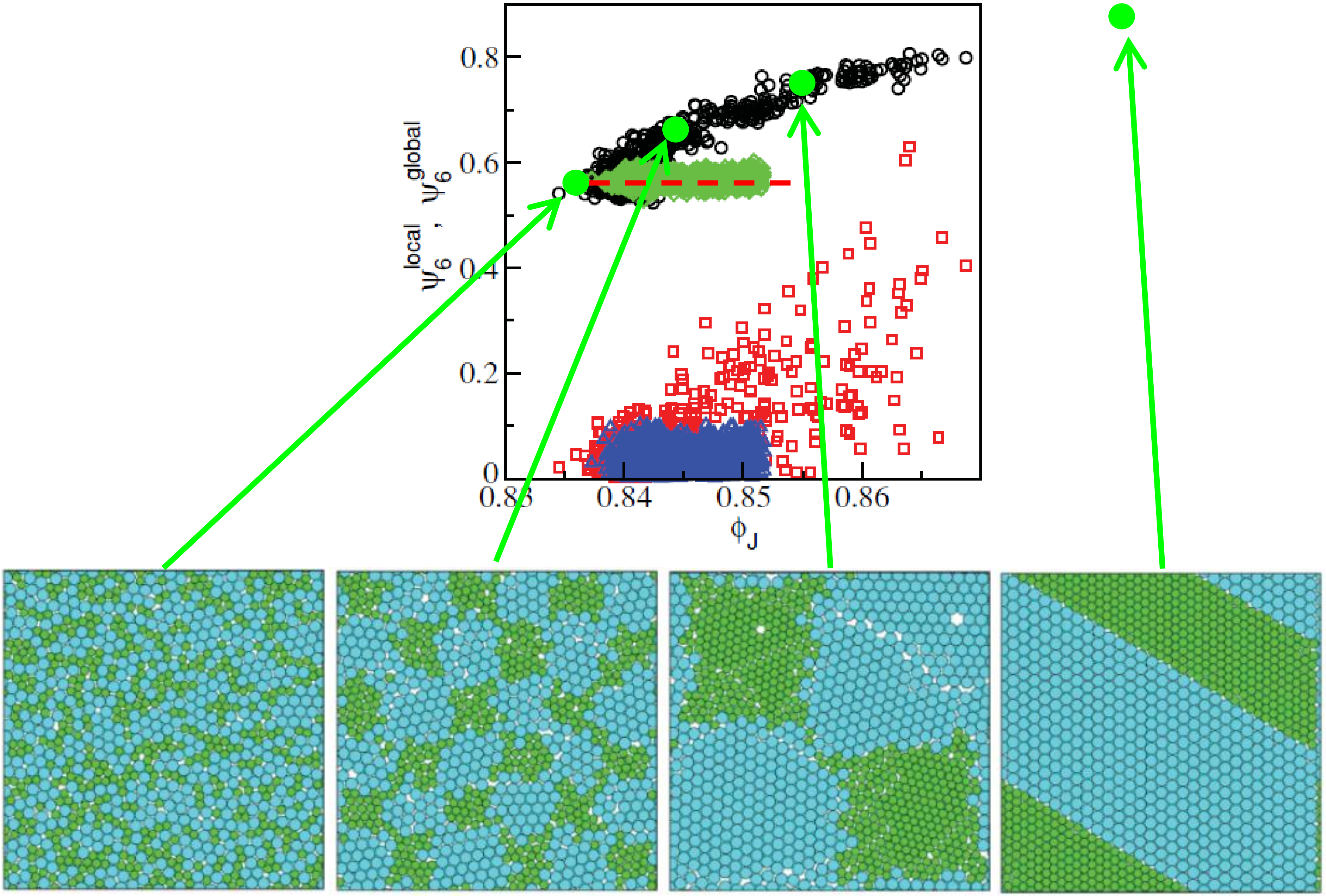
- *MCT should work better in Higher Dimensions*

  ???

- *MCT should work better for Long-Ranged Systems*
- *Dynamic (MCT) transition point should mark the qualitative change of the free energy landscape (inherent structures)*

More puzzles than answers on configurational properties beyond dynamic (MCT) transition point.

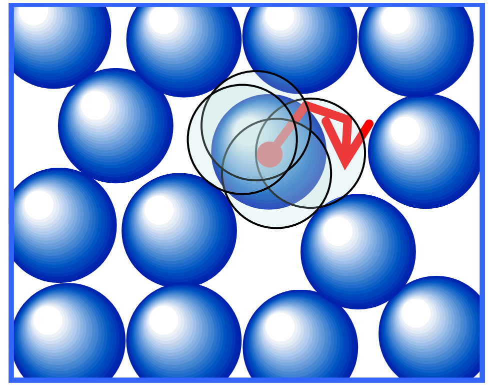
- *Is the "order" we found really a mosaic size?*
- *How does the order affect slow dynamics?*
- *How many length scales exist?*
- *etc…*



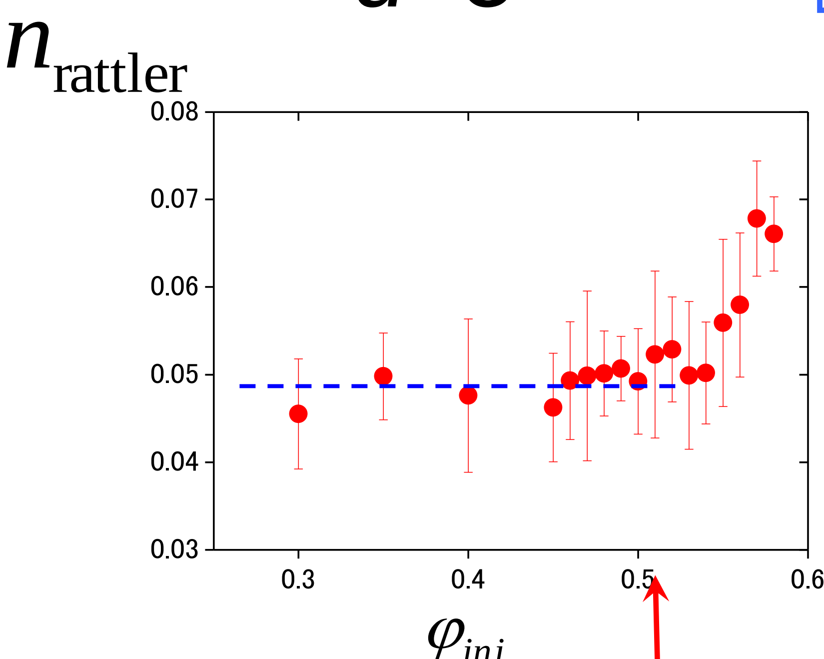
Schreck *et al*. *PRE* (2011)

Jamming Transition versus Glass Transition

Fraction of Rattlers

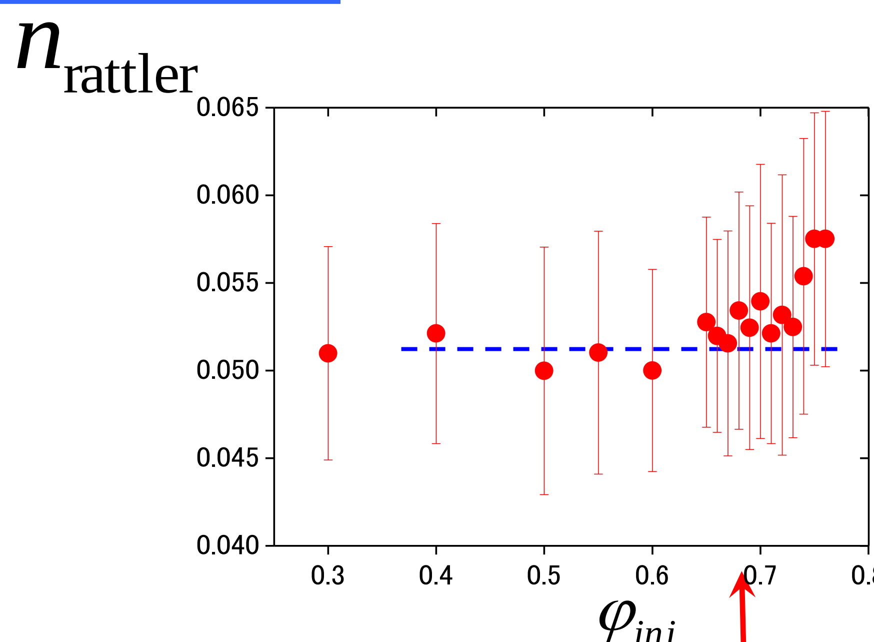


d=3



$\varphi_{\mathrm{MCT}} = 0.51$

d=2

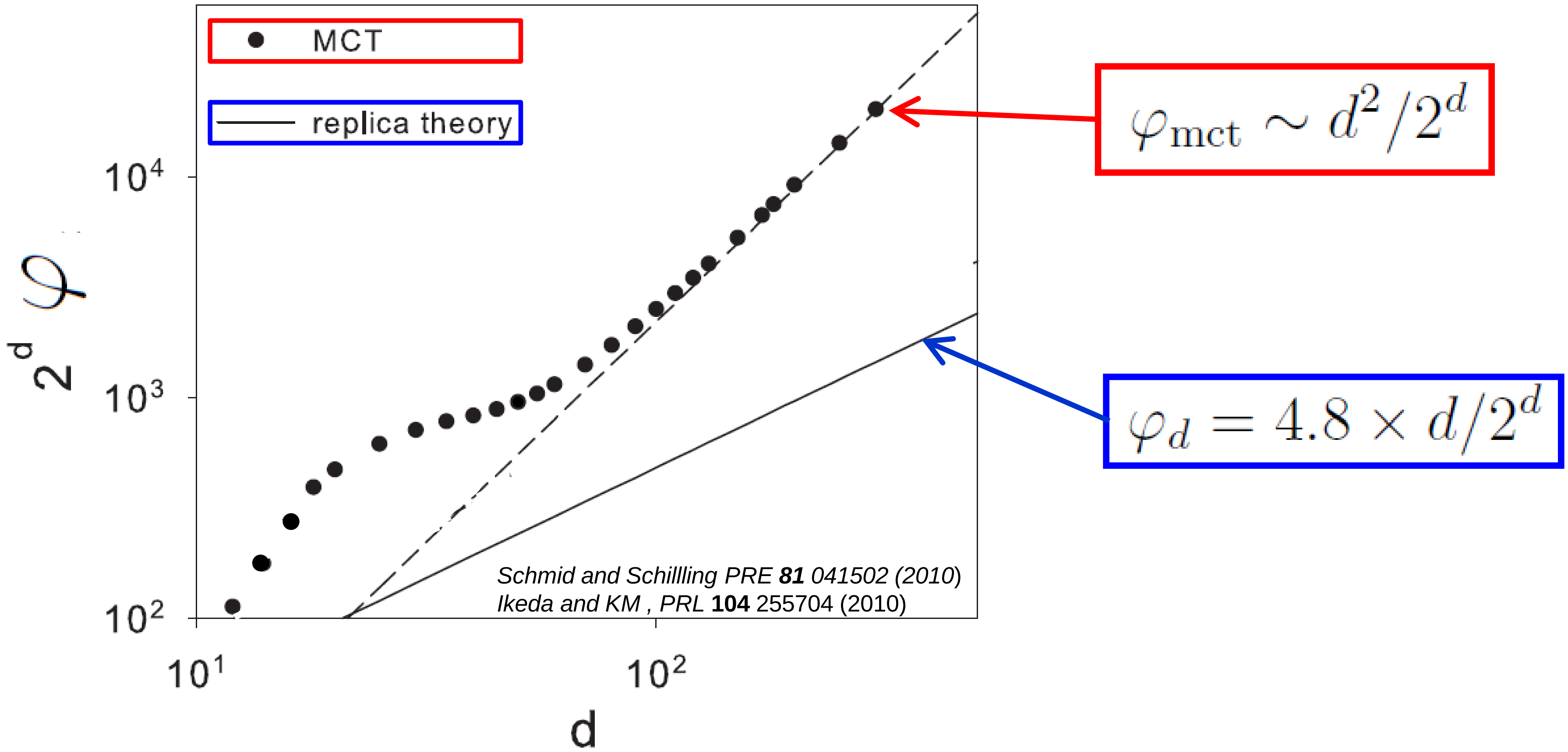


$\varphi_{\mathrm{MCT}} = 0.69$

See also Chaudhuri, Berthier, Sastry, PRL **104** (2010) 165701

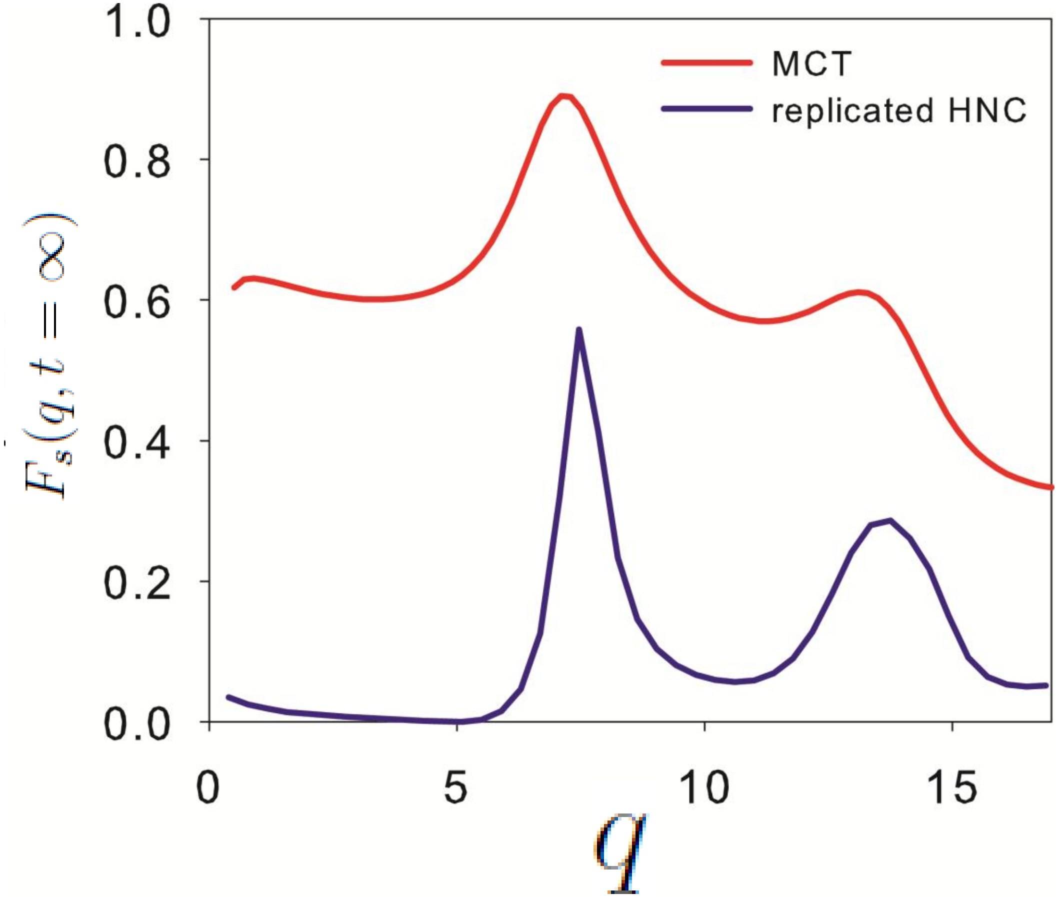
Mode-Coupling Theory vs. Replica Theory

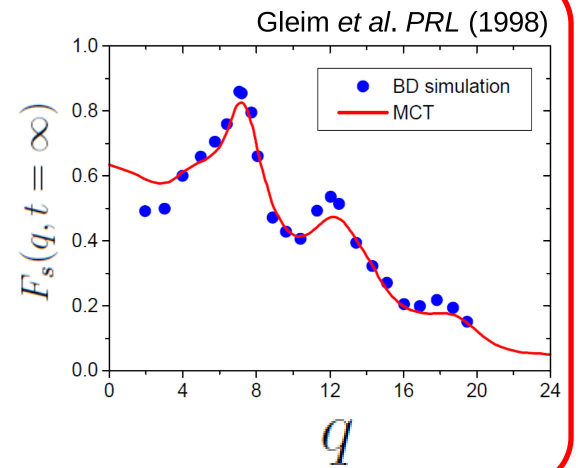
- MCT vs. Replica theory in $d=\infty$



Mode-Coupling Theory vs. Replica Theory

- MCT vs. Replica theory in $d = 3$





MCT wins over Replica. But maybe simply because HNC is a bad approximation.

INTRODUCTION

- Mean Field Scenario of the Glass Transition

If MCT is really a mean field description,

◆ *Does MCT work better in higher dimensions?*

◆ *Do MCT and Replica Theory consistently describe the dynamic transition?*

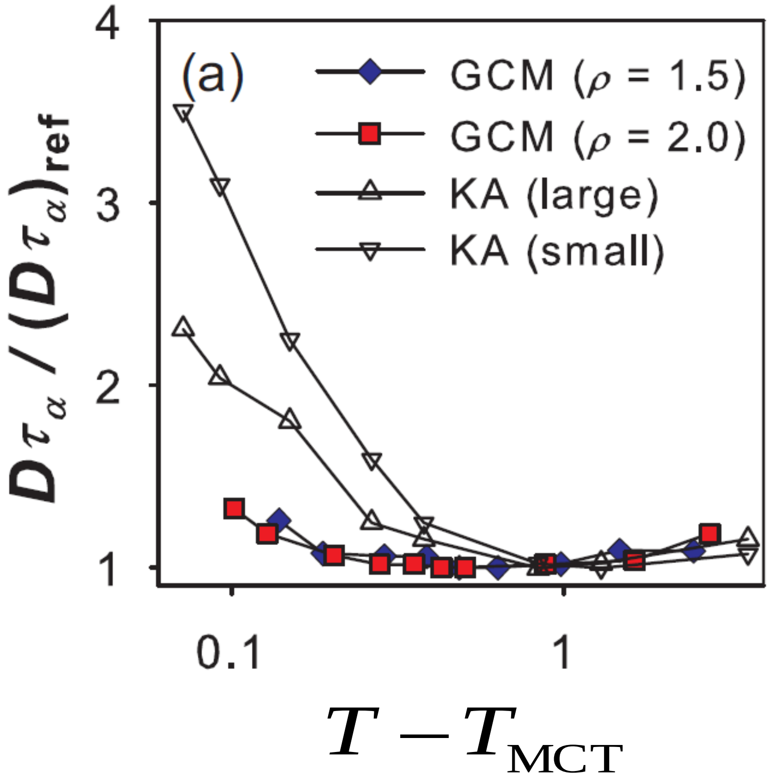
MCT transition point coincides with Dynamic transition point of replica theory?

For hard spheres $\varphi_{mct} \underset{?}{=} \varphi_d$

Glass Transition of Long-Ranged Systems

Monatomic GCM vitrifies!
And MCT works unprecedentedly well!!
And dynamic heterogeneities are weak!!!

Weaker violation of Stokes-Einstein relation



Glass Transition in Higher Dimensions

Replica Theory vs MCT for hard sphere glasses at d > 4

◆ MCT in arbitrary dimensions

$$\frac{\partial F(q,t)}{\partial t} = -\frac{Dq^2}{S(q)}F(q,t) + \int_0^t \mathrm{d}t' \quad M(q,t-t')\frac{\partial F(q,t')}{\partial t'}$$

$$M(q,t) = \frac{\rho D}{2}\int \frac{\mathrm{d}^d k}{(2\pi)^d}\left[kc(k) + (q-k)c(q-k)\right]^2 F(k,t)F(q-k,t)$$

◆ Replica Theory with Hyper-Netted Chain *Parisi and Zamponi Rev. Mod. Phys.* ***82*** *789 (2010)*

$$\begin{cases} \ln g(r) = \beta v(r) + \displaystyle\int \frac{\mathrm{d}\vec{q}}{(2\pi)^d} \mathrm{e}^{i\vec{q}\cdot\vec{r}} \frac{\rho h^2(q)}{1+\rho h(q)}, \\ \ln \tilde{g}(r) = \displaystyle\int \frac{\mathrm{d}\vec{q}}{(2\pi)^d} \mathrm{e}^{i\vec{q}\cdot\vec{r}} \left\{ \frac{\rho h^2(q)}{1+\rho h(q)} - \frac{\rho[h(q)-\tilde{h}(q)]^2}{1+\rho[h(q)-\tilde{h}(q)]} \right\} \end{cases}$$

Regular HNC equation

HNC equation between replicas

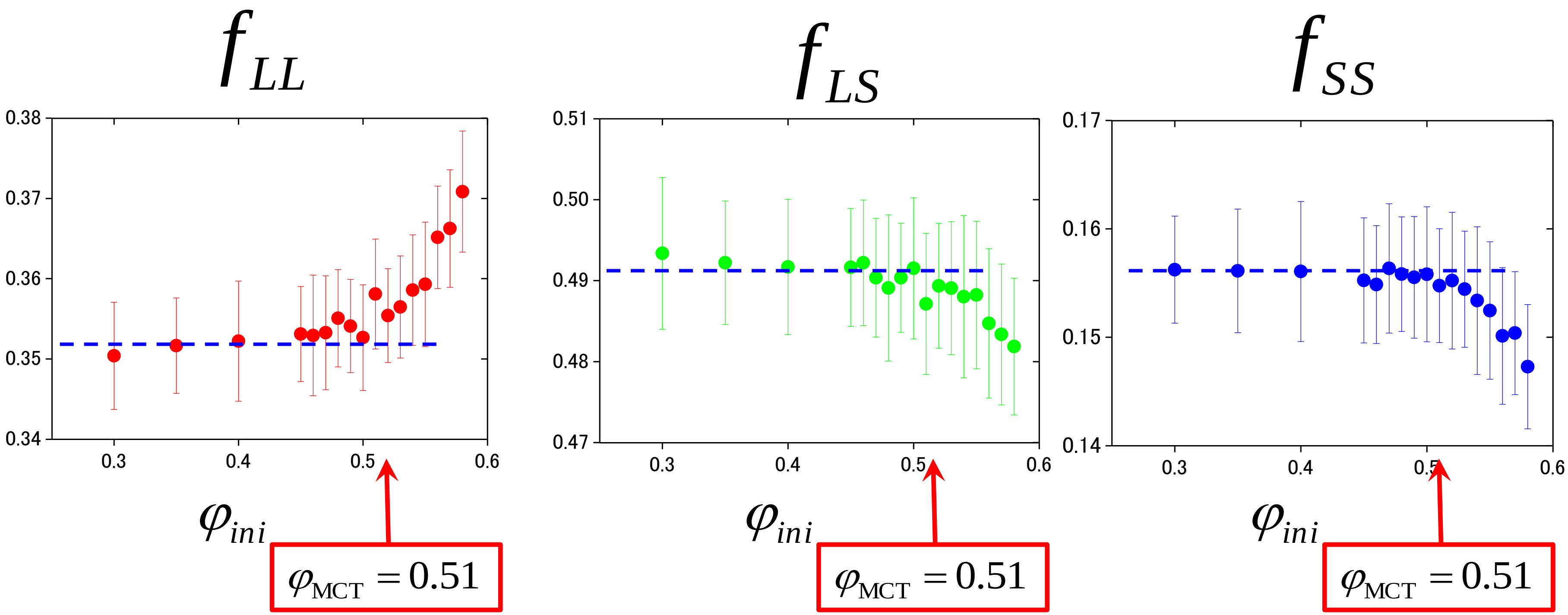
Jamming Transition versus Glass Transition

Compositional Orders

Ozawa, Kuroiwa, Ikeda, and KM (in preparation)

The fraction of pairs of Large-Large, Small-Large, and Small-Small particles

d=3



INTRODUCTION

Mean Field "Theories" of Glass transition

◆ Thermodynamics: Replica Liquid Theory

Mezard, Parisi , Zamponi ,etc…

$$\begin{cases} \ln g(r) = \beta v(r) + \int \frac{\mathrm{d}\vec{q}}{(2\pi)^d} \mathrm{e}^{i\vec{q}\cdot\vec{r}} \frac{\rho h^2(q)}{1+\rho h(q)}, \\ \ln \tilde{g}(r) = \int \frac{\mathrm{d}\vec{q}}{(2\pi)^d} \mathrm{e}^{i\vec{q}\cdot\vec{r}} \left\{ \frac{\rho h^2(q)}{1+\rho h(q)} - \frac{\rho[h(q)-\tilde{h}(q)]^2}{1+\rho[h(q)-\tilde{h}(q)]} \right\} \end{cases}$$

◆ Dynamics: Mode-Coupling Theory (MCT)

Gotze etc…

$$\frac{\partial F(q,t)}{\partial t} = -\frac{Dq^2}{S(q)} F(q,t) + \int_0^t \mathrm{d}t' \ M(q,t-t') \frac{\partial F(q,t')}{\partial t'}$$

$$M(q,t) = \frac{\rho D}{2} \int \frac{\mathrm{d}^d k}{(2\pi)^d} \left[k c(k) + (q-k) c(q-k) \right]^2 F(k,t) F(q-k,t)$$

INTRODUCTION

- *Mean Field "Theories" of Glass transition*

◆ Thermodynamics: Replica Liquid Theory *Mezard, Parisi , Zamponi ,etc…*

$$\begin{cases} \ln g(r) = \beta v(r) + \displaystyle\int \frac{\mathrm{d}\vec{q}}{(2\pi)^d} \mathrm{e}^{i\vec{q}\cdot\vec{r}} \frac{\rho h^2(q)}{1+\rho h(q)}, \\ \ln \tilde{g}(r) = \displaystyle\int \frac{\mathrm{d}\vec{q}}{(2\pi)^d} \mathrm{e}^{i\vec{q}\cdot\vec{r}} \left\{ \frac{\rho h^2(q)}{1+\rho h(q)} - \frac{\rho[h(q)-\tilde{h}(q)]^2}{1+\rho[h(q)-\tilde{h}(q)]} \right\} \end{cases}$$

◆ Dynamics: Mode-Coupling Theory (MCT) *Gotze etc…*

$$\frac{\partial F(q,t)}{\partial t} = -\frac{Dq^2}{S(q)} F(q,t) + \int_0^t \mathrm{d}t' \; M(q,t-t') \frac{\partial F(q,t')}{\partial t'}$$

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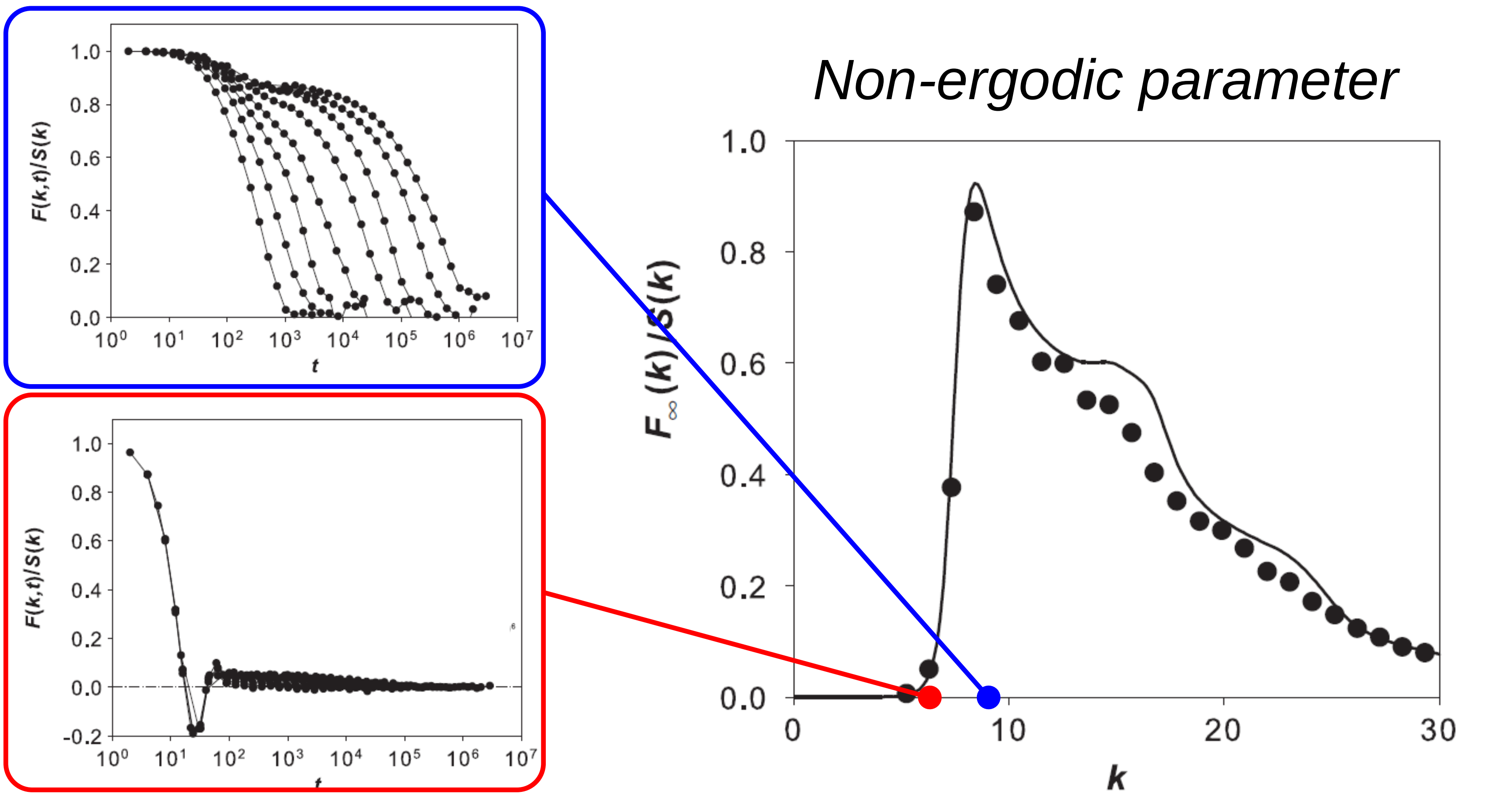
Glass Transition of Long-Ranged Systems

Monatomic GCM vitrifies!

And MCT works unprecedentedly well!!

And dynamic heterogeneities are weak!!!



Glass Transition of Long-Ranged Systems

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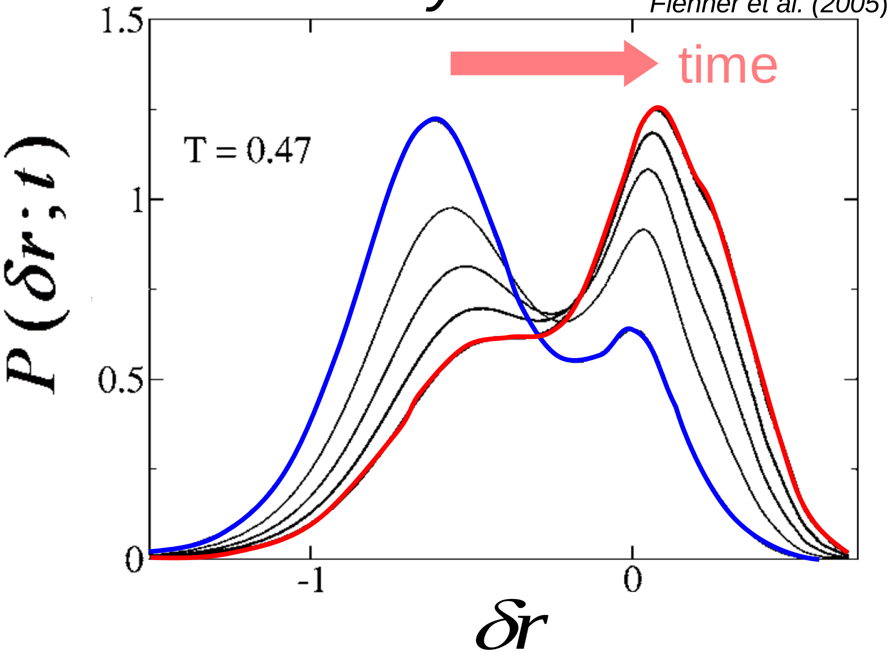
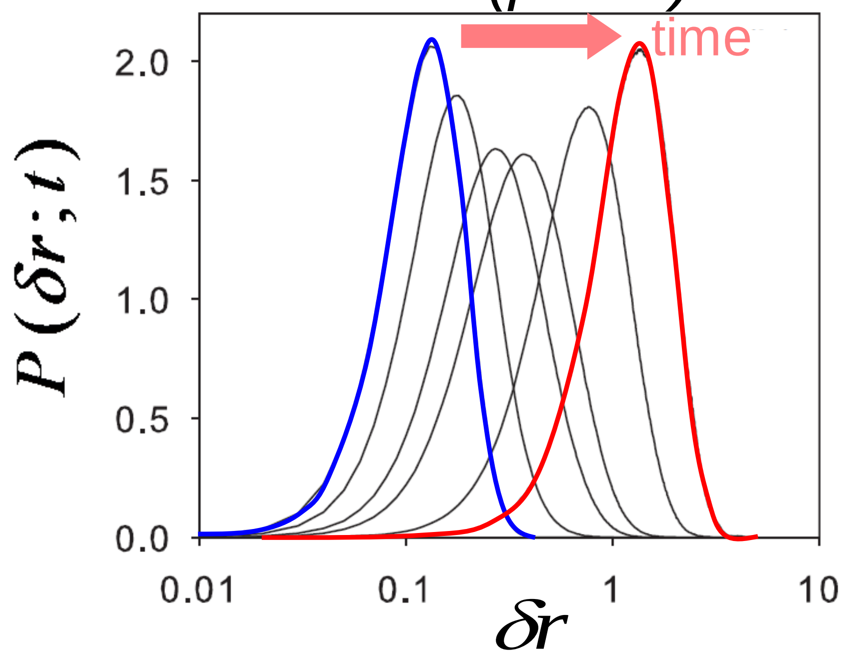
Distribution of the Particle Displacement δr

KA-LJ system



Bimodal distribution of fast and slow particles

GCM (ρ=2.0)



Single-peaked and Gaussian shape

Glass Transition of Long-Ranged Systems

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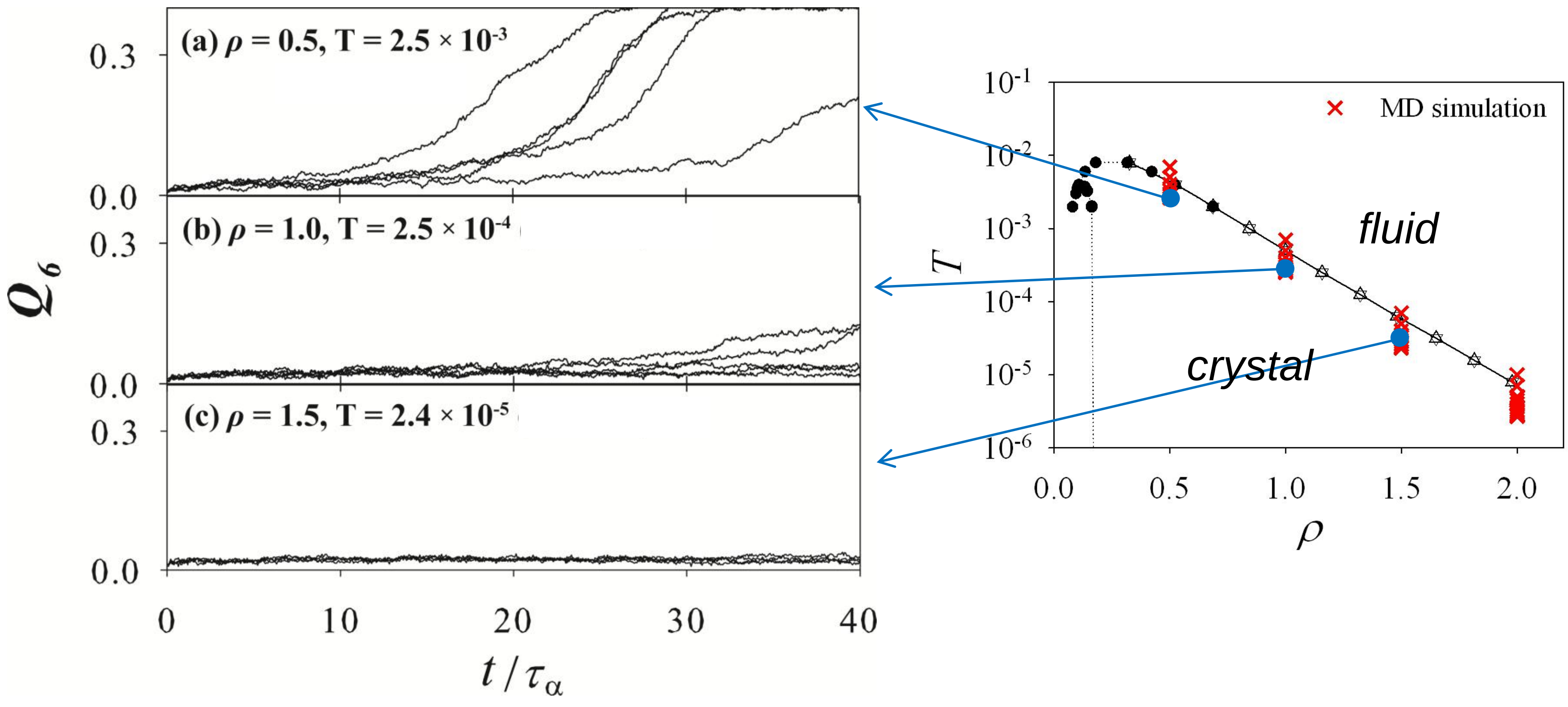
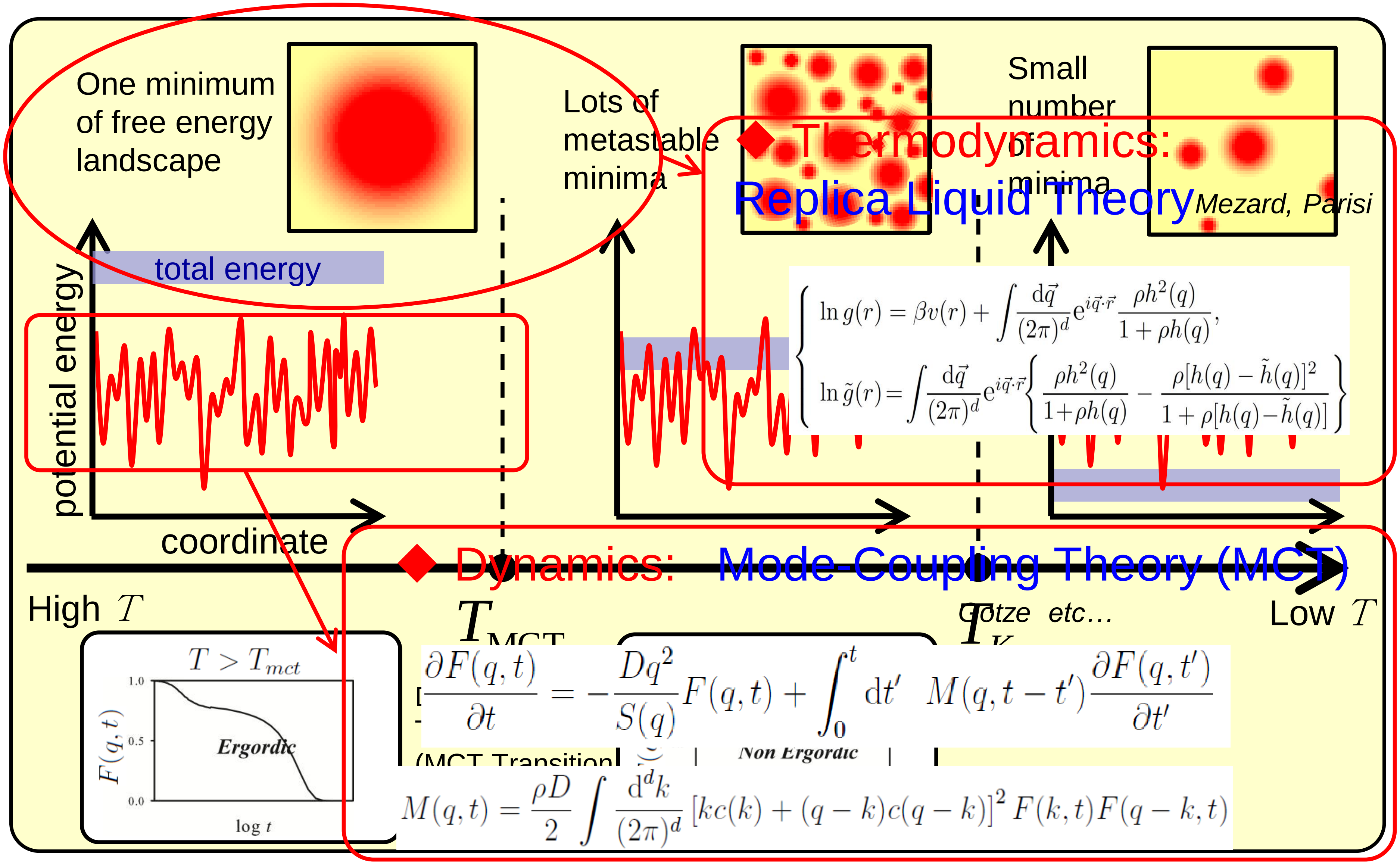
And dynamic heterogeneities are weak!!!



Mean Field "Theory" of the Glass transition



◆ Thermodynamics: Replica Liquid Theory *Mezard, Parisi*

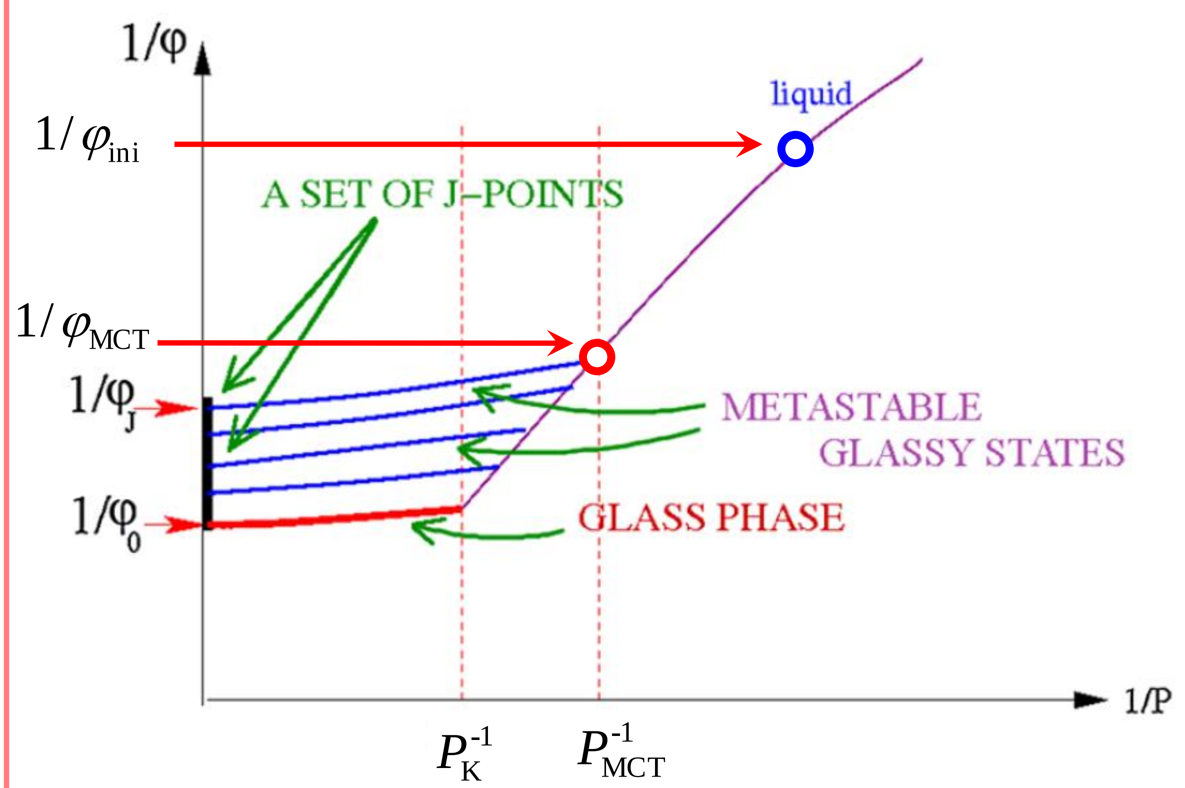
$$\begin{cases} \ln g(r) = \beta v(r) + \displaystyle\int \frac{\mathrm{d}\vec{q}}{(2\pi)^d} \mathrm{e}^{i\vec{q}\cdot\vec{r}} \frac{\rho h^2(q)}{1+\rho h(q)}, \\ \ln \tilde{g}(r) = \displaystyle\int \frac{\mathrm{d}\vec{q}}{(2\pi)^d} \mathrm{e}^{i\vec{q}\cdot\vec{r}} \left\{ \frac{\rho h^2(q)}{1+\rho h(q)} - \frac{\rho[h(q)-\tilde{h}(q)]^2}{1+\rho[h(q)-\tilde{h}(q)]} \right\} \end{cases}$$

◆ Dynamics: Mode-Coupling Theory (MCT) *Gotze etc…*

$$\frac{\partial F(q,t)}{\partial t} = -\frac{Dq^2}{S(q)} F(q,t) + \int_0^t \mathrm{d}t' \; M(q,t-t') \frac{\partial F(q,t')}{\partial t'}$$

$$M(q,t) = \frac{\rho D}{2} \int \frac{\mathrm{d}^d k}{(2\pi)^d} \left[k c(k) + (q-k) c(q-k) \right]^2 F(k,t) F(q-k,t)$$

Jamming Transition versus Glass Transition



Mari, Krzakala and Kurchan, PRL (2009)

$$\varphi_J = \lim_{P\to\infty} \varphi(P)$$

$$= 0.64 \quad \text{for} \quad \varphi_{ini} < \varphi_{\text{mct}}$$

$$> 0.64 \quad \text{for} \quad \varphi_{ini} > \varphi_{\text{mct}}$$

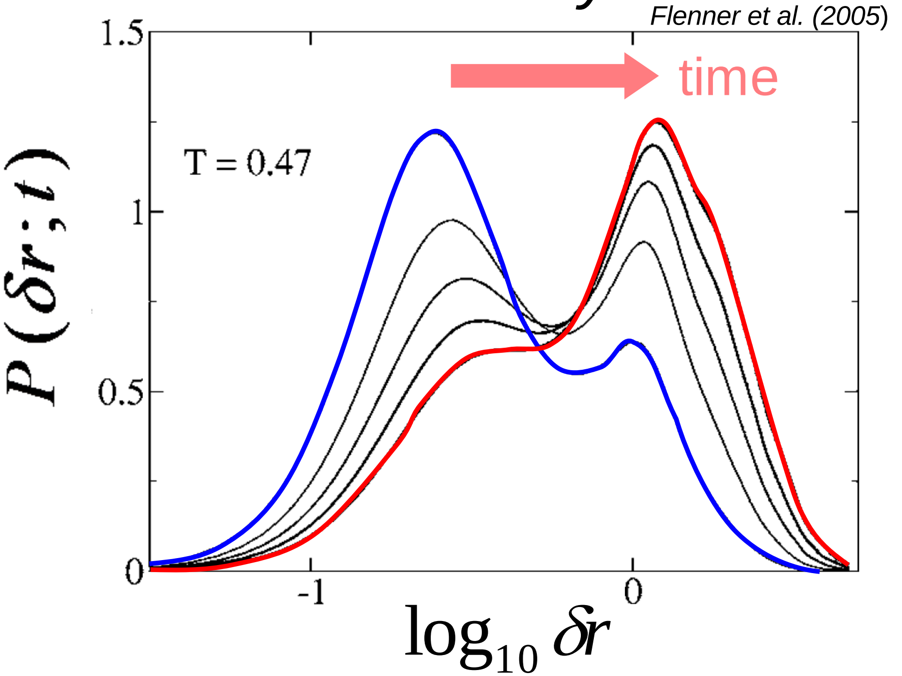
Sastry, Stillinger (1999)
Brummer, Reichman (2005)
Zamponi, Parisi (2009)
Mari, Krzakala, Kurchan (2009)

Glass Transition of Long-Ranged Systems

MCT works unprecedentedly well!!
And dynamic heterogeneities are weak!!!

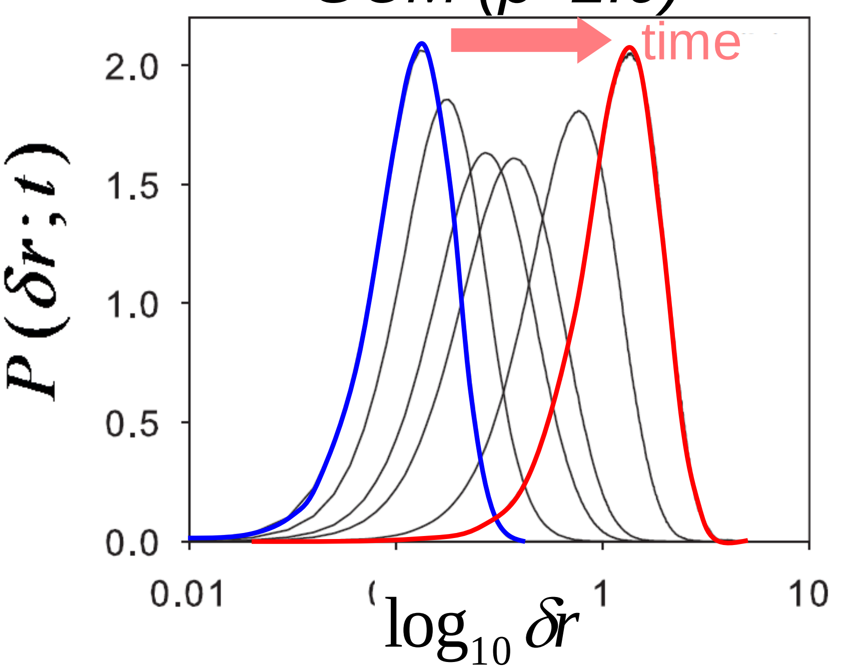
Distribution of the Particle Displacement δr

Lennard-Jones system



Bimodal distribution of fast and slow particles

GCM (ρ=2.0)



Single-peaked and Gaussian shape

Glass Transition of Long-Ranged Systems

Phase Diagram of Monatomic GCM