Random first-order transition of a spin glass model in three dimensions

– Toward a mean-field theory for glass transitions –

Koji Hukushima

University of Tokyo, Dep. of Basic Sciences

Integrated Sciences

14 August 2015

In collaboration with

Takashi Takahasi.

Japan-France Joint Seminar

Outline

Outline

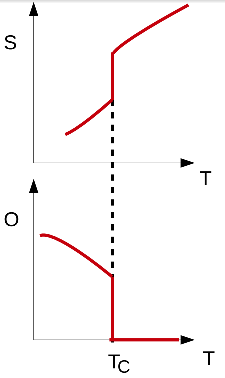
Order of phase transition

Ehrenhest's criterion

Phase transition is described by a singularity of free energy.
Phase transition with a singularity in nth order differential of free energy is called nth order phase transition.

1st order transition

- Internal energy, entropy and volume have a jump at T_c.
- Order parameter also has a jump.
- latent heat and delta-function-type divergence in specific heat.



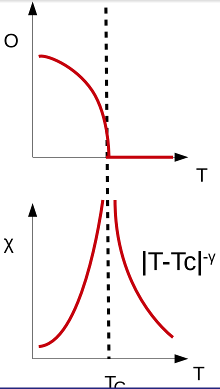
Order of phase transition

Ehrenhest's criterion

Phase transition is described by a singularity of free energy.
Phase transition with a singularity in nth order differential of free energy is called nth order phase transition.

2nd order transition

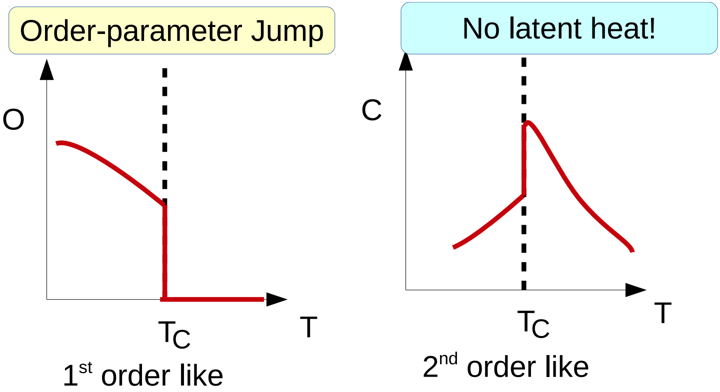
- Internal energy, entropy S, order parameter O change continuously at critical temperature.
- Specific heat, susceptibility χ follow power-law divergence at T_c
- divergence of length scale ξ
- universality class by critical exponents.



1.5 order phase transition?

- There exists infinite order phase transition like KT transitions.
- Meanwhile, a kind of phase transitions, not 1st order and not 2nd order, has attracted much attention...

Random first-order transition (RFOT)



RFOT and spin glasses

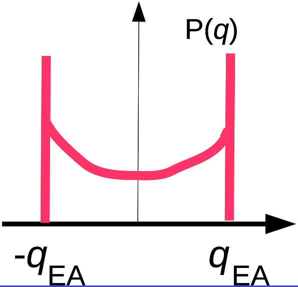
RFOT has been found in some spin glass models with one-step replica symmetry breaking.

1 step RSB

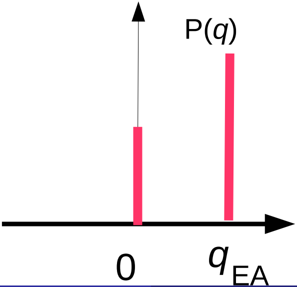
- p-state Potts glass with $p \geq 4$
- p-spin glass with $p > 2$

Overlap distribution $P(q)$

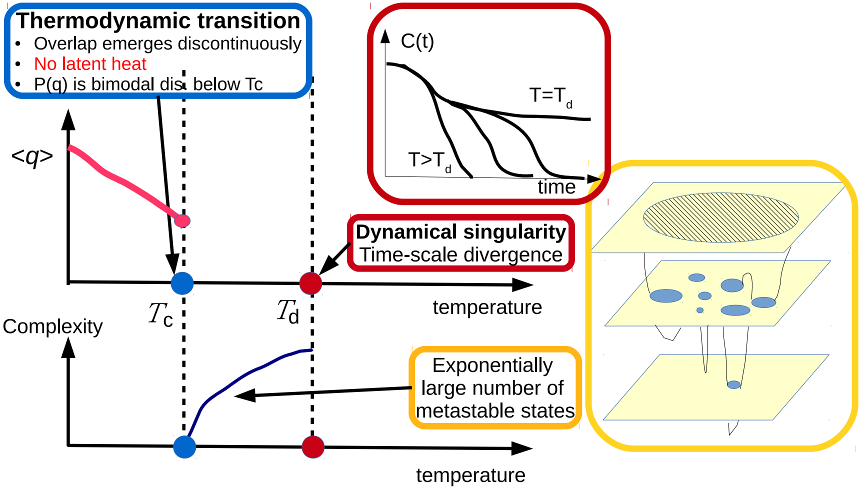
$P(q)$ for full RSB



$P(q)$ for 1RSB



Some features of a 1RSB transition



Random First-Order Transition (RFOT)

$\Longrightarrow$ the phenomenology of glass transitions

Does RFOT provides a good theory of glass transitions?

Some statistical-mechanical models of RFOT

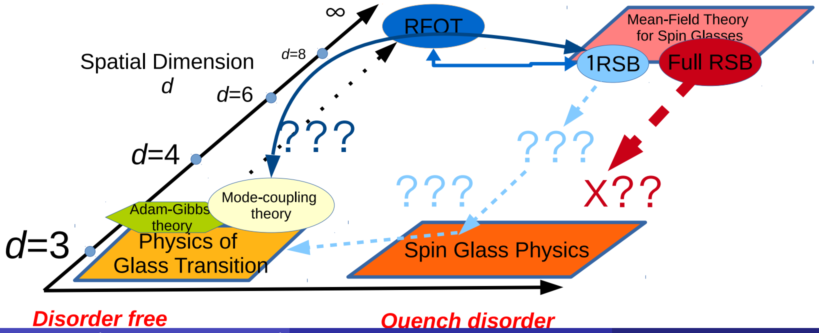
- mean-field **Potts glass model**
- mean-field p-spin glass model
- Biroli-Mézard model (lattice glass model) on Bethe lattice
- K-SAT, ...

They are all mean-field models with **1RSB** transition.

Does RFOT provides a good theory of glass transitions?

Two difficulties –mean-field theory and quench disorder–

1. One of the next issues to be addressed is to clarify whether predictions from the mean-field theory survive in finite dimensional models.
   Today's issue
2. The correct theory of glass transitions must be free from quench disorder.
   Universality class??



Outline

RFOT occurs in a three dimensional Potts glass model?

Potts glass Hamiltonian in three dimensions

$$\mathcal{H}_J(\boldsymbol{S}) = -\sum_{(ij)} J_{ij}\delta\left(S_i, S_j\right), \quad \text{Potts variable: } S_i = \{0, 1, \cdots, p-1\}$$

Questions

- Does the model have a SG phase transition beyond a mean-field theory? Is it RFOT?
- Low-temperature properties are described by replica symmetry breaking?
- Most of researchers believe that dynamical singularity at T_d is smeared out in finite dimensions. Does the singularity completely disappear?

Summary of the previous numerical studies

3 dimensional Potts glass models

- No phase transition for $p = 3$, Scheucher et al(1990).
- No phase transition for $p = 10$, Brangian et al(2002).
- Finite T transition for $p = 3$, Lee-Katzgraber-Young(2006).
- Finite T transition for $p = 4$ JANUS project, Cruz et. al(2009).
- Finite T transition for $p = 5$ and 6 JANUS project, Baños et. al(2010).

- It is found that p-state PG model with $p = 3, 4, 5$ and 6 shows a finite temperature SG transition by extended-ensemble MC simulations.
- The transitions are continuous and there is no finite discontinuous jump of the order parameter.
- No features of RFOT/1RSB were found.

Comment from Cammarota et al (2013)

PHYSICAL REVIEW B **87**, 064202 (2013)

Fragility of the mean-field scenario of structural glasses for disordered spin models in finite dimensions

Chiara Cammarota,[1,2,*] Giulio Biroli,[1,†] Marco Tarzia,[2,‡] and Gilles Tarjus[2,§]
[1]*IPhT, CEA/DSM-CNRS/URA 2306, CEA Saclay, F-91191 Gif-sur-Yvette Cedex, France*
[2]*LPTMC, CNRS-UMR 7600, Université Pierre et Marie Curie, boîte 121, 4 Pl. Jussieu, 75252 Paris cédex 05, France*
(Received 11 October 2012; revised manuscript received 18 January 2013; published 21 February 2013)

At the mean-field level, on fully connected lattices, several disordered spin models have been shown to belong to the universality class of "structural glasses" with a "random first-order transition" (RFOT) characterized by a discontinuous jump of the order parameter and no latent heat. However, their behavior in finite dimensions is often drastically different, displaying either no glassiness at all or a conventional spin-glass transition. We clarify the physical reasons for this phenomenon and stress the unusual fragility of the RFOT to *short-range* fluctuations, associated, e.g., with the mere existence of a finite number of neighbors. Accordingly, the solution of fully connected models is only predictive in very high dimension, whereas despite being also mean-field in character, the Bethe approximation provides valuable information on the behavior of finite-dimensional systems. We suggest that before embarking on a full blown account of fluctuations on all scales through computer simulation or renormalization-group approach, models for structural glasses should first be tested for the effect of short-range fluctuations and we discuss ways to do it. Our results indicate that disordered spin models do not appear to pass the test and are therefore questionable models for investigating the glass transition in three dimensions. This also highlights how nontrivial is the first step of deriving an effective theory for the RFOT phenomenology from a rigorous integration over the short-range fluctuations.

DOI: 10.1103/PhysRevB.87.064202 PACS number(s): 64.70.Q−, 75.10.Nr, 64.70.pm

Comment from Cammarota et al (2013)

Detect 1RSB transition/RFOT in finite dimensions,

1. The number of Potts states, p, have to be large enough.
2. A rate of antiferromagnetic coupling have to be increased for preventing a ferromagnetic ordering.
3. The connectivity must be increased in order to keep the frustration. (Large p suppresses the frustration in general)

Thus, in a naive sense, it is very hard to meet these conditions simultaneously on a three dimensional lattice. It might be possible in higher dimensions like $d = 9, 10, \ldots$.

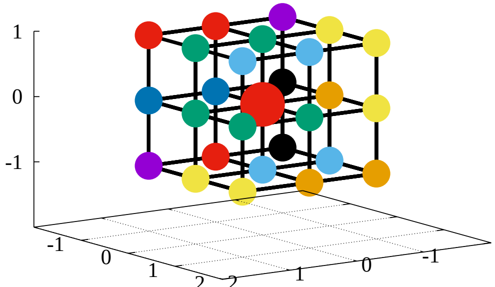
Our strategy:

- we don't want to go to high dimensions.
- Instead, interaction range is enlarged up to 1st, 2nd and 3rd neighbors.

Our Model

7-state Potts glass model

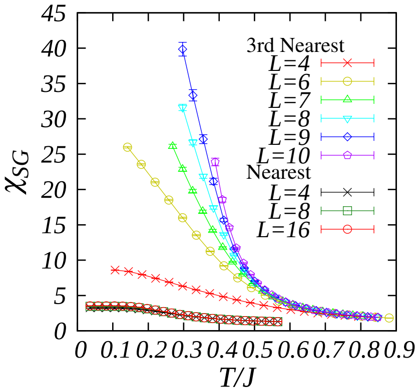
- 3rd neighbor random interactions with $\pm J$ type. (# of neighbors $= 26$).
- System sizes: $L = 4, \ldots, 10$, Number of samples: $256 \sim 1024$.
- Exchange MC(parallel tempering).



Outline

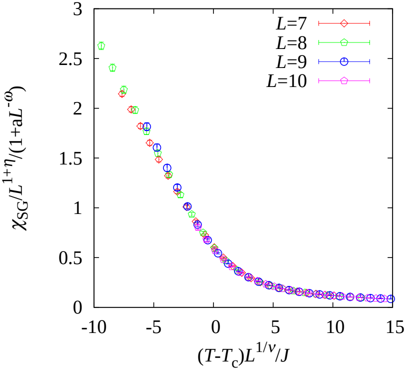
MC results for 7-state PG in three dimensions

non-linear susceptibility χ_{SG}



- 7-state PG model exhibits a finite temperature SG transition at $T_c/J \simeq 0.42$.

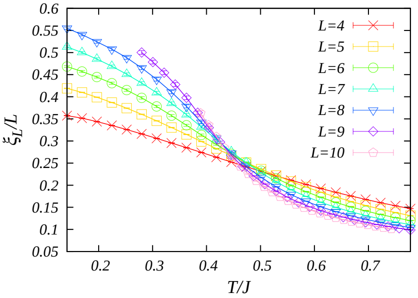
Finite-size scaling for χ_{SG}



- $T_c/J = 0.42(1)$
- $1/\nu = 1.53(1) \quad \Longleftrightarrow \nu = 2/d$
- $\eta = 0.43(2) \quad \Longleftrightarrow \gamma \simeq 0.94$

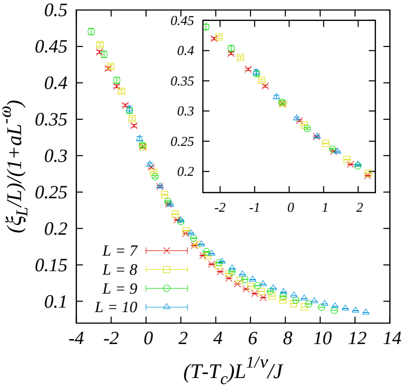
MC results for 7-state PG in three dimensions: 2

Scaled correlation length $\xi_{\rm SG}/L$



- Length scale also diverges at $T_c/J \simeq 0.42$.

FSS for ξ_L/L

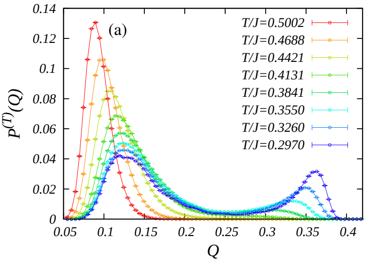


- $T_c/J = 0.421(3)$
- $\nu = 0.68(9) \Longleftrightarrow \nu = 2/d$

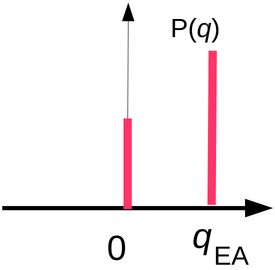
MC results for 7-state PG in three dimensions: 3

Order-parameter distribution

$$P(q) = \left\langle \delta\left(q - \sqrt{q^{(2)}}\right)\right\rangle$$



Temp. dep for $L = 9$.

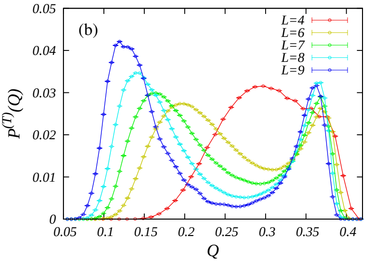


- a bimodal distribution of $P(q)$ is compatible to 1step RSB.

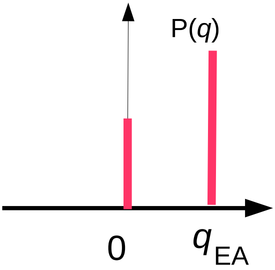
MC results for 7-state PG in three dimensions: 3

Order-parameter distribution

$$P(q) = \left\langle \delta\left(q - \sqrt{q^{(2)}}\right)\right\rangle$$

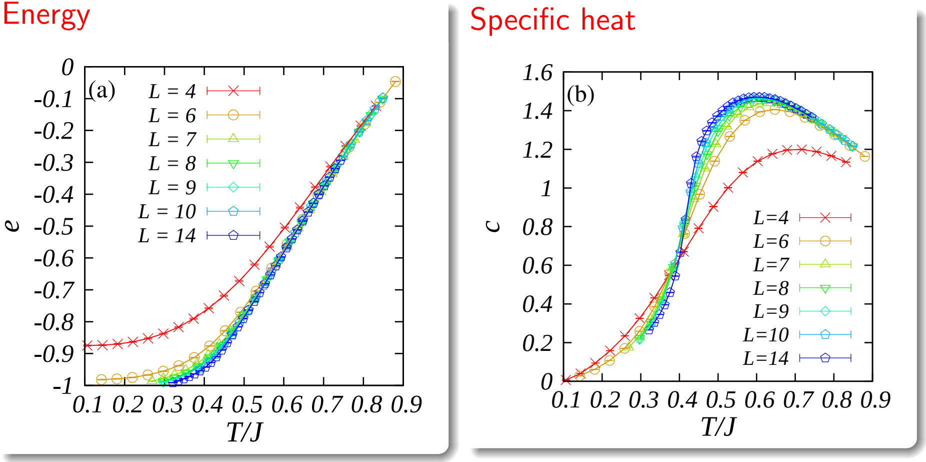


L dep at $T \simeq 0.7 T_c$.



- a bimodal distribution of $P(q)$ is compatible to 1step RSB.

MC results for 7-state PG in three dimensions: 4



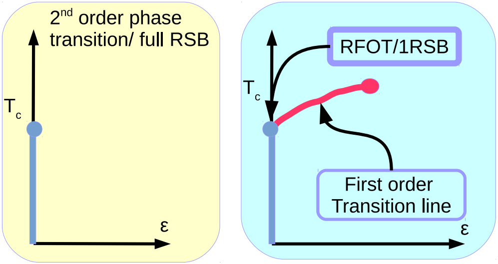
- No divergence of c is found at $T = T_c$, meaning no latent heat.
- These indicate that it is Random First Order transition.

Phase diagram of ϵ-coupled system

Phase transition under a symmetry-broken field:

Predictions for an ϵ-coupled system

$$\mathcal{H}_J(\boldsymbol{S}_\alpha, \boldsymbol{S}_\beta) = \mathcal{H}_J(\boldsymbol{S}_\alpha) + \mathcal{H}_J(\boldsymbol{S}_\beta) - \epsilon \sum_i \delta(S_{i,\alpha}, S_{i,\beta})$$



$0 < \epsilon < \epsilon^*$

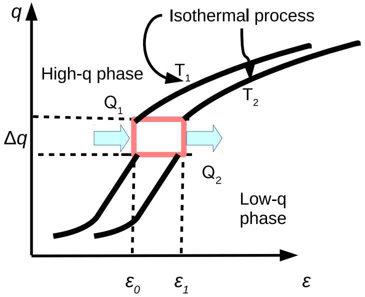
- discontinuous jump in q
- 1st order phase transition with latent heat

$\epsilon^* < \epsilon$

- crossover in q
- no phase transition

Clausius-Clapeyron relation of ϵ-coupled system

Carnot cycle in the ϵ-coupled system



Carnot theorem

$$\frac{Q_1}{T_1} = \frac{Q_2}{T_2}$$

As $T_1 - T_2 = \Delta T$, the first law gives the work W of the cycle

$$W = Q_1 - Q_2 = Q_1 - \frac{T_2}{T_1} Q_1 = Q_1 \frac{\Delta T}{T_1}$$

The work W is also expressed by the area as

$$\Delta q \Delta \epsilon = Q_1 \frac{\Delta T}{T_1}, \Longrightarrow \frac{\Delta T}{\Delta \epsilon} = \frac{T \Delta q}{Q_1} \Longrightarrow \frac{dT}{d\epsilon} = \frac{T \Delta q}{Q_1}$$

From Clausius-Clapeyron relation, ...

1. First-order phase boundary is monotonic upward curve in $T-\epsilon$ phase diagram
   - $\Delta q \geq 0$ and $Q_1 \geq 0$
2. If RFOT occurs in the limit $\epsilon = 0$

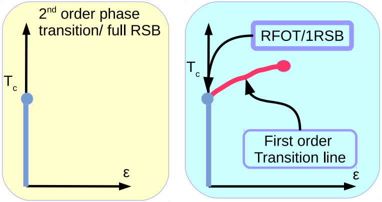
$$\left.\frac{dT}{d\epsilon}\right|_{\epsilon=0} = \infty,$$

because $Q_1 = 0$ and $\Delta q > 0$.

3. A mean-field prediction for annealed system gives $T_c(\epsilon) = T_c(0) + O(\sqrt{\epsilon})$ with $\Delta q =$ const., yielding $\Longrightarrow Q_1 = \sqrt{\epsilon} + \cdots$.
4. About critical end point...

CC relation

$$\frac{dT}{d\epsilon} = \frac{T\Delta q}{Q_1}$$

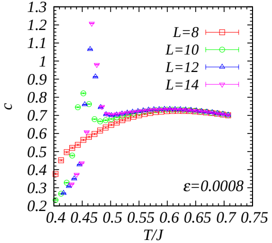


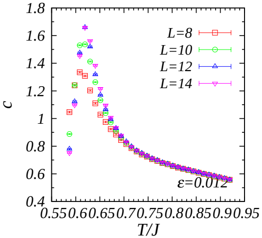
Thermodynamics of the ϵ-coupled system

$0 < \epsilon < \epsilon^*$:

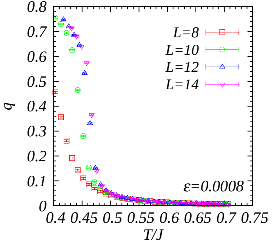
$\epsilon^* < \epsilon$:

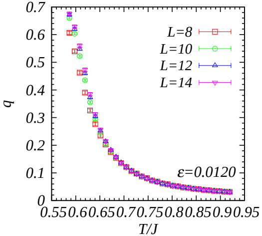
Specific heat



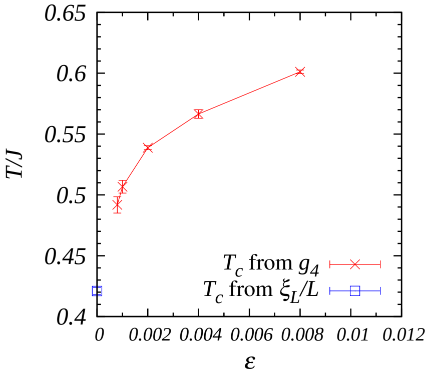


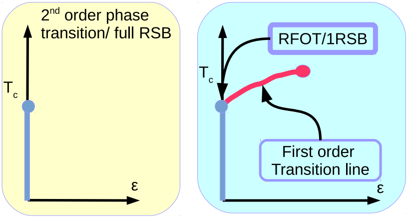
Overlap





Phase diagram of $3d$ Potts glass model in $\epsilon - T$





- Our result is consistent with 1st order transition temperature with infinite slope at $\epsilon = 0$, suggesting RFOT at $\epsilon = 0$.
- Critical endpoint:$0.008 < \epsilon^* < 0.012$

Dynamics –auto-correlation function and susceptibility–

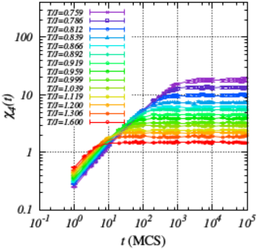
- Autocorrelation function : $C(t;t_w) = \frac{1}{N}\sum_i \frac{\boldsymbol{S}_i(t_w)\cdot\boldsymbol{S}_i(t+t_w)}{1-1/p}$
- Dynamical susceptibility (four-point correlation function) χ_4:

$$\chi_4(t;t_w) = N\left[\langle C(t;t_w)^2\rangle - \langle C(t;t_w)\rangle^2\right]$$

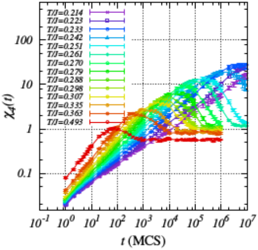
  - $\lim_{t\to\infty}\lim_{t_w\to\infty}\chi_4(\infty;\infty) = \chi_{SG}$: Static spin-glass susceptibility

- (Left)χ_4 increases monotonically for no-RFOT case
- (right)χ_4 has a peak at finite time t and its height diverges at $T = T_d$ for RFOT case.

non-RFOT case

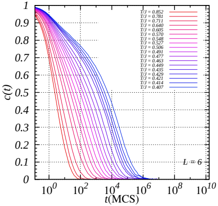


RFOT case

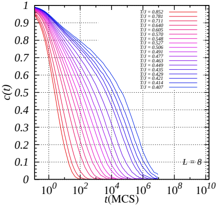


Dynamical properties in $3d$ Potts glass model –Auto-correlation function $C(t)$–

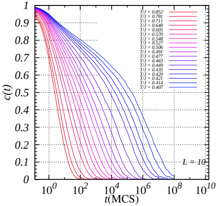
$L = 6$



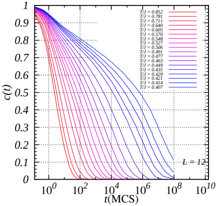
$L = 8$



$L = 10$



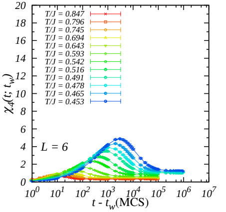
$L = 12$



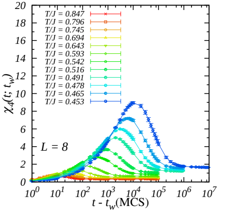
- Static SG transition is located on boundary between blue and red.
- No plateau is found, in contrast to the mean-field prediction
- No dynamical singularity at T_d is also found.

Dynamical properties in $3d$ Potts glass model –dynamical susceptibility $\chi_4(t)$–

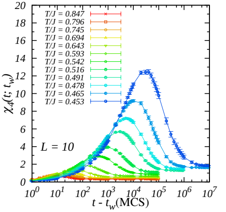
$L = 6$



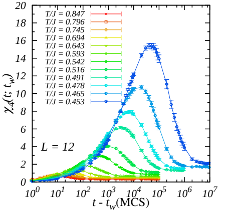
$L = 8$



$L = 10$

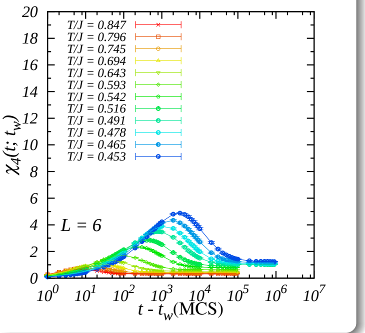


$L = 12$

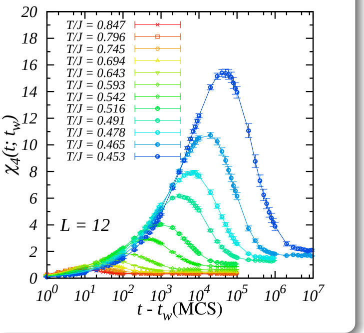


Dynamical properties in $3d$ Potts glass model –dynamical susceptibility $\chi_4(t)$–

$L = 6$



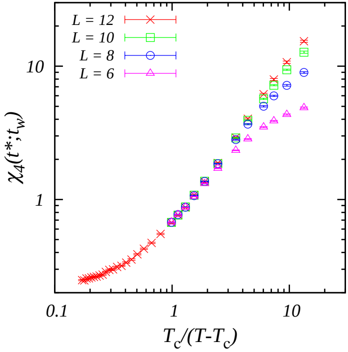
$L = 12$



- Before equilibrium limit $t \to \infty$, $\chi_4(t)$ has a peak at certain time scale
- The time scale and the peak height have a divergent tendency
- χ_4 in equilibrium limit diverges at T_c.

Dynamical properties in $3d$ Potts glass model

Temperature dependence of the peak in χ_4



- Peak height $\chi_4(t^*)$ in χ_4 diverges at T_c not T_d: $\chi_4(t^*) \sim |T - T_c|^{-\gamma^*}$
- $\chi_4(t^*)$ has singularity stronger than static $\chi_4(\infty)$: $\chi_4(\infty) \sim |T - T_c|^{-\gamma}$

$\boxed{\gamma^* > \gamma}$ $\Longrightarrow$ **Separation between static and dynamics singularities**

Outline

Summary

- Random first-order transition (RFOT) of spin glasses
- 7-state Potts glass model in three dimensions with 1st, 2nd, and 3rd neighbor couplings.

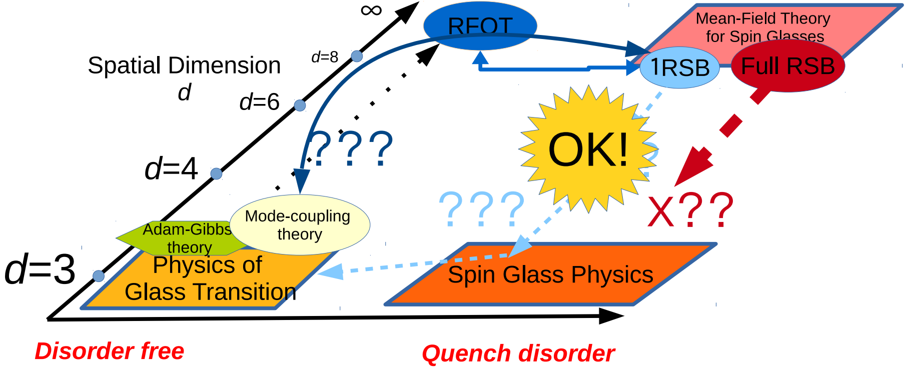
Our findings Phys. Rev. E 91, 020102(R)(2015)

- SG transition at finite temperature T_c.
- A critical exponent $\nu = 0.68(9) \sim 2/d$.
- Overlap has a jump at T_c without latent heat.
- $P(q)$ has double-peak structure at and below T_c.

- These features are compatible to 1RSB.
- This model is a strong candidate which displays RFOT in three dimensions.
- A dynamical singularity in flucutuation is found, indicating a possibility of $T_d \simeq T_c$.

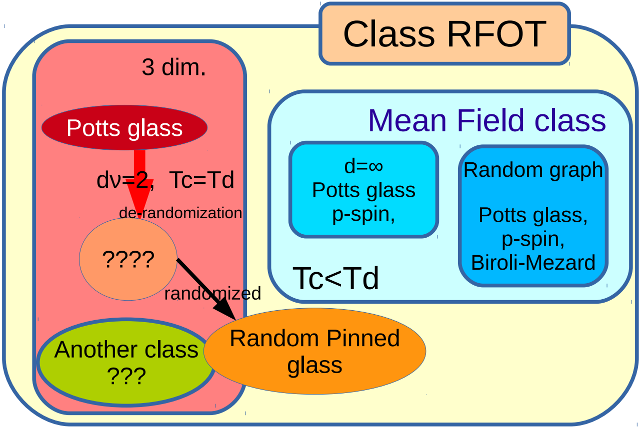
Summary

This research is one step toward the understanding of thermodynamic glass transitions as a transition from liquid to disordered solid.



Summary

This research is one step toward the understanding of thermodynamic glass transitions as a transition from liquid to disordered solid.



Thank you for your attention.

Financial support

- 2013-2018 Grant-in-Aid for Scientific Research on Innovative Areas, MEXT, Japan "Initiative for High-Dimensional Data-Driven Science through Deepening of Sparse Modeling"
- JPS Core-to-Core program 2013-2015, "Non-equilibrium dynamics of soft matter and information"