

An extended ensemble Monte Carlo study for a simple glass model

Koji Hukushima

<mailto:hukusima@phys.c.u-tokyo.ac.jp>

The University of Tokyo, Komaba,
Graduate school of Arts and Sciences

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Outline

- 1 A simple lattice glass model : Biroli-Mézard (BM) model
- 2 Extended ensemble MC
- 3 Test in BM model on a random graph
- 4 BM model on a regular graph in two dimensions
- 5 Summary



General question

Glassy materials are ubiquitous, but the nature of glass still remains to be unclear.

One of the most fundamental questions is that

existence of **thermodynamical** glass transition?

The spin-glass transitions are found both in experiments and in theoretical models.

Does the lattice model in finite dimensions exhibit a thermodynamic transition?



A simple lattice glass model: Biroli-Mézard model (2002)

- A given graph $G(V,E)$
 - Random graph
 - Regular graph ...
- An occupation variable σ_i is defined on each site

$$\sigma_i = \begin{cases} 1 & \text{for occupied,} \\ 0 & \text{for empty} \end{cases}$$

- Particle configuration:

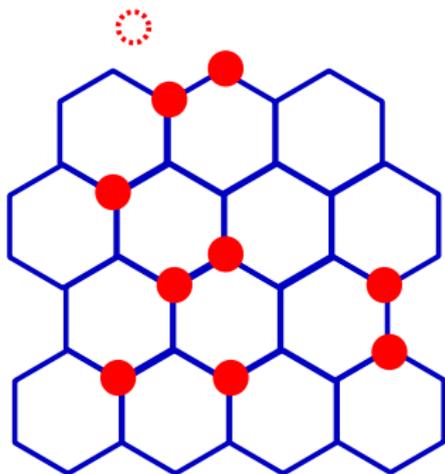
$$\sigma = (\sigma_i)_{i=1, \dots, N}$$

- Energy :

$H(\sigma) = \infty$ # of particles in the neighbor sites is greater than a parameter l .

$H(\sigma) = 0$ Otherwise

BM model with $l = 1$



Equilibrium statistical mechanics of BM model

- Grand partition function

$$Z(\mu) = \sum_{\sigma} C(\sigma) e^{\mu \sum_{i=1}^N \sigma_i}$$

where $C(\sigma)$ is a indicator function,

$$C(\sigma) = \begin{cases} 1 & \text{for a possible configuration } \sigma \\ 0 & \text{otherwise.} \end{cases}$$

- $C(\sigma)$ is generally expressed as multi-body interactions.
- Probability $P(\sigma)$:

$$P(\sigma) = \frac{1}{Z(\mu)} C(\sigma) \exp \left(\mu \sum_{i=1}^N \sigma_i \right)$$

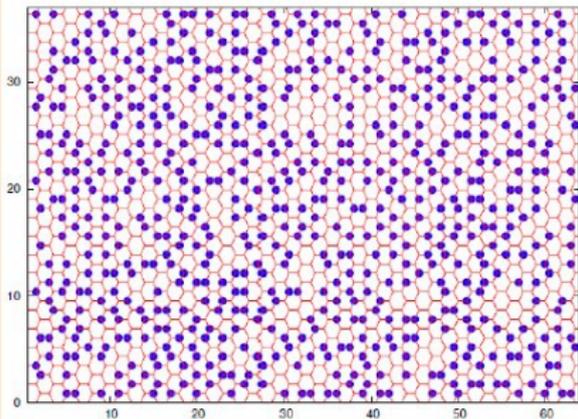
- Expectation value $A(\mu) = \langle \hat{A} \rangle_{\mu} = \sum_{\sigma} \hat{A}(\sigma) P(\sigma)$.



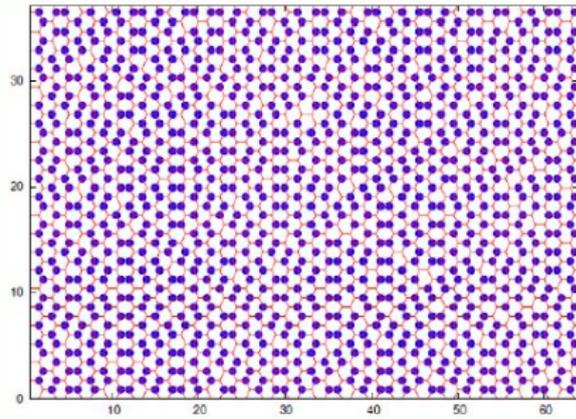
Phase transition of the BM model

A typical snapshot of BM model with $l = 1$

$$\mu = 0.2$$



$$\mu = 7.0$$

A typical snapshot of BM model with $l = 1$

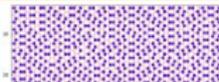
$$\mu = 0.2$$



$$\mu = 3.0$$



$$\mu = 6.0$$

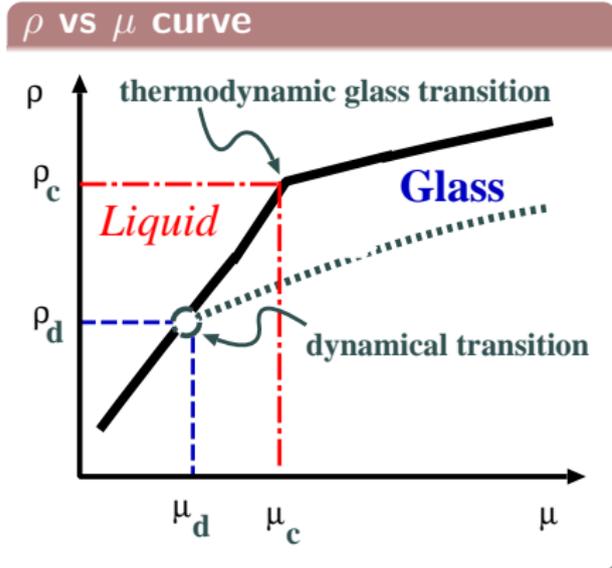


$$\mu = 7.0$$



Theoretical analyses: Rivoire et al(2004) , Krzakala-Tarzia-Zdeborová(2008)

- The model in a random graph by cavity method.
- **One-step replica-symmetry-breaking transition** occurs at ρ_c .
- Average density $\rho(\mu)$ is continuous, but smooth at some density ρ_c .
- Dynamical transition occurs at $\rho_d < \rho_c$. For $\rho > \rho_d$ **local-update algorithm, like simulated annealing, cannot reach equilibrium.**



Questions

Physics: Does there exist **thermodynamic glass transition** in a statistical-mechanical model beyond mean-field analysis?

- the BM model defined on a honeycomb lattice where connectivity is 3.

Algorithm: How can we go across **“dynamical transition”** to reveal thermodynamic transition?

- Florent provided a promising strategy in his talk, but... we study in a straightforward way by using an extended ensemble MC method



Slow relaxation in MCMC

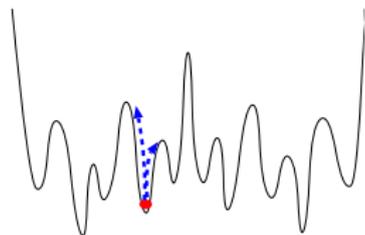
Under some circumstances, transitions in Markov chain are strongly suppressed. Configurations get trapped into some small area of configuration space.

ergodicity breaking \approx slow relaxation/mixing

One may often face this difficulty in some physically interesting problems.

- ① **slowing down** of phase transition
 - critical slowing down of 2nd order transition
 - nucleation of 1st order transition

- ② **rugged free energy**
(Spin) Glasses, proteins, optimizations...



many metastable states = multi-modal dist.



Some development of MCMC algorithm

1 non-local update (cluster algorithm)

- Swendsen-Wang (1987), Wolf (88): based on Fortuin-Kasteleyn representation.
- pivot update algorithm for polymer simulation

2 Extended ensemble MC

Original probability distribution to be solved is modified or extended.

- **Multicanonical MC** : Berg-Neuhaus, (1991)
 - entropic sampling : Lee
 - Broad histogram MC : Oliveira (1998)
 - Flat histogram MC , Transition Matrix MC : Wang (1999)
 - Wang-Landau method....
- **Simulated tempering** : Marinari-Parisi(1992),
 - Expanded ensemble method : Lyubartsev et. al. (1992)
- **Exchange MC method** : Hukushima-Nemoto(1996),
 - Metropolis coupled Markov chain MC(Geyer) , Parallel tempering



From SA to exchange MC

- ① Temperature schedule
 - Practically important.
 - Temperature is always lowered, but heating may be useful for escaping from local minima.
- ② Sampling from distribution
 - Detailed balance conditions are not satisfied when temperature is lowered.
 - When temperature is fixed, this corresponds to MCMC. At low temperatures, the difficulty of slow relaxation(mixing) is faced.

A goal is to construct an MCMC algorithm in which **temperature keeps changing back and forth with preserving detailed balance conditions.**

- Simulated tempering and exchange MC(parallel tempering).
- A dual method is multicanonical MC, where energy value changes a wide range.

Exchange Monte Carlo Method (1)

Replicated System : For a given model $\mathcal{H}(X)$, M replicas of the system is introduced:

$$\mathcal{H}_{\text{eff}}(\{X\}) = \sum_{m=1}^M \beta_m \mathcal{H}(X_m),$$

“extended state” : $\{X\} = \{X_1, X_2, \dots, X_M\}$.

“Extended” probability distribution

$$P_{\text{eq}}(\{X\}; \{\beta\}) = \prod_{m=1}^M P_{\text{eq}}(X_m; \beta_m) = \prod_{m=1}^M \frac{1}{Z(\beta_m)} \exp(-\beta_m \mathcal{H}(X_m))$$

Monte Carlo steps

- 1 Update each replica configuration (Local update)

$$X_m \implies X'_m$$

- 2 Exchange of two configurations of two replicas X_m and X_n

$$\{X_m, X_n\} \implies \{X_n, X_m\}$$



Exchange Monte Carlo Method (2)

Detailed Balance conditions

$$P(\{\dots, X, \dots, X', \dots\}; \{\dots, \beta_m, \dots, \beta_n, \dots\}) \times W(X, X'; \beta_m, \beta_n) \\ = P(\{\dots, X', \dots, X, \dots\}; \{\dots, \beta_m, \dots, \beta_n, \dots\}) W(X', X; \beta_m, \beta_n).$$

$$\frac{W(X, X'; \beta_m, \beta_n)}{W(X', X; \beta_m, \beta_n)} = \exp(-\Delta),$$

where

$$\Delta(X, X'; \beta_m, \beta_n) = (\beta_n - \beta_m)(\mathcal{H}(X) - \mathcal{H}(X')).$$

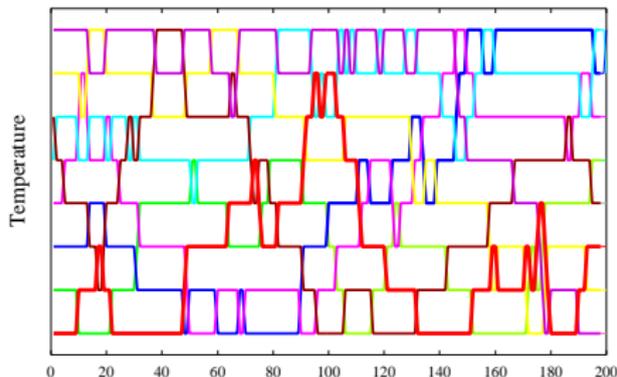
Transition Probability for exchange process

$$W(X, X'; \beta_m, \beta_n) = \begin{cases} \min[1, \exp(-\Delta)], & \text{for Metropolis type,} \\ \frac{1}{2} \left(1 + \tanh\left(-\frac{\Delta}{2}\right)\right), & \text{for heat-bath type.} \end{cases}$$



Exchange Monte Carlo Method (3)

Monte Carlo Procedure



- 1 Each replica is updated **simultaneously** and **independently** as a canonical ensemble for a few MC steps

$$\{X_m\} \implies \{X'_m\}$$

- 2 An exchange process between X_m and X_{m+1} is tried and accepted with probability $W(X_m, X_{m+1})$.

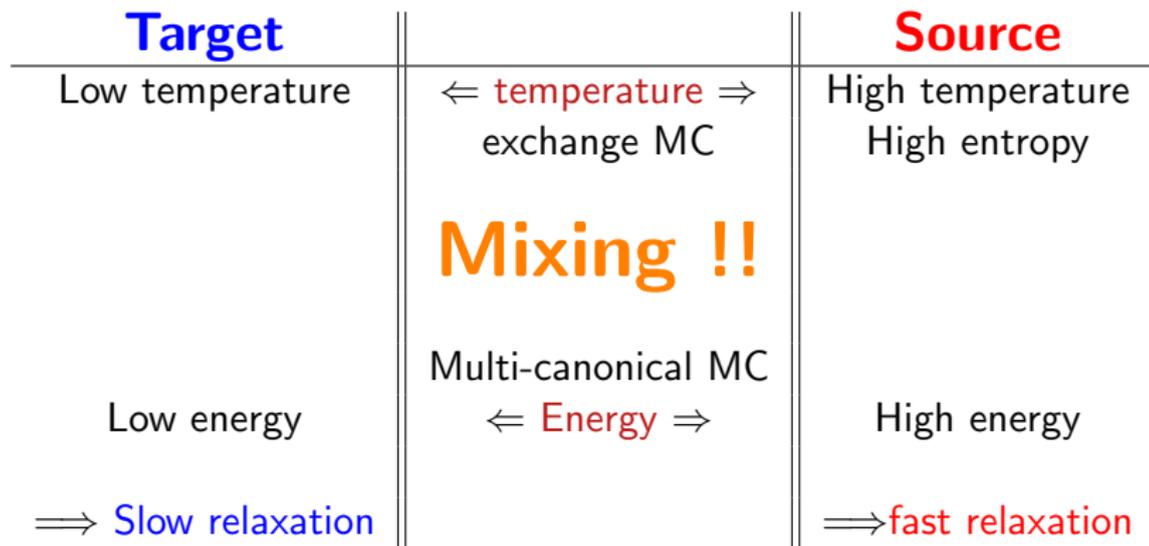
$$\{X_m, X_{m+1}\} \implies \{X_{m+1}, X_m\}$$

- Each replica wanders in the parameter space like random walker.
 - Self-organized **annealing** and **heating**
 - one may have a chance to escape from **meta-stable state** at high temp.
- Sampling from equilibrium distribution at each temperature.



Strategy of extended ensemble MCs

- Acceleration of relaxation ... (reduction of mixing time)



Slow relaxation found in the “TARGET” might be modified with the help of fast relaxation in the “SOURCE”.



Possible extensions of Extended ensemble MC

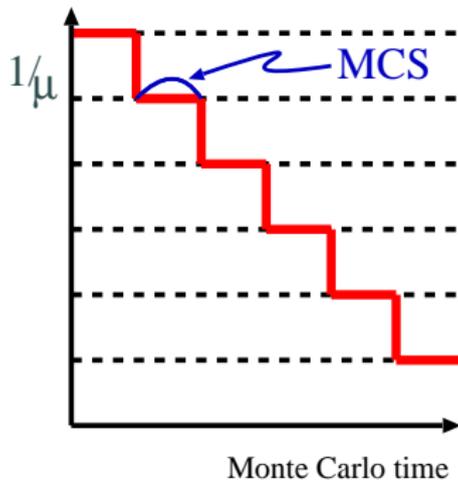
	Multi-canonical MC	Simulated tempering exchange MC (Parallel tempering)
$Z(\beta) = \sum \exp(-\beta E)$	Energy E	Temperature β
$Z(\mu) = \sum \exp(\mu n)$	Particle number n	Chemical Potential μ
magnetic interaction $E' = -HM$	Magnetization M	Magnetic field H
$E = E^{(1)} + kE^{(2)}$ free particle+interaction	$E^{(2)}$	k

- An easy system with high entropy or at high temperature must be included in the parameter space.
- An extension to multiple parameters is OK.

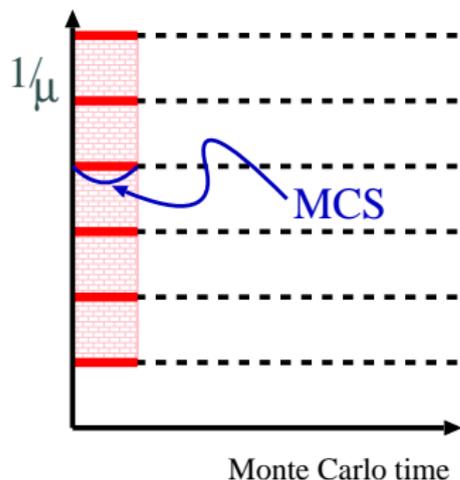


Comparison between SA and EMC

parameter schedule of SA



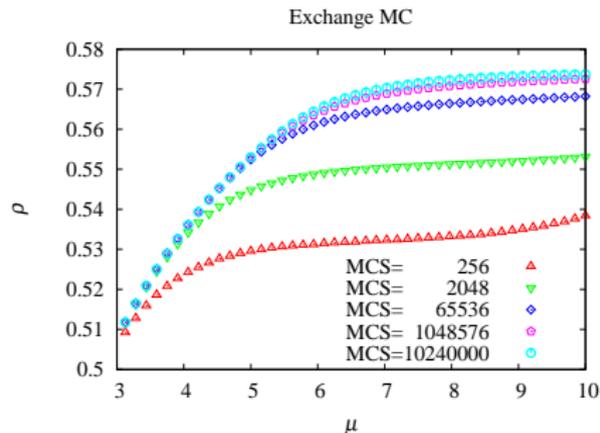
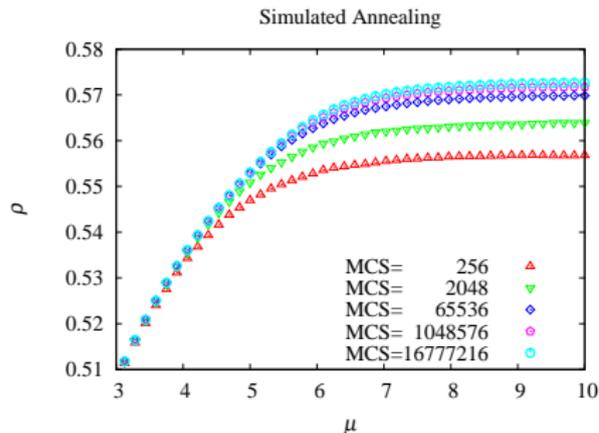
EMC(parallel tempering)



- The same set of μ s is used in SA and EMC.
- A constant number of **Monte Carlo steps**(MCS) is performed at each μ . The annealing rate in SA is proportional to $1/\text{MCS}$.
- Total MCS of SA and EMC is in common.

MCS dependence of $\rho(\mu)$ ρ - μ curve of BM model on random graph with $N = 512$

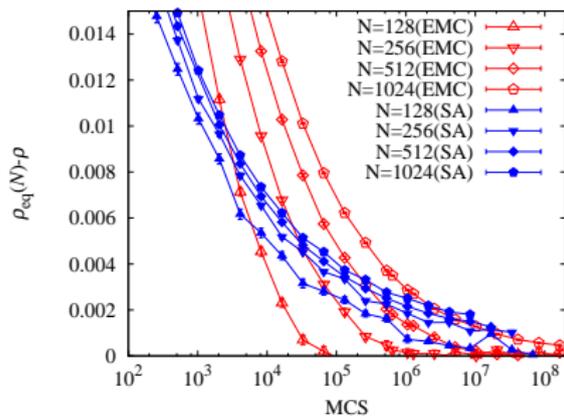
- regular random graph: $C = 3$
- model parameter : $l = 1$ (allowed occupation number in neighbor sites)

 ρ - μ curve of BM model on random

Annealing limit and equilibrium limit

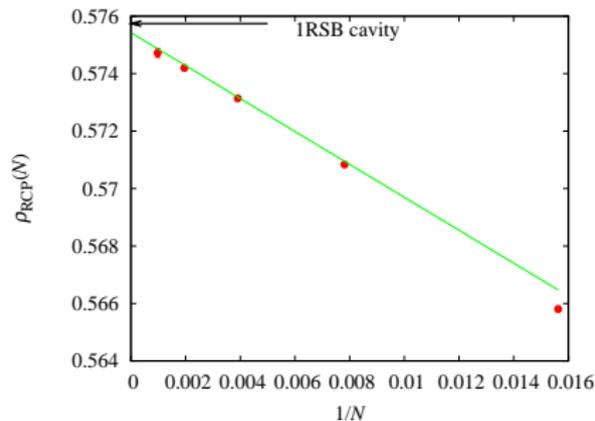
$\rho_{\text{eq}}(N) - \rho$ vs MC step at $\mu = 10$

- $N = 128, 256, 512$ and 1024 .



Size dep. of the densest packing

$\rho_{\text{RCP}}(N)$



- For large N limit, SA data may saturate to a finite gap predicted by the cavity method, but no tendency is found in EMC data up to MCS and sizes observed at least.
- Extrapolated value of the densest packing obtained by EMC with **finite N** is consistent with that of the cavity method.

Glassy property of BM model with $C = 3$ and $l = 1$

- Density $\hat{\rho} = \frac{1}{N} \sum_i \sigma_i$.
- Overlap of density fluctuation

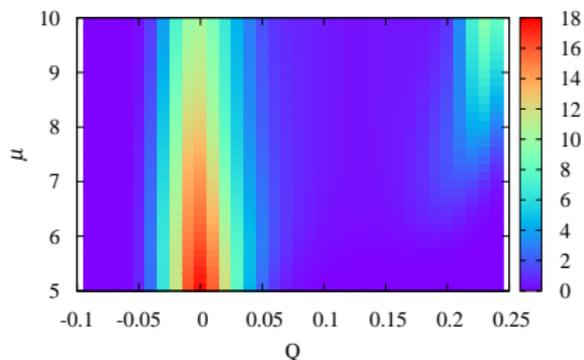
$$\hat{q} = \frac{1}{N} \sum_{i=1}^N (\sigma_i - \hat{\rho}) (\sigma'_i - \hat{\rho}')$$

where σ and σ' are configurations of two independent systems.

- Overlap distribution $P(q)$

$$P(q) = \langle \delta(q - \hat{q}) \rangle$$

Overlap dist. $P(q)$ with $N = 512$



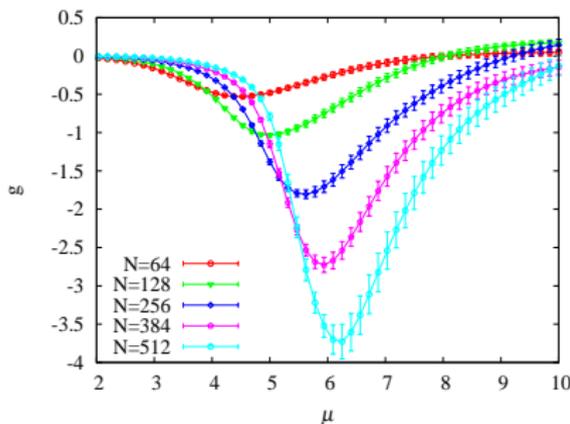
- This supports a transition from liquid to some glassy states.
- Two-peak structure of $P(q)$ is consistent with 1RSB picture.

Glassy transition of BM model with $C = 3$ and $l = 1$

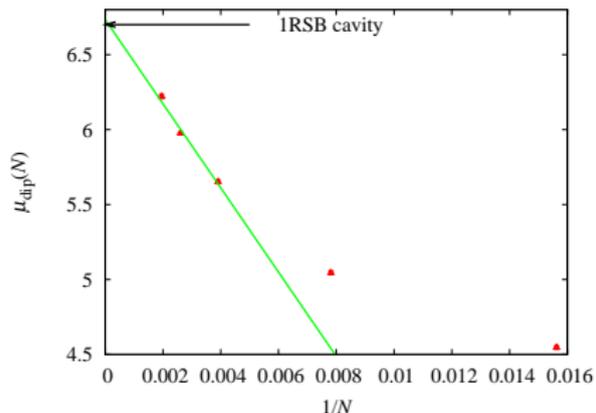
Binder parameter

$$g_\mu = \frac{1}{2} \left(3 - \frac{\langle \hat{q}^4 \rangle}{\langle \hat{q}^2 \rangle^2} \right)$$

- A negative dip appears at 1RSB transition.



Extrapolation of glass transition

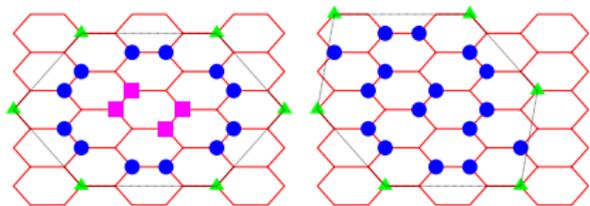


- $\mu_K \simeq 6.7$ (thanks to Florent).
- This is consistent with the 1RSB cavity analysis.

BM model with on a honeycomb lattice

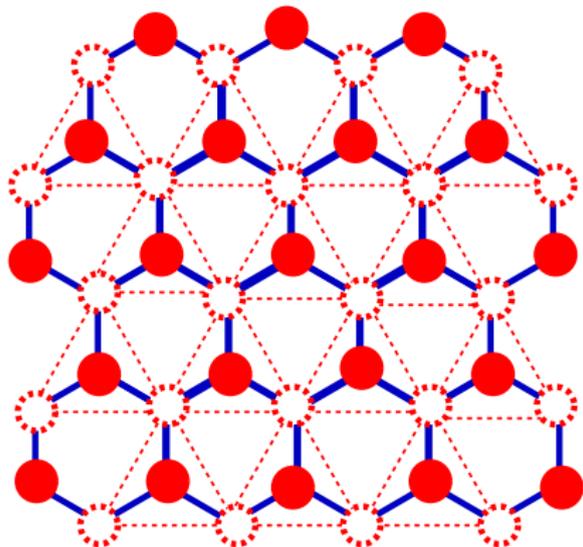
- $C = 3$: Honeycomb (HC) lattice
- $l = 0$: exactly solved model
 - Baxter's hard hexagon model
 - continuous phase transition from liquid to trigonal crystal.
- $l = 1$: not yet.

densest packing for $l = 1$



Complex mixtures are expected to be realized for dense region.

hard-trigons crystal for $l = 0$



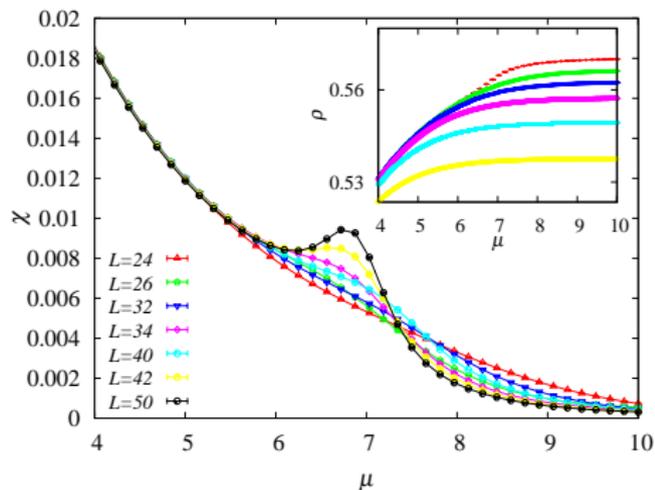
$\rho(\mu)$ curve and density fluctuation of BM in HC

- density fluctuation

$$\begin{aligned}\chi(\mu) &= \frac{\partial \rho(\mu)}{\partial \mu} \\ &= N \langle (\hat{\rho} - \rho(\mu))^2 \rangle\end{aligned}$$

- Anomalous behavior in χ is found around $\mu \sim 7.0$
- χ has a finite jump at transition?!

density fluctuation χ

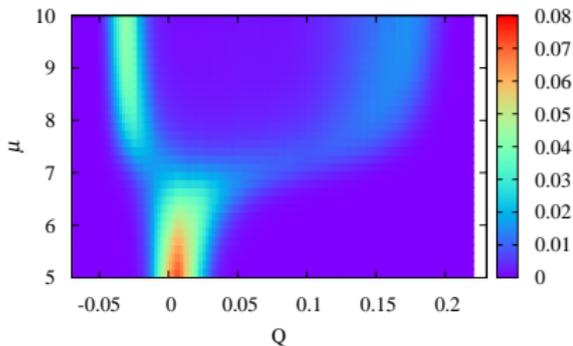


- linear size L : 24 to 50.

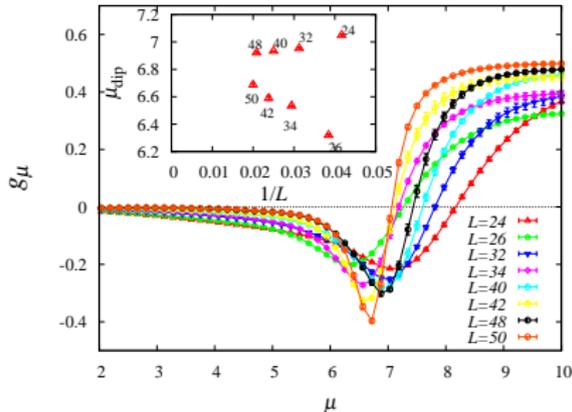
DEX-SMI

Evidence of thermodynamic transition at finite μ

Overlap distribution



Binder parameter



- At high dense region, $P(q)$ has a double-peak structure, often found in 1RSB phase.
- The transition point is estimated as $\mu_s \simeq 6.8$ from dips of g . Surprisingly, the value is very close to the cavity estimate for random graph model $\mu_K \simeq 6.7$.

Summary

- A simple lattice glass model, Biroli-Mézard (BM) model has been studied by using an exchange Monte Carlo (EMC) method.
- Efficiency of EMC method has been found in applications to the BM model defined on a regular random graph.
 - Time needed for equilibrium for EMC is shorter than that for the simulated annealing (SA).
 - Presumably, dynamical arrest also appears in EMC for large size, but no tendency is found up to 10^3 .
 - Results obtained by EMC with relatively small sizes are consistent with those predicted by the cavity analysis.
- A thermodynamic phase transition is found in the BM model in a two-dimensional honeycomb lattice.
 - 1RSB feature
 - $\mu_K^{\text{honeycomb}} \sim 6.8$ is very close to $\mu_K^{C=3} = 6.7\dots$
 $Z(\mu) = Z(BP)(1 + \dots \text{non-singular part})???$

Thank you for your attention.

