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Domain-Wall Free Energy of Spin-Glass Models

from an extended-ensemble approach

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OUTLINE

- Exchange Monte Carlo Method
- Brief review of earlier SG simulations
- Domain-wall free energy
- Numerical Results
- Conclusions

Introduction

Hardly-relaxing problem in Monte Carlo simulations

Systems with conflicting constraint such as spin glass, optimization problems, proteins,...

- Numerous local free-energy minima
- Rapid growth of characteristic times as temperature decreases

Recent improvements of MC algorithms

Extended ensemble method

Multicanonical method : Berg-Neuhaus, '91

Simulated tempering : Marinari-Parisi, '92

Exchange MC method : Hukushima-Nemoto, '96

Exchange Monte Carlo Method (1)

Effective Hamiltonian

For a given Hamiltonian $\mathcal{H}(X)$

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

where $\{X\} = \{X_1, X_2, \cdots, X_M\}$: is the state of the extended ensemble.

Partition Function and Equilibrium Distribution

$$Z_{\rm EMC} = {\rm Tr}_{\{X\}} e^{-\mathcal{H}_{\rm eff}(\{X\})} = \prod_{m=1}^{M} Z(\beta_m)$$

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

Monte Carlo dynamics

- Update config. for each replica

$$X_m \Longrightarrow X_m^{'}$$

- Exchange config. of two replicas X_m and X_n

$$\{X_m, X_n\} \Longrightarrow \{X_n, X_m\}$$

Exchange Monte Carlo Method (2)

Detailed Balance Conditions

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

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

where

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

Replica-exchange transition probability

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

Exchange Monte Carlo Method (3)

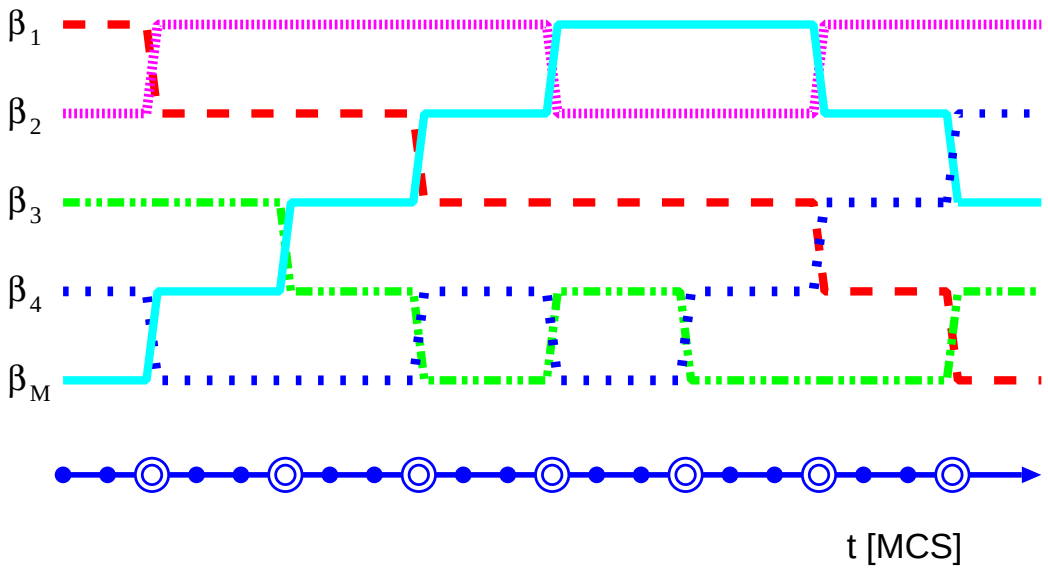
Monte Carlo Procedure

1. Each replica is simulated simultaneously and independently as canonical ensemble for a few MC steps.

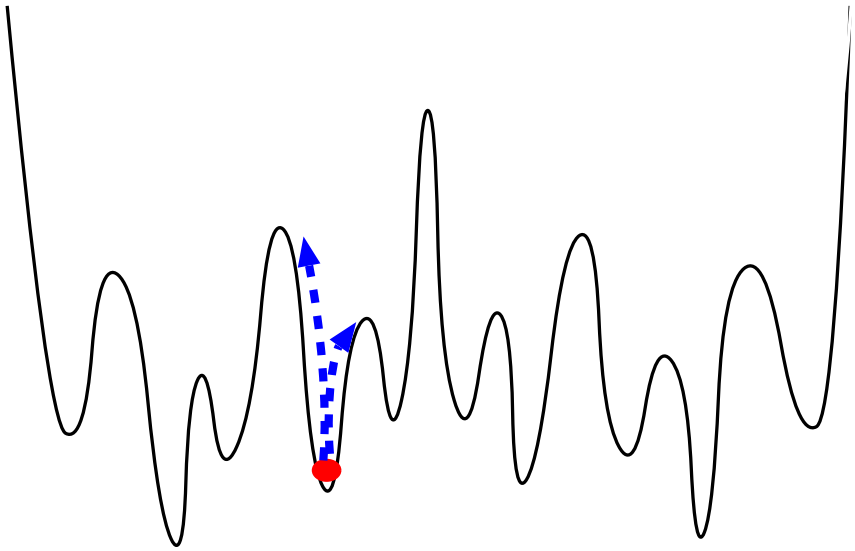
$$\{X_m\} \Longrightarrow \{X_m^{'}\}$$

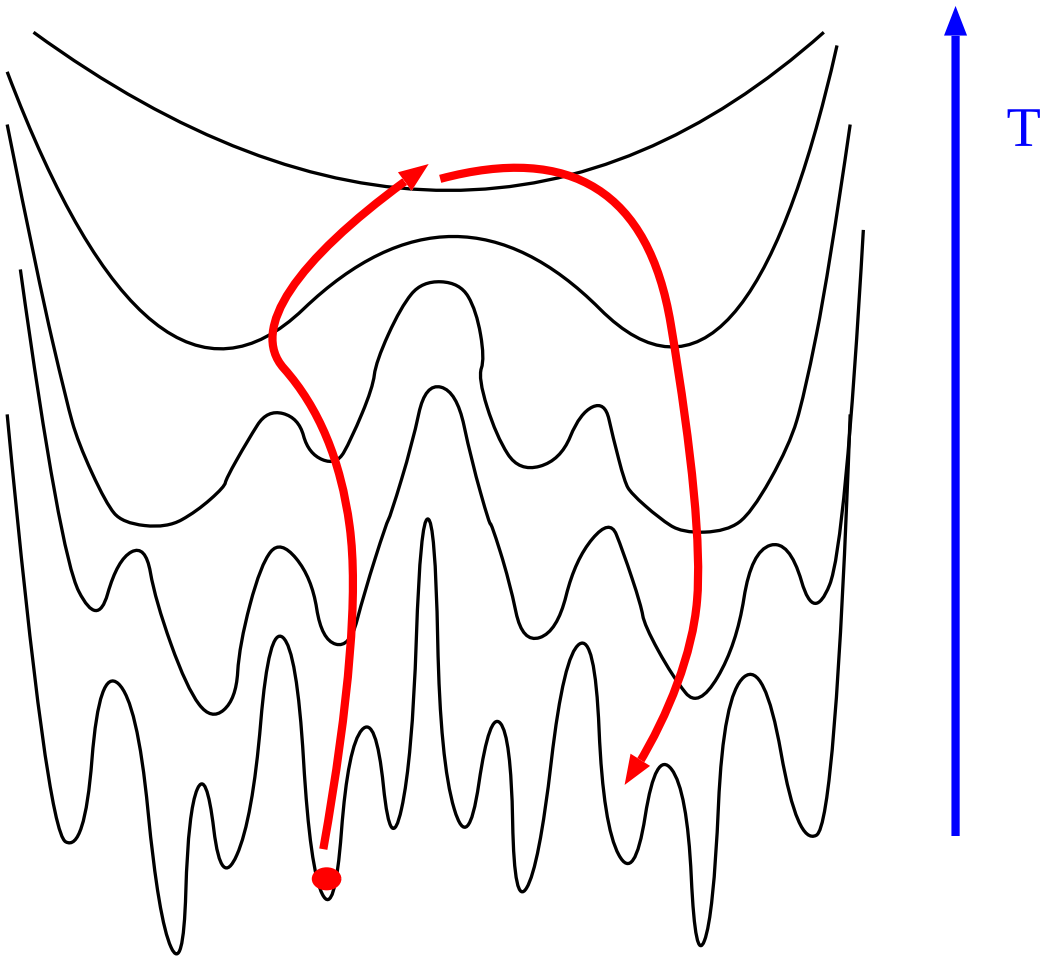
2. Exchange of two configurations X_m and X_{m+1} is tried and accepted with probability $W(X_m, X_{m+1})$

$$\{X_m, X_m + 1\} \Longrightarrow \{X_m + 1, X_m\}$$



Rugged free-energy landscape




T

$3d \pm J$ Ising SG model

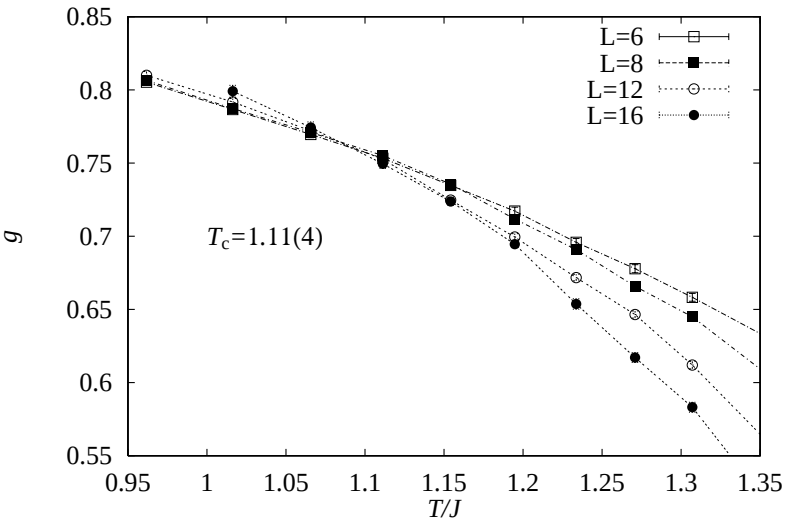
- Model

$$\mathcal{H} = \sum_{ij} J_{ij} S_i S_j, \quad P(J_{ij}) = \frac{1}{2}\delta(J_{ij}-J)+\frac{1}{2}\delta(J_{ij}+J).$$

- Dynamical properties (Ogielski-Morgenstern)
  - divergence of correlation time at $T_c \neq 0$
  - spin auto-correlation function $q(t)$ seems to vanish in the long time limit

    $q(t) \sim t^{-\lambda}$ at $T < T_c$

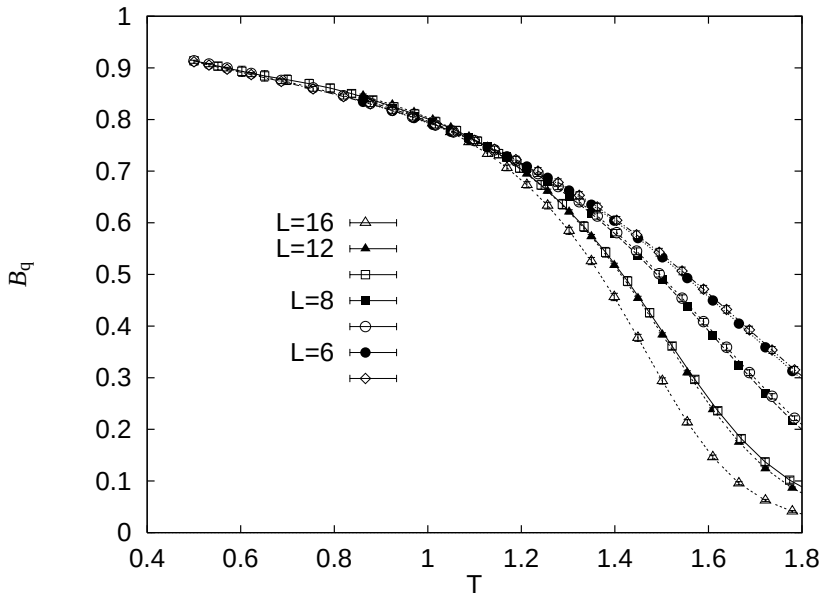
- Static properties (Bhatt-Young, Kawashima-Young)
  - Binder parameter $g = \frac{1}{2}\left(3 - \frac{[\langle q^4 \rangle]}{[\langle q^2 \rangle]^2}\right)$



marginal low temperature phase ??

$3d \pm J$ Ising SG model

- Binder parameter (K.H, Nemoto and Takayama, unpublished)



- Multi-overlap ensemble (Berg and Janke)

  nontrivial scaling behavior even below T_c.

- careful finite-size scaling (Palassini and Caracciolo)

  zero-temperature transition is excluded.

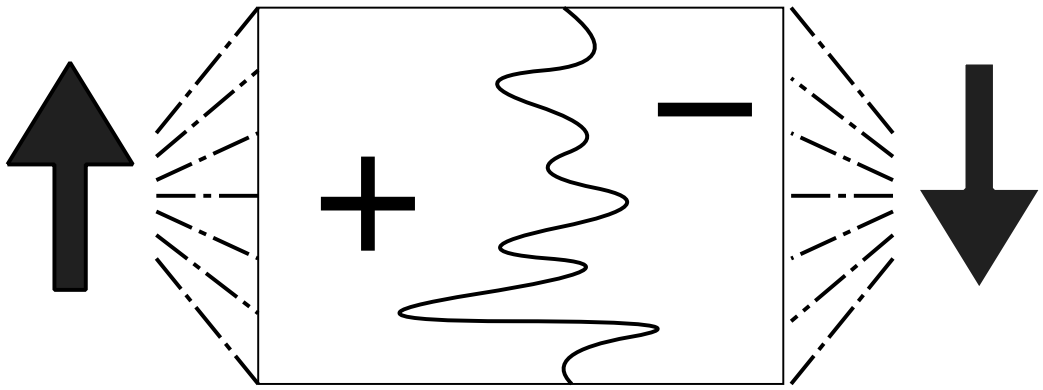
Possible Scenario

1. A standard continuous phase transition at T_c
2. An essential singularity at T_c like KT transition

Domain-Wall Free Eenergy

a singular part of free enrgy

$\sim$ domain-wall free energy $\Delta F \equiv F_{\rm APBC} - F_{\rm PBC}$



scaling regime

$$\Delta F(T, L) \sim L^{\theta}, \tag{1}$$

where θ is related to the rigidity.

$\theta > 0$ ordered phase

$\theta < 0$ disordered phase

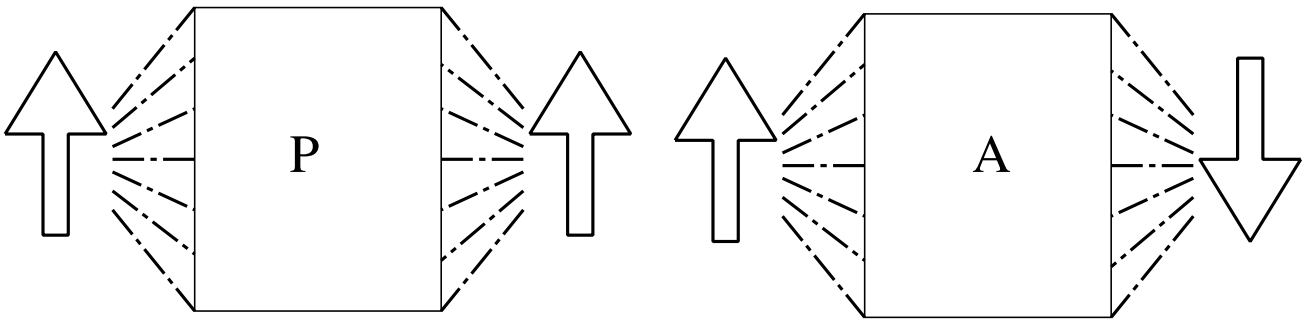
finite-size scaling

$$\Delta F(T, L) \sim f((T - T_c)L^{1/\nu})$$

similar to the Binder parameter.

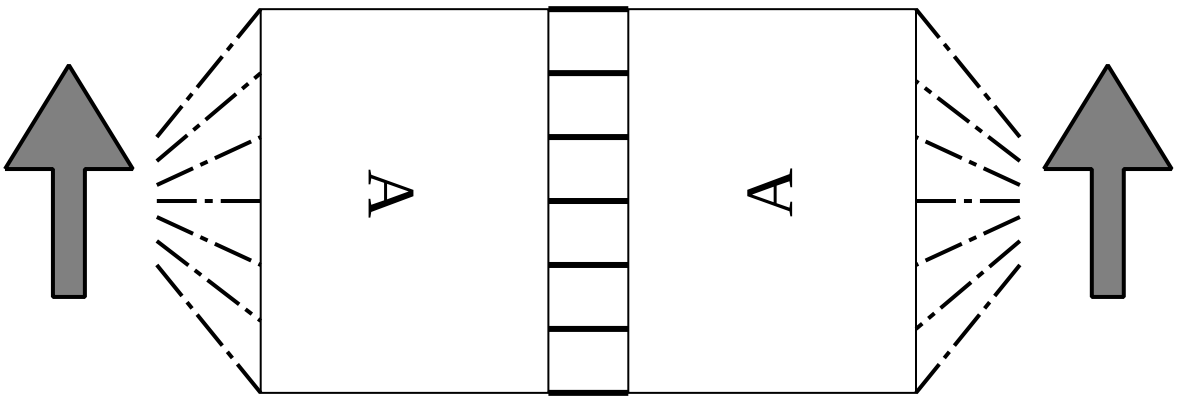
Boundary Conditions

Random (spin-fixed) boundary condition used in DWRG study



$$J^J_{\rm eff} = \tfrac{1}{2}(F_{\rm P} - F_{\rm A})$$
$$J_L = \sqrt{\langle (J^J_{\rm eff})^2 \rangle_J - \langle J^J_{\rm eff} \rangle^2_J}$$

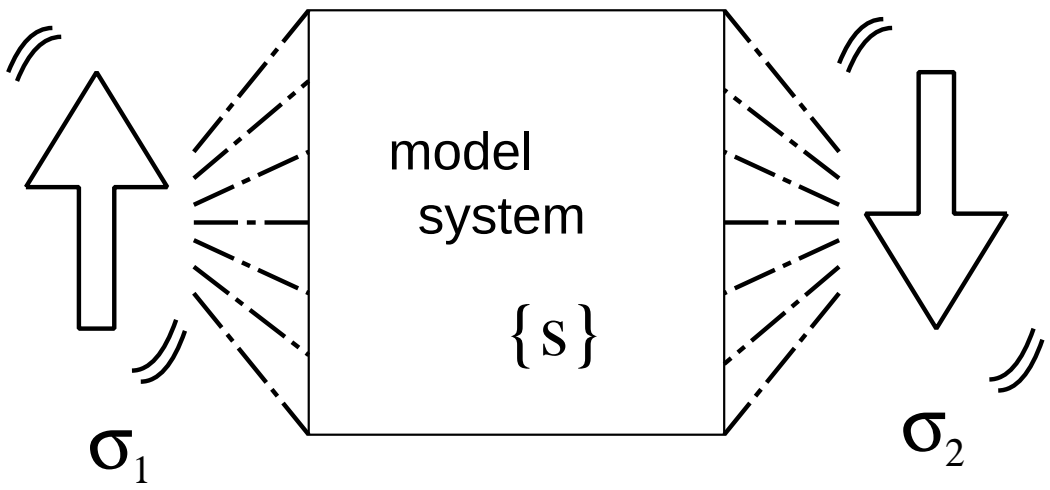
Replica Boundary Conditions proposed by Ozeki



- $J_{\rm int} > 0$: Periodic boundary condition
- $J_{\rm int} < 0$: Anti-periodic BC

$$\Delta F_{\rm R} = F^R_{\rm P} - F^R_{\rm A} \geq 0$$

How to estimate Domain-Wall Free Eenergy



total Hamiltonian

$$\mathcal{H}_{\rm tot}(\{S\},\sigma_1,\sigma_2) = \mathcal{H}_{\rm model}(\{S\}) + \mathcal{H}_{\rm boundary}(\{S\},\sigma)$$

Boundary Conditions

Periodic BC (Fixed spins) $\rightarrow \sigma_1 = \sigma_2$

Anti-Periodic BC $\rightarrow \sigma_1 = -\sigma_2$

Probability distribution for BCs $\{\sigma\}$

$$P(\sigma_1 = \pm\sigma_2; T) = \frac{{\rm Tr}_{\{S\}}\delta_{\sigma_1=\pm\sigma_2}\exp(-\beta\mathcal{H}_{\rm tot})}{Z_{\rm tot}(T)} = \frac{Z_{\rm (A)PBC}}{Z_{\rm tot}}$$

Domain-Wall Free-Energy: $\Delta F \equiv F_{\rm APBC} - F_{\rm PBC}$

$$\exp(\beta\Delta F) = \frac{Z(PBC)}{Z(APBC)} = \frac{P(\sigma_1 = \sigma_2)}{P(\sigma_1 = -\sigma_2)}$$

How to estimate Domain-Wall Free Eenergy (2)

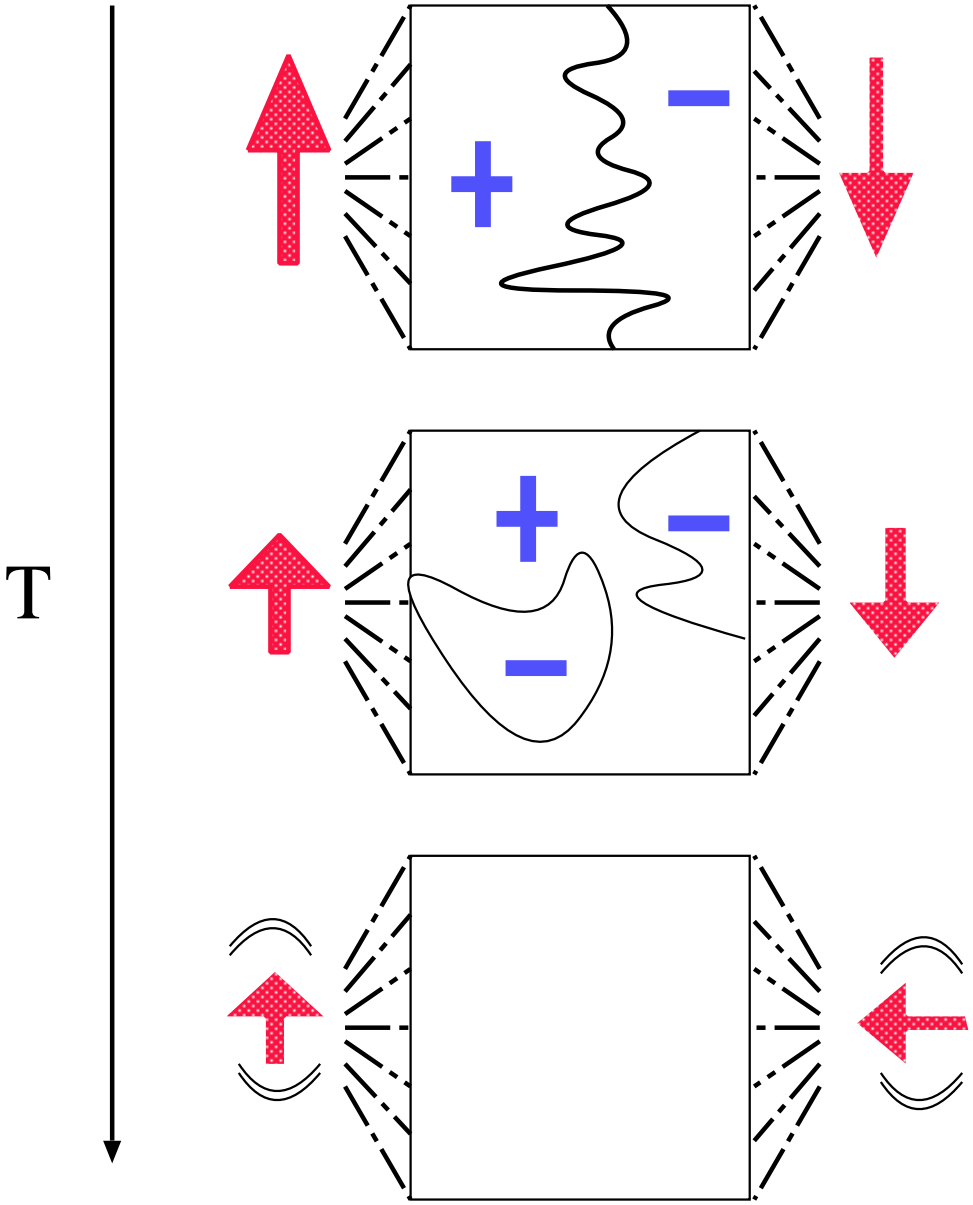
- Boundary spins are coupled with bulk spins whose number is $O(L^{d-1})$
- At low temperatures, metastable state corresponding to each boundary condition

$\longrightarrow$ **This is a typical slow relaxaing problem**

In order to overcome this difficulty,

Cluster MC method (Hasenbusch's work)

Exchange MC method (present work)

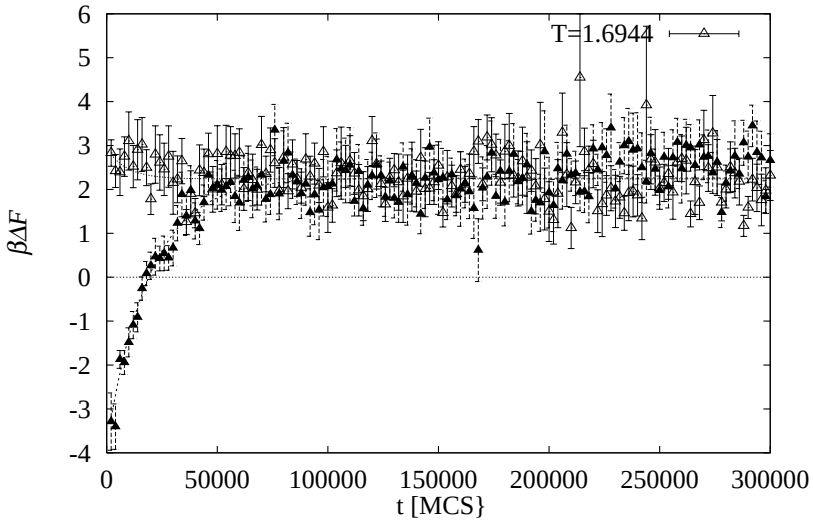


Equilibration check

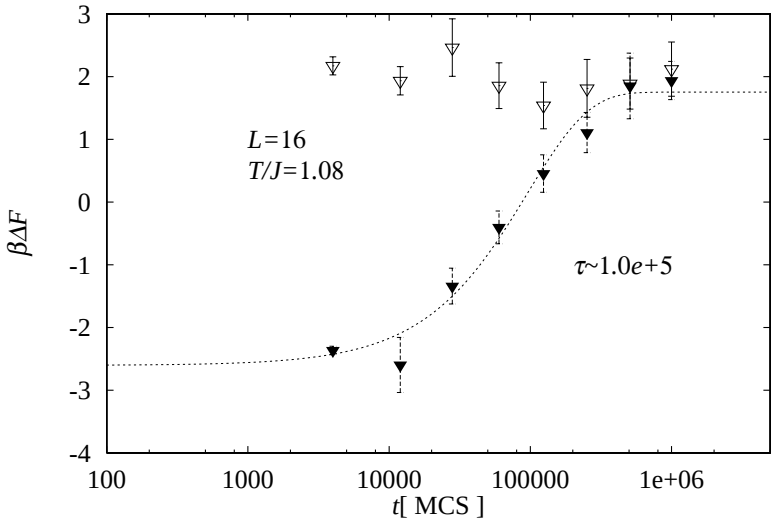
A comparison between two estimations starting from different initial spin conditions

- Periodic boundary conditions for all replicas
- Anti-parallel BC

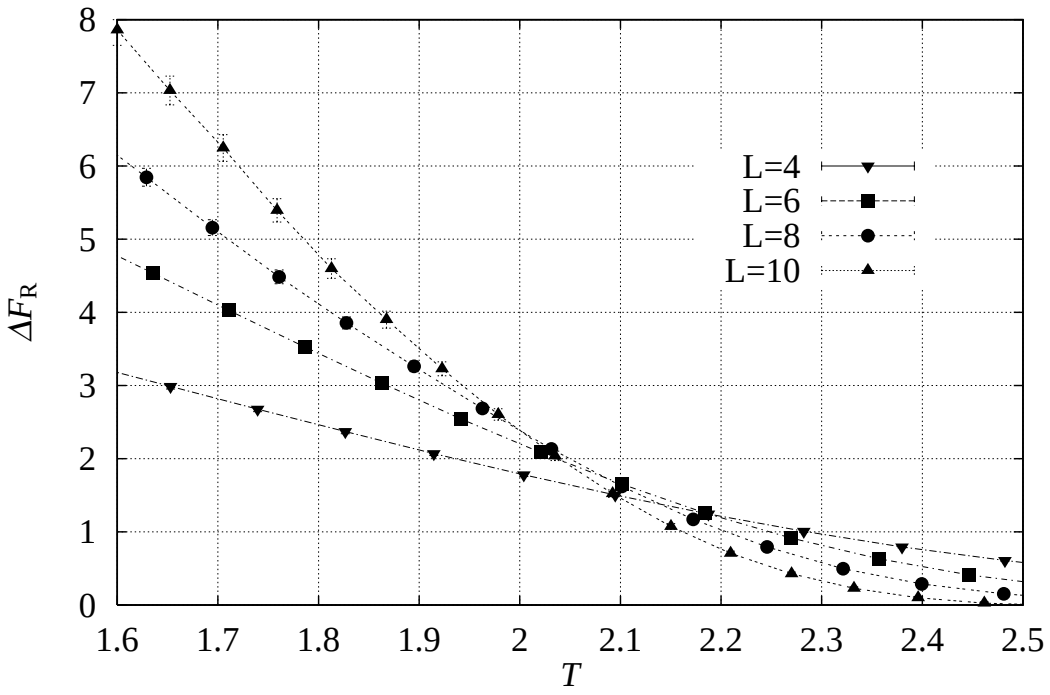
4D $\pm J$ Ising model



3D $\pm J$ Ising model



Domain-Wall Free-Eenrgy for 4D $\pm J$ Ising SG Model

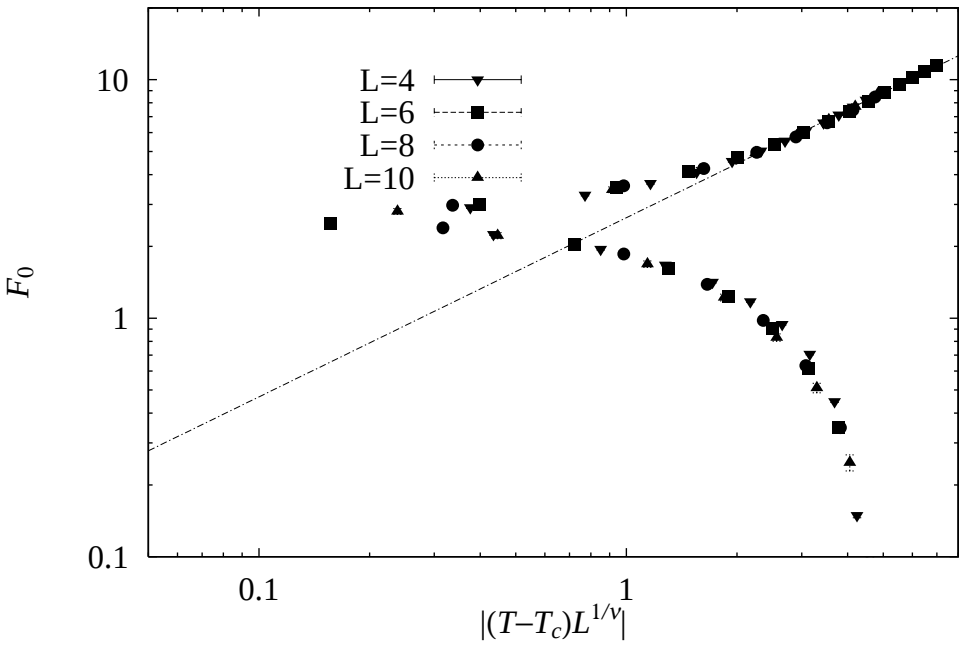


Crossing temperature is shift as L increases.

$\rightarrow$ correction to the FSS

$$\Delta F_{\mathrm{R}} \sim F_0((T-T_{\mathrm{c}})L^{1/\nu}) + L^{-\omega} F_1((T-T_{\mathrm{c}})L^{1/\nu}))$$

Finite-Size Scaling and stiffness exponent



Estimated valuses are

$$T_{\rm c} = 2.00(4),\ \nu = 0.92(6) \text{ and } \omega = 1.5(9).$$

Assumption

Large length scale $\Delta F_{\rm R} \sim L^{\theta}$ is also described by the finite-size scaling form.

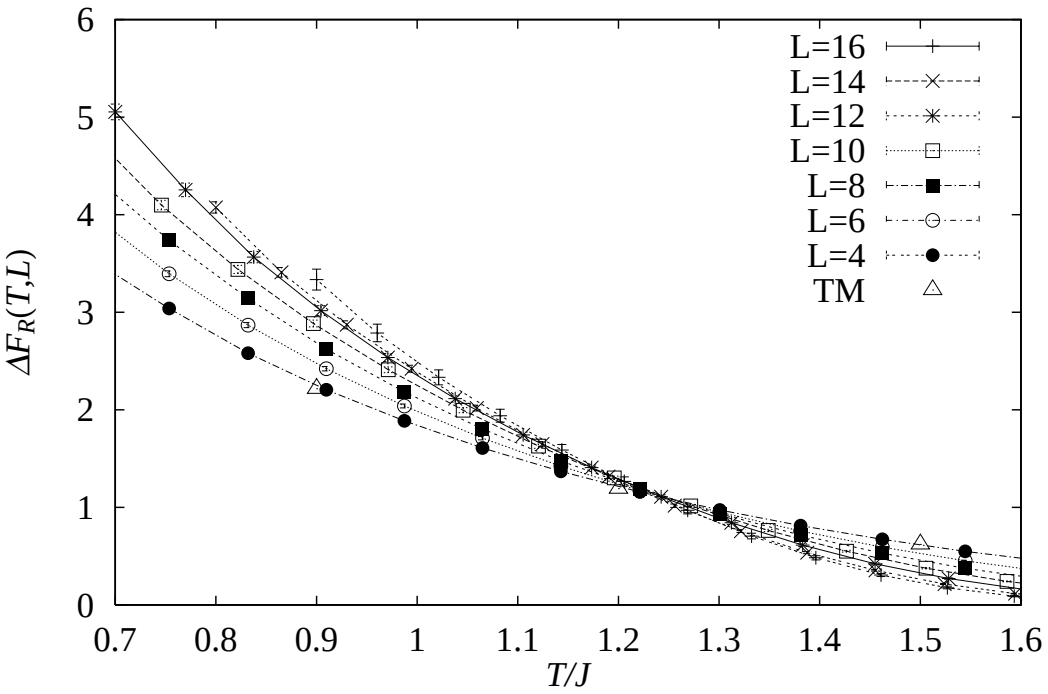
$$F_0(x) \sim x^{\mu} \quad \text{at} \quad x \to \infty$$

$$\mu = \theta\nu$$

Result $\theta = 0.82(6)$

Gound state calculation(A. K. Hartmann, '99)
$\theta = 0.65(4)$ up to $L = 7$.

DWFE of 3D $\pm J$ Ising SG Model



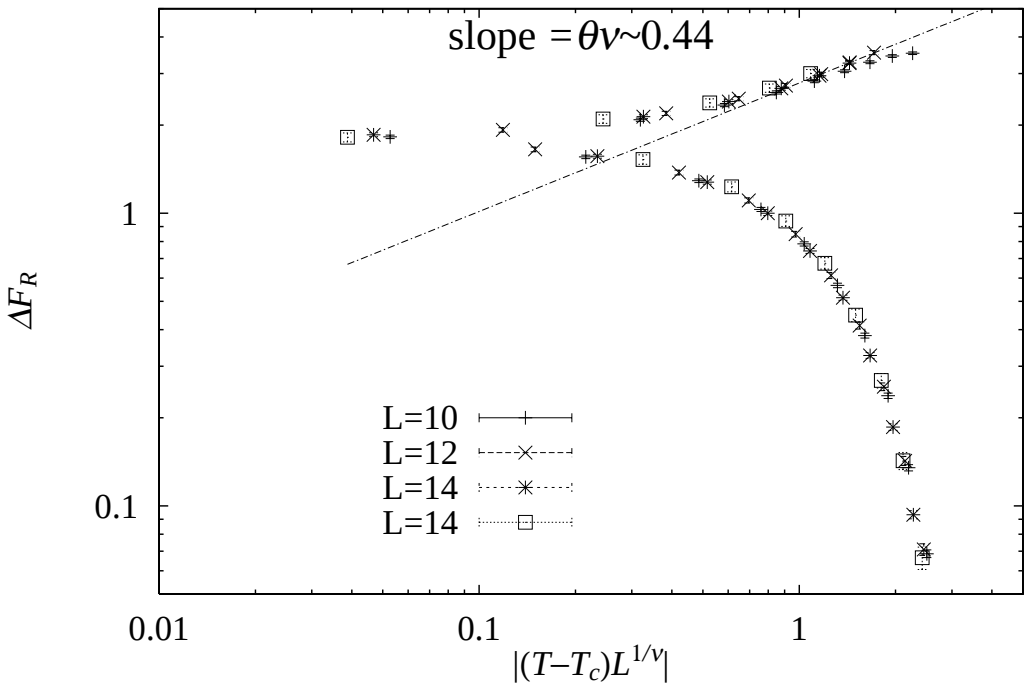
Resouces

L	# of samp.	MC sweeps	CPU time
4	2,500	5.2×10^4	8.6 Hours·Alpha21164
6	3,818	1.76×10^5	4.7 Days·Alpha21164
8	2,514	3.36×10^5	9.6 Days·Alpha21164
10	2,122	9.92×10^5	1.9 Months·Alpha21164
12	1,200	1.47×10^6	1.1 Months·VPP500
14	1.734	2.12	3.5 Months·VPP500
16	642	4.24	3.6 Months·VPP500

VPP500(Fujitsu) $\sim 7.5\times10^7$ spin updates / second

Alpha 21164 433Mhz $\sim 2.7\times10^7$ spin updates / second

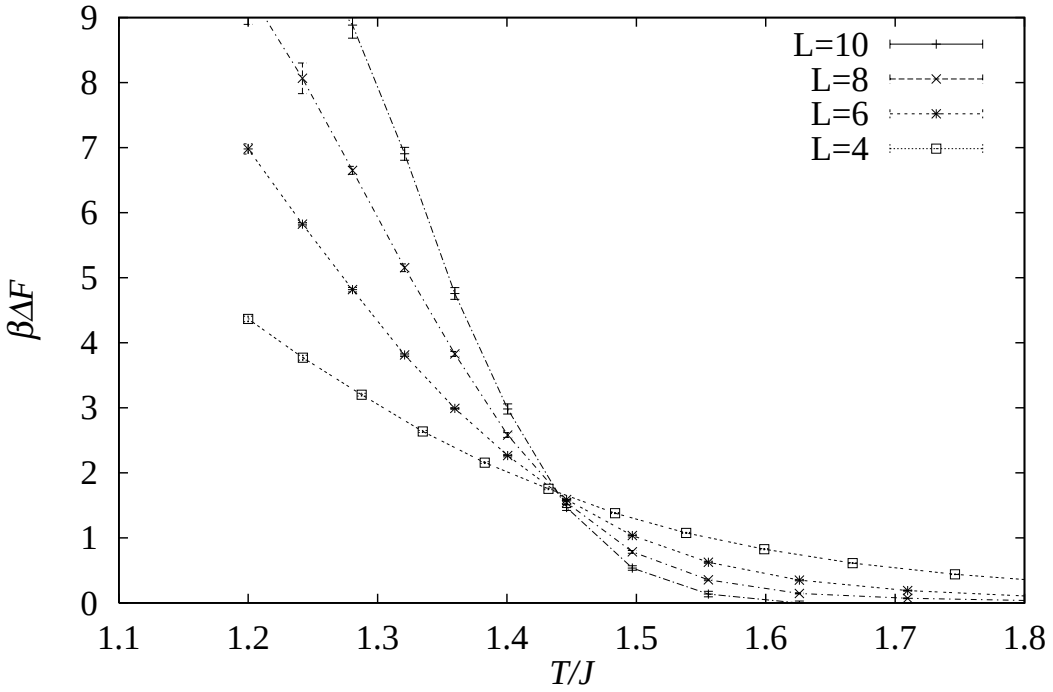
Finite-size scaling analysis of 3D $\pm J$ Ising SG Model



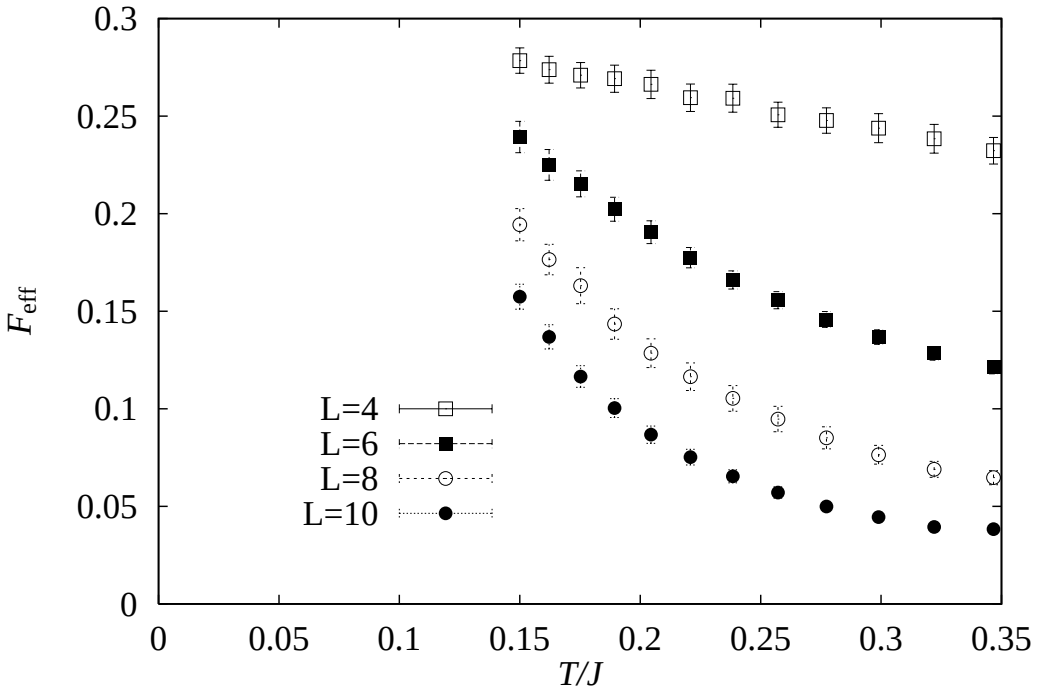
- $T_{\rm c} = 1.13(5)$
- $\nu = 1.8(2)$
- $\theta\nu = 0.44(5) \longrightarrow \theta \sim 0.24$

Other applications

3D simple ferromagnetic Heisenberg model



3D $\pm J$ Heisenberg SG model



No finite-temperature SG trasition

CONCLUSIONS

- In three dimensions, spin-glass phase transition occurs at finite temperature with strong ordering.
  - finite order parameter in the low-temp. phase.
  - no KT like phase.