Stochastic Cutoff Method for Long-Range Interacting Systems

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1. Introduction

Monte Carlo (MC) simulations for long-range interacting systems are hard because it requires $\mathcal{O}(N^2)$ computations per 1 MC step.

We have developed an efficient Monte-Carlo method for long-range interacting systems called Stochastic CutOff (SCO) method.

M. Sasaki and F. Matsubara: J. Phys. Soc. Jpn. **77**(2008) 024404.

Features of the SCO method

1) Computational time per 1 MC step is reduced greatly.
2) The detailed balance condition is satisfied strictly.
3) Applicable to general long-range interacting systems.

Basic idea

Eliminate most of distant (and weak) interactions
by the Stochastic Potential Switching (SPS) Algorithm.

Another method based on similar strategy:

K. Fukui and S. Todo: J. Comp. Phys. **228** , 2629 (2009).

2 Stochastic CutOff (SCO) method

Hamiltonian $\mathcal{H} = \sum_{i<j} V_{ij}\{S\}$

Flowchart of the SPS Algorithm[1]

[1] C. H. Mak, J. Chem. Phys., **122**, 214110 (2005).

1) Switch the potential

$$V_{ij}\{S\} \rightarrow \begin{cases} \tilde{V}_{ij}\{S\} & p = P_{ij}\{S\} \\ \bar{V}_{ij}\{S\} & p = 1 - P_{ij}\{S\} \end{cases}$$

2) Perform a standard MC with the switched Hamiltonian

$$\mathcal{H}' = \sum{}' \tilde{V}_{ij}\{S\} + \sum{}'' \bar{V}_{ij}\{S\},$$

3) Return to 1).

$$P_{ij}\{S\} = \exp\left[\beta(\Delta V_{ij}\{S\} - \Delta V_{ij}^{\max})\right], \qquad \Delta V_{ij}\{S\} = V_{ij}\{S\} - \tilde{V}_{ij}\{S\},$$

$$\Delta V_{ij}^{\max} \geq \max_{\{S\}} \Delta V_{ij}\{S\}, \qquad \bar{V}_{ij}\{S\} = V_{ij}\{S\} - \beta^{-1} \log[1 - P_{ij}\{S\}],$$

In the SCO method, we simply set $\tilde{V}_{ij}$ to 0 to reduce computational time in step 2).

How many interactions are survived as $\bar{V}_{ij}$ in step 1)?

When $V_{ij} = \mathcal{O}(r_{ij}^{-\alpha})$ and r_{ij} is large enough,

$$\begin{aligned} p(V_{ij} \to \bar{V}_{ij}) &= 1 - \exp[\beta(V_{ij}\{S\} - V_{ij}^{\max})] \\ &\approx \beta(V_{ij}\{S\} - V_{ij}^{\max}) = \mathcal{O}(\beta r_{ij}^{-\alpha}) << 1 \end{aligned}$$

# of potentials switched to $\bar{V}$

$$\sim \int_1^L \mathrm{d}r N r^{d-1} \beta r^{-\alpha} \sim \begin{cases} \beta N, & (d < \alpha) \\ \beta N \log(N), & (d = \alpha) \\ \beta N^{(2d-\alpha)/d}, & (d > \alpha) \end{cases}$$

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$$\sim \int_1^L \mathrm{d}r \underbrace{N r^{d-1}}_{\text{\# of pairs}} \underbrace{\beta r^{-\alpha}}_{\text{probability}} \sim \begin{cases} \beta N, & (d < \alpha) \\ \beta N \log(N), & (d = \alpha) \\ \beta N^{(2d-\alpha)/d}, & (d > \alpha) \end{cases}$$

Furthermore, we can reduce the computational time in step 1) by using an efficient method[1].

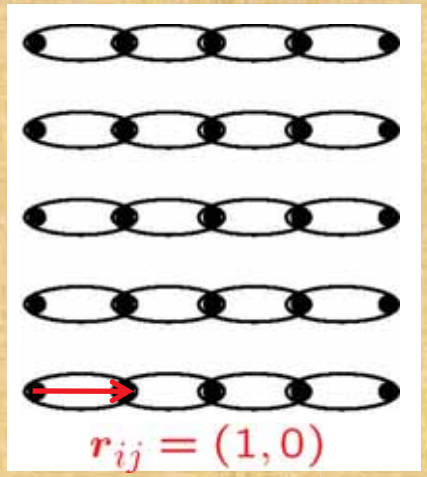
[1] M. Sasaki and F. Matsubara: J. Phys. Soc. Jpn. **77** (2008) 024404.

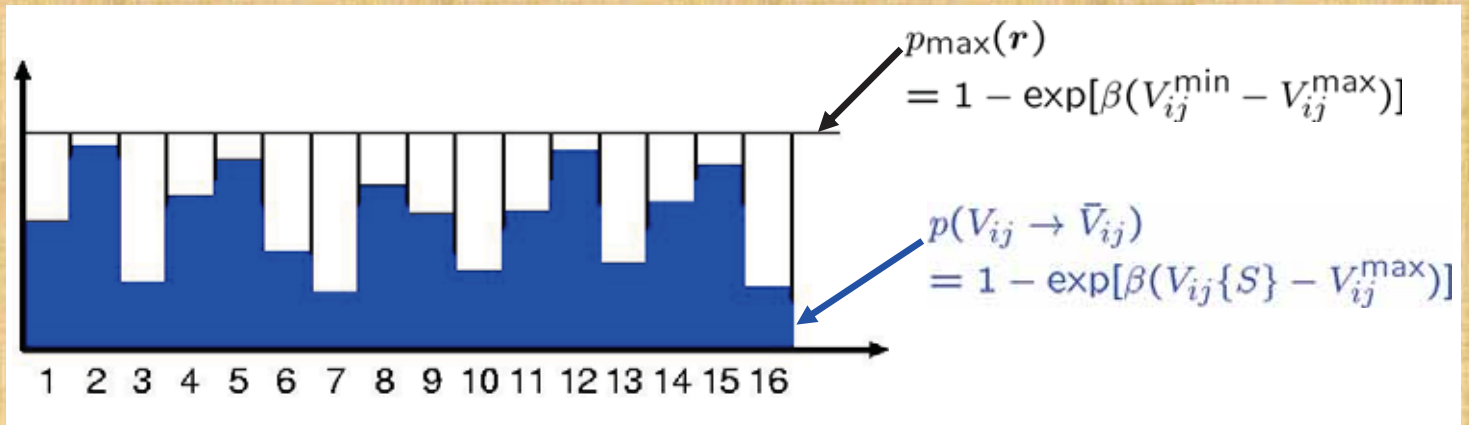
$$t_{\mathrm{MC}} \sim \begin{cases} \beta N, & (d < \alpha) \\ \beta N \log(N), & (d = \alpha) \\ \beta N^{(2d-\alpha)/d}, & (d > \alpha) \end{cases}$$

3. Potential Switching in Lattice Systems

We consider to switch a set of potentials for which $r_{ij} = r$.

Point: There exists a maximum value of $p(V_{ij} \to \bar{V}_{ij})$





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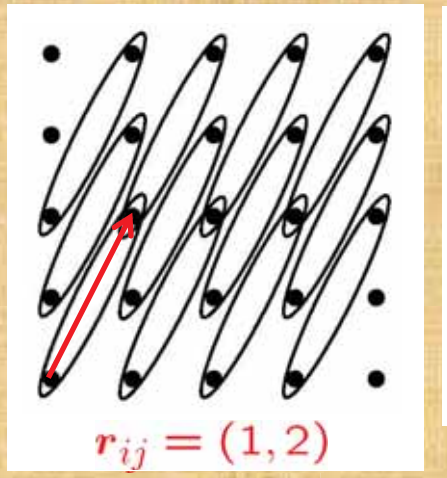

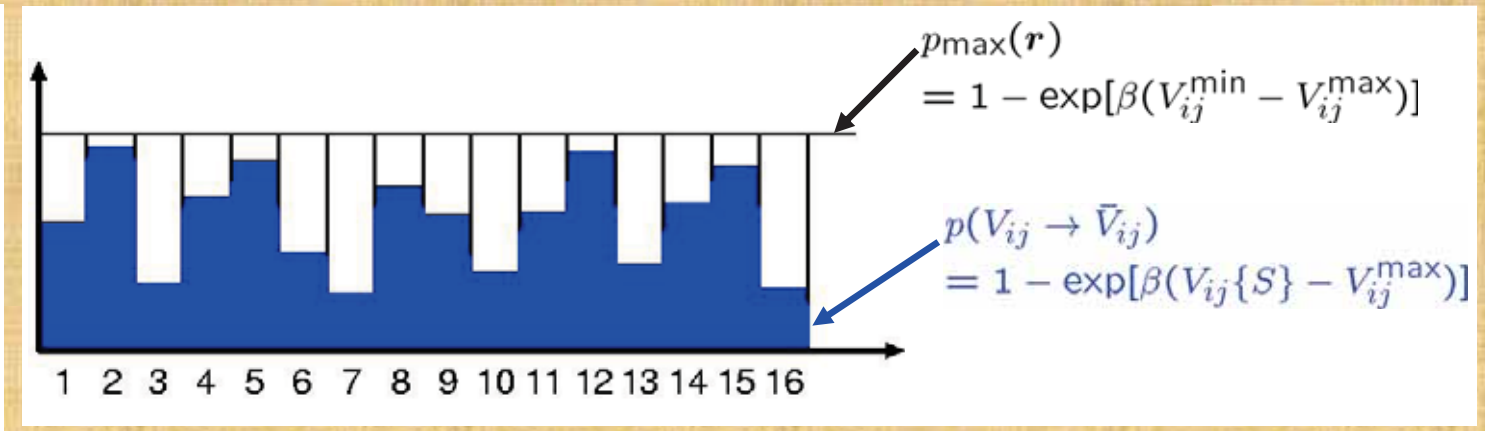

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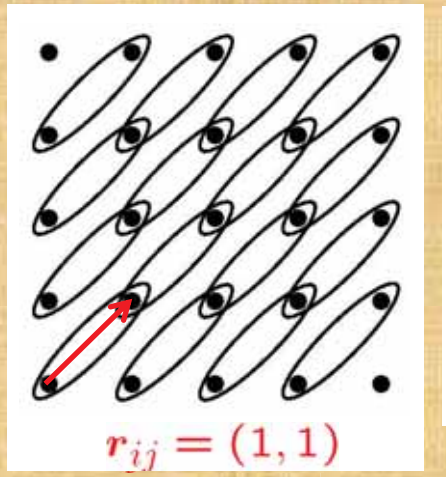

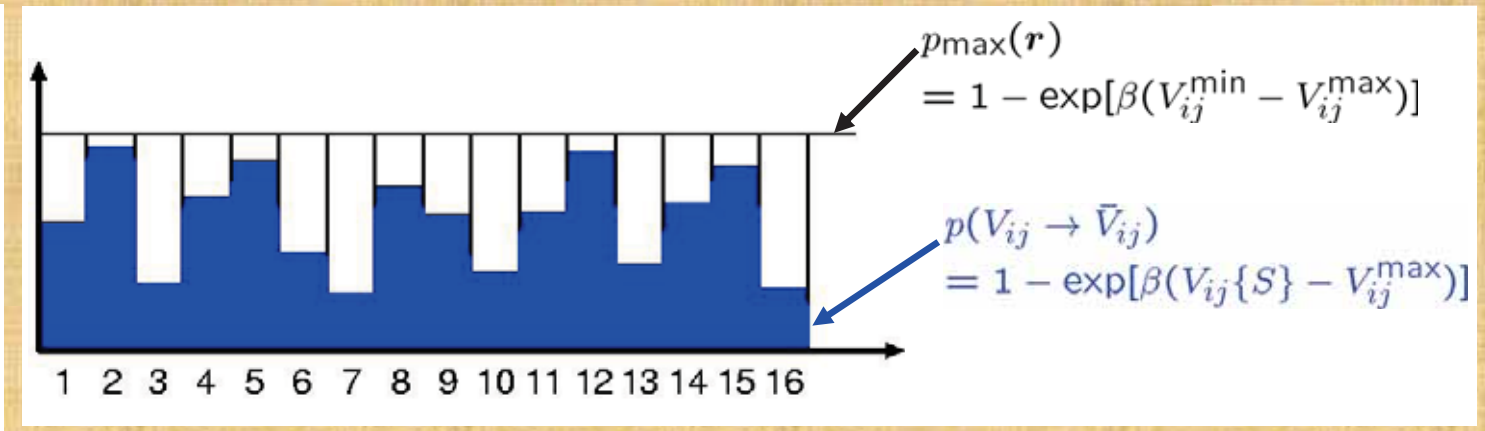

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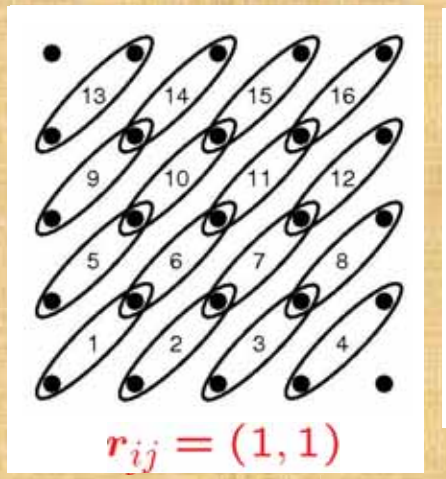

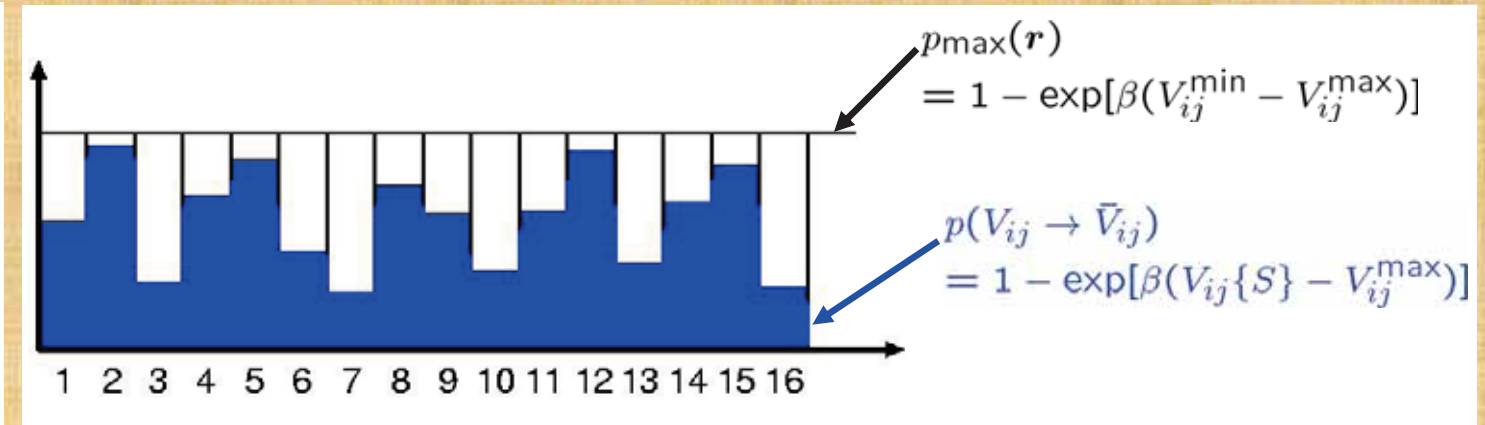

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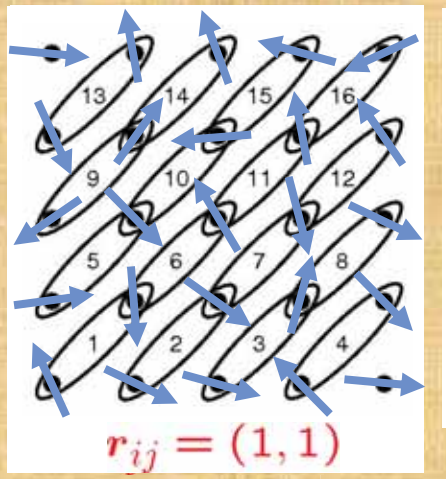

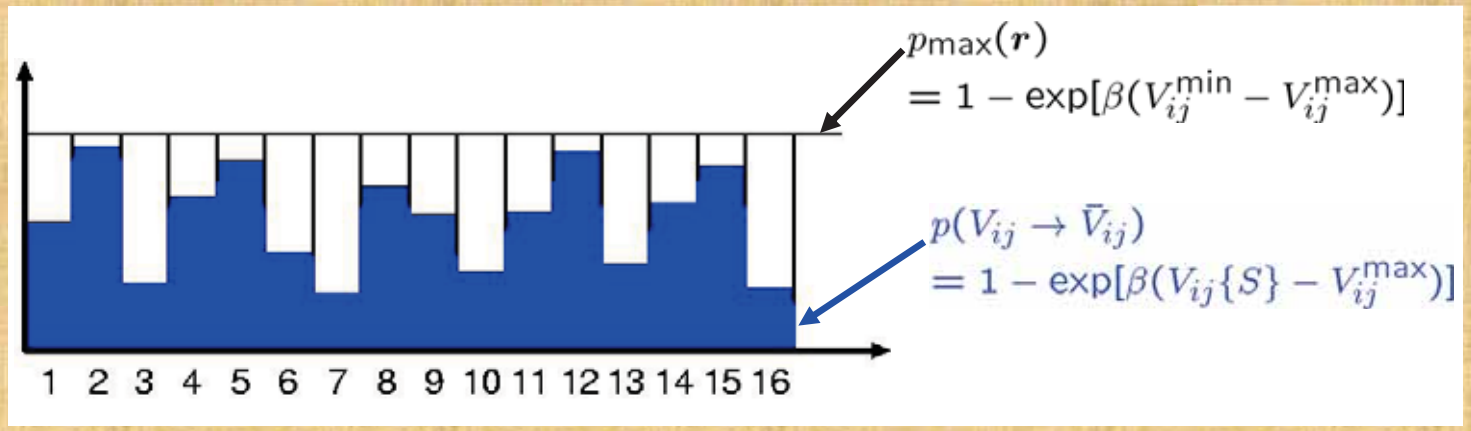

The way to switch potentials

A) Choose candidates switched to $\bar{V}_{ij}$ with probability $p_{\max}(\boldsymbol{r})$. The pairs not chosen as a candidate are switched to $0 (= \tilde{V}_{ij})$.

B) Switch each of the candidates to $\bar{V}_{ij}$ with probability $p(V_{ij} \to \bar{V}_{ij})/p_{\max}(\boldsymbol{r})$. Otherwise, switch to 0.

The way to choose candidates

The probability g(n) that trials to choose a candidate successively end in failure n-1 times before the first success is given by $g(n) = (1 - p_{\max})^{n-1} p_{\max}$.

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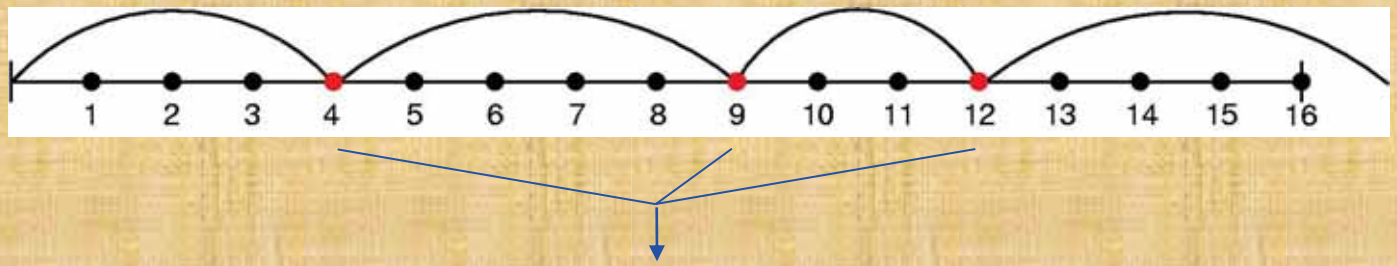

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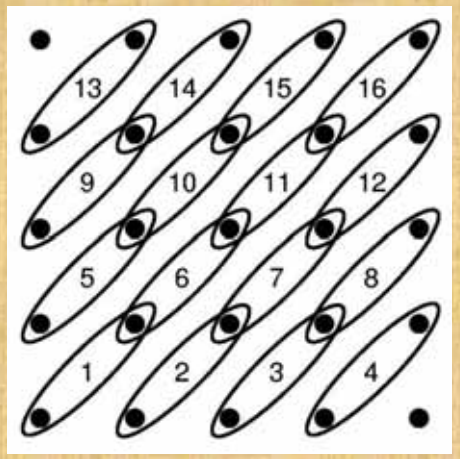

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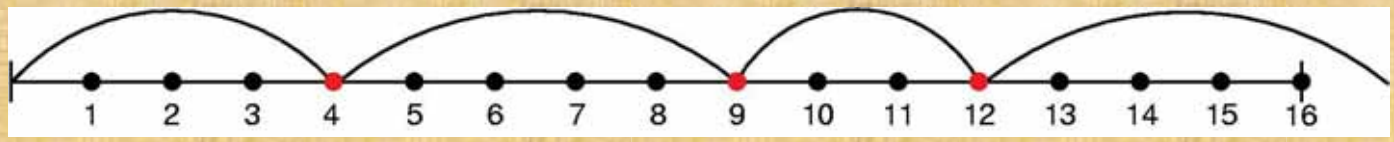

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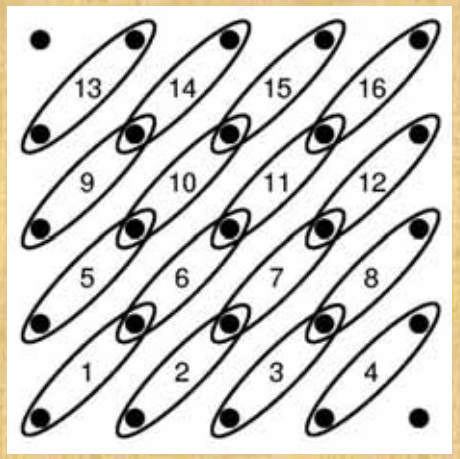


computational time ~ # of candidates ≪ # of potentials

4.Application to a magnetic dipolar system on a square lattice

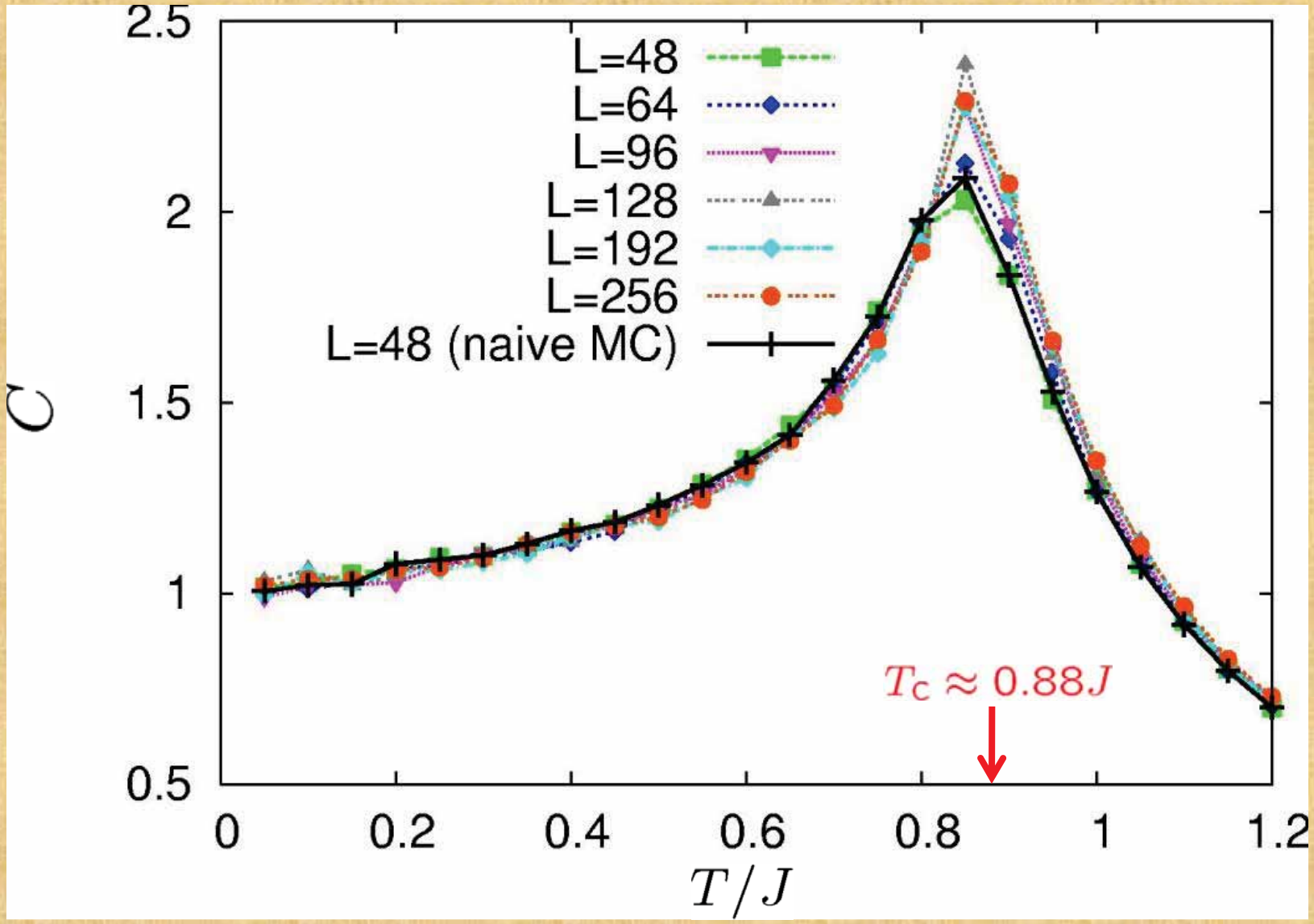
$$\mathcal{H} = \underbrace{-J \sum_{n.n.} \boldsymbol{S}_i \cdot \boldsymbol{S}_j}_{\text{exchange (ferro)}} + \underbrace{D \sum_{i<j} \left(\frac{\boldsymbol{S}_i \cdot \boldsymbol{S}_j}{r_{ij}^3} - 3 \frac{(\boldsymbol{S}_i \cdot \boldsymbol{r}_{ij})(\boldsymbol{S}_j \cdot \boldsymbol{r}_{ij})}{r_{ij}^5} \right)}_{\text{magnetic dipolar interaction}}, \quad \left(J > 0, \frac{D}{J} = 0.1 \right)$$

- classical Heisenberg spins
- open boundary
- simulated annealing
  (100,000 MCS at each temperature)

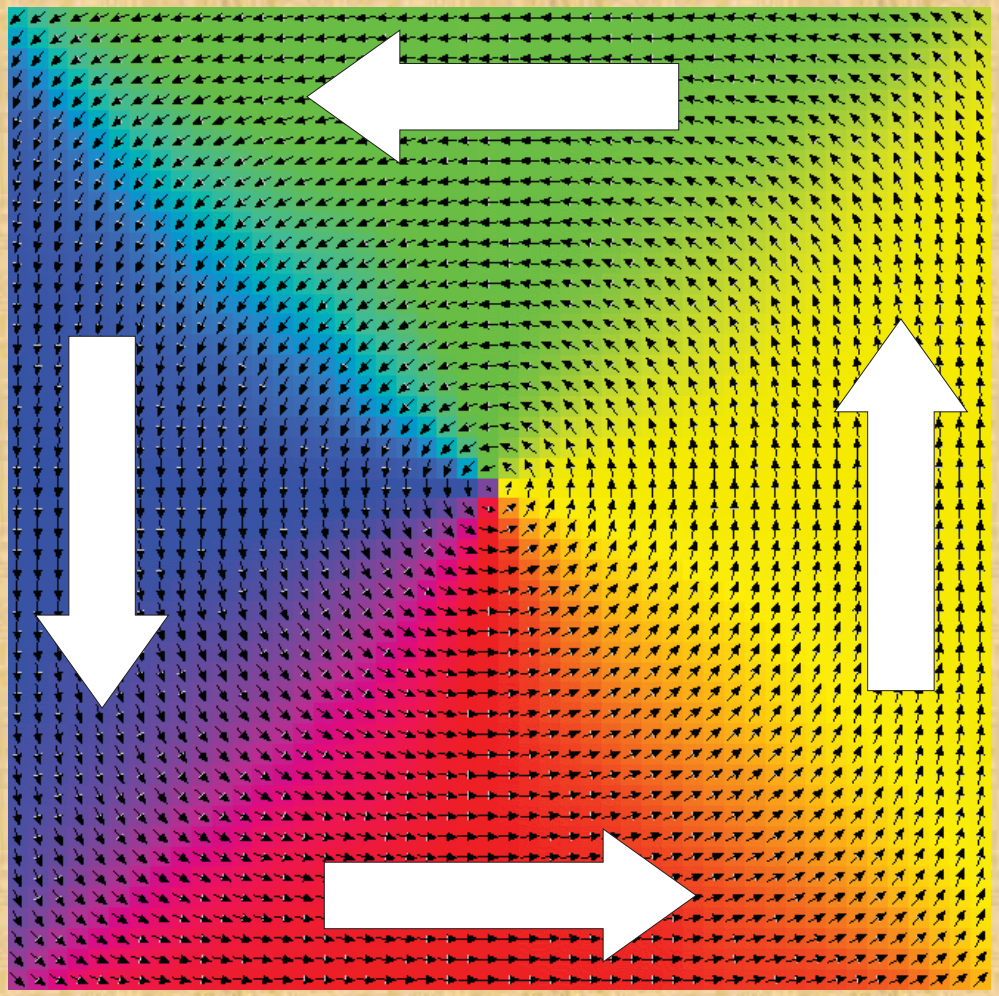
This model undergoes a phase transition to a circularly ordered state at $T_C \approx 0.88J$.

J. Sasaki and F. Matsubara: J. Phys. Soc. Jpn. **66** (1996) 2138.

1) Specific heat



2) Configuration at T=0.05J.



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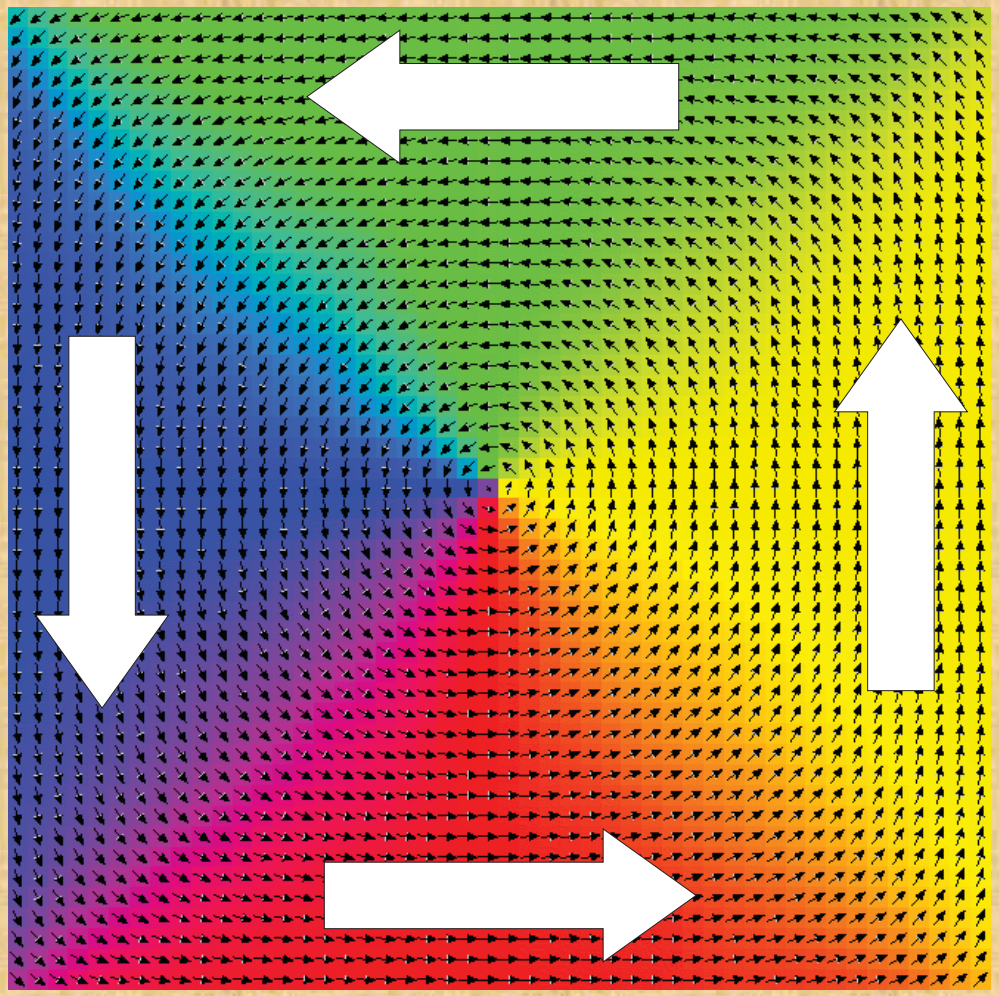
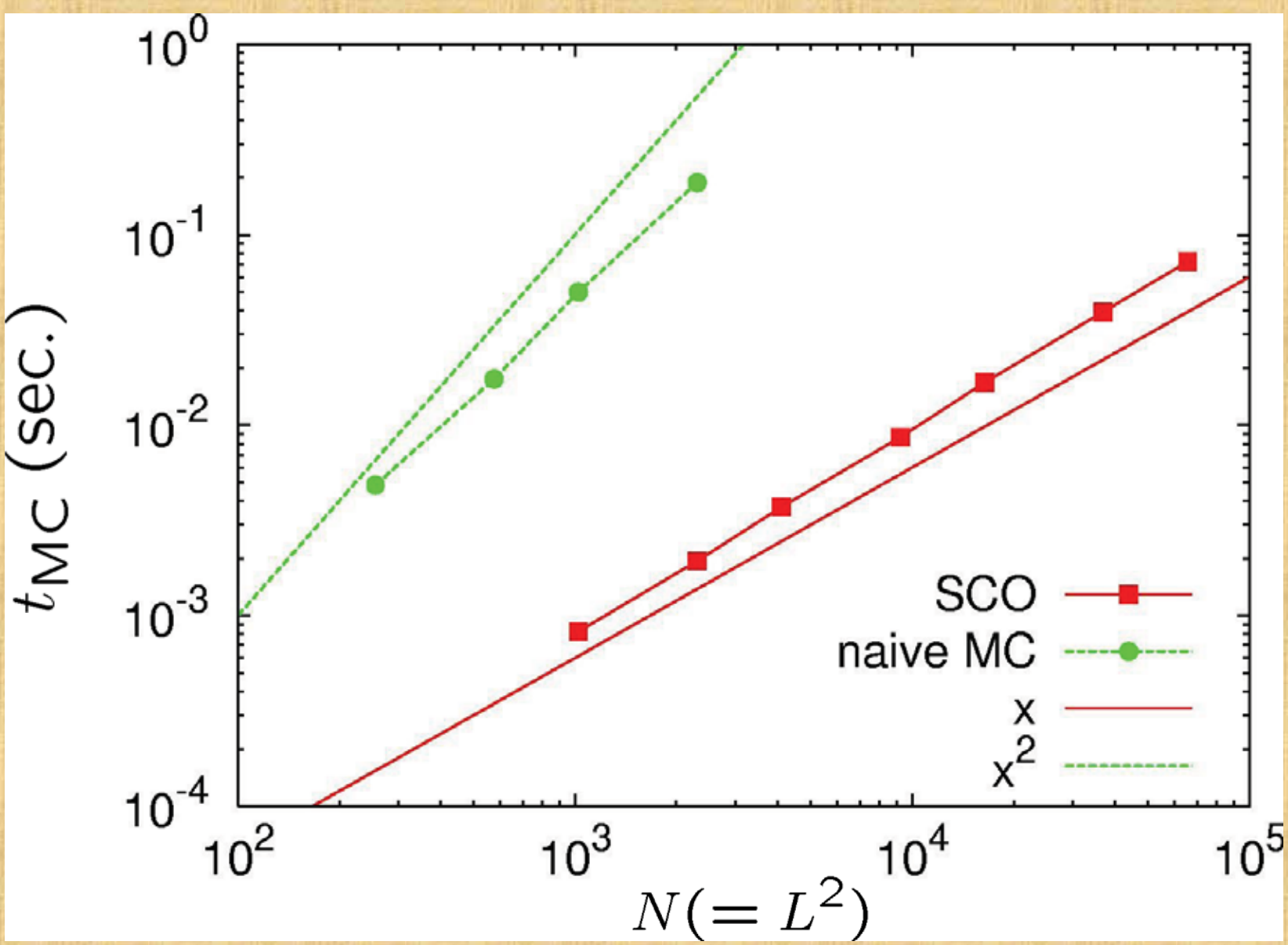
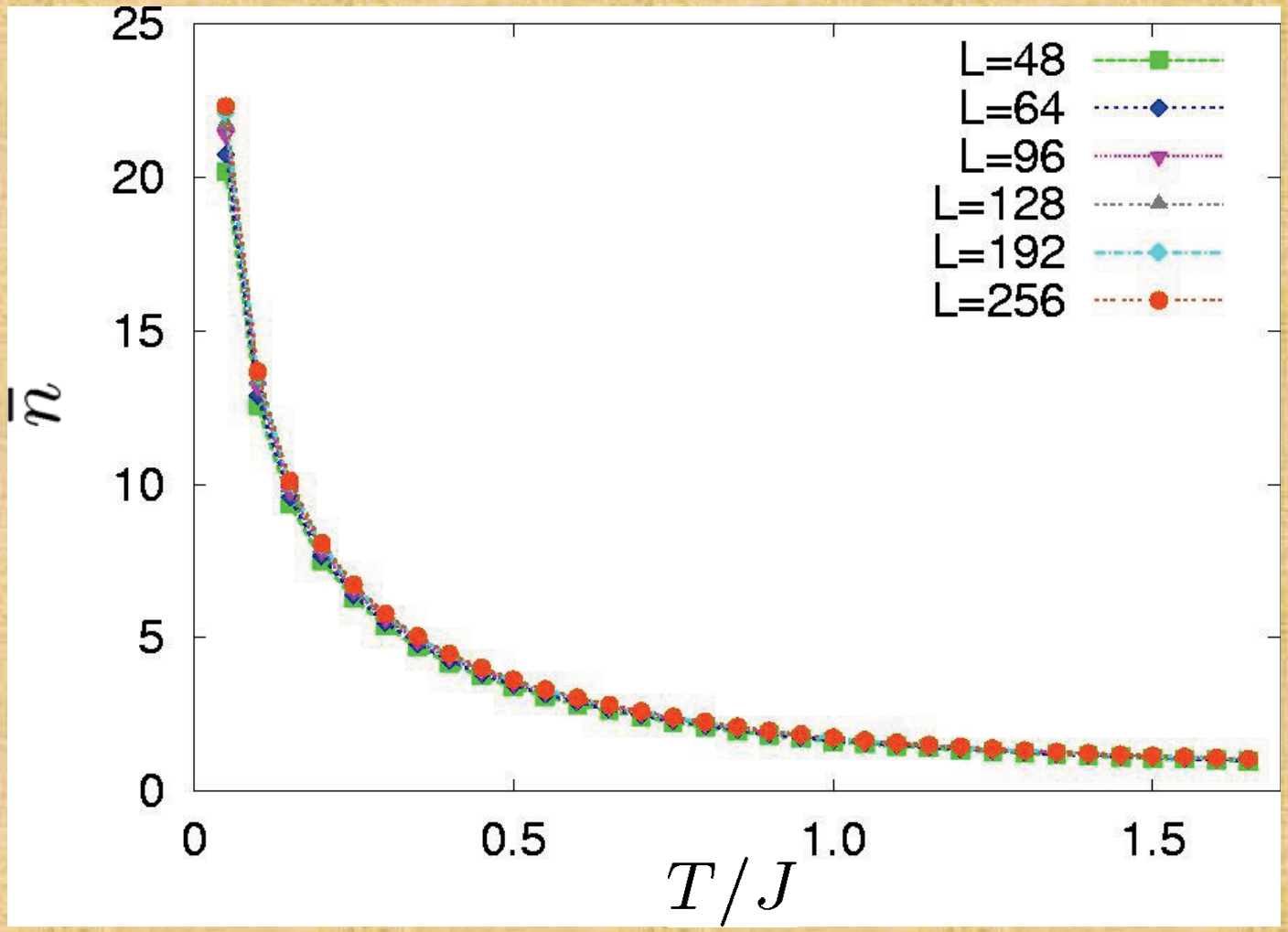


The SCO method gives correct results.

3) Computational time per 1 MCS



4) Number of potentials survived as $\bar{V}$ (per spin)



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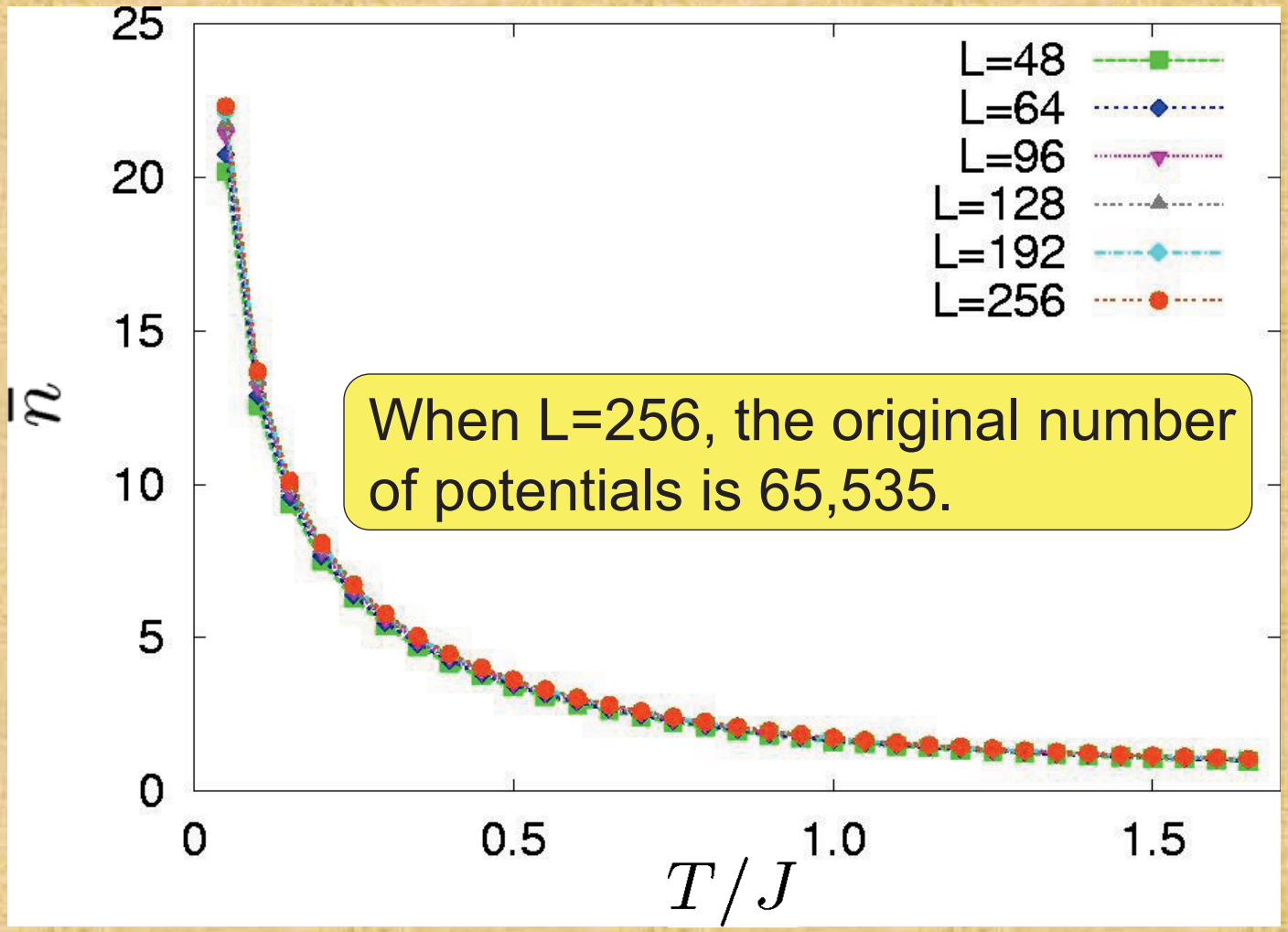

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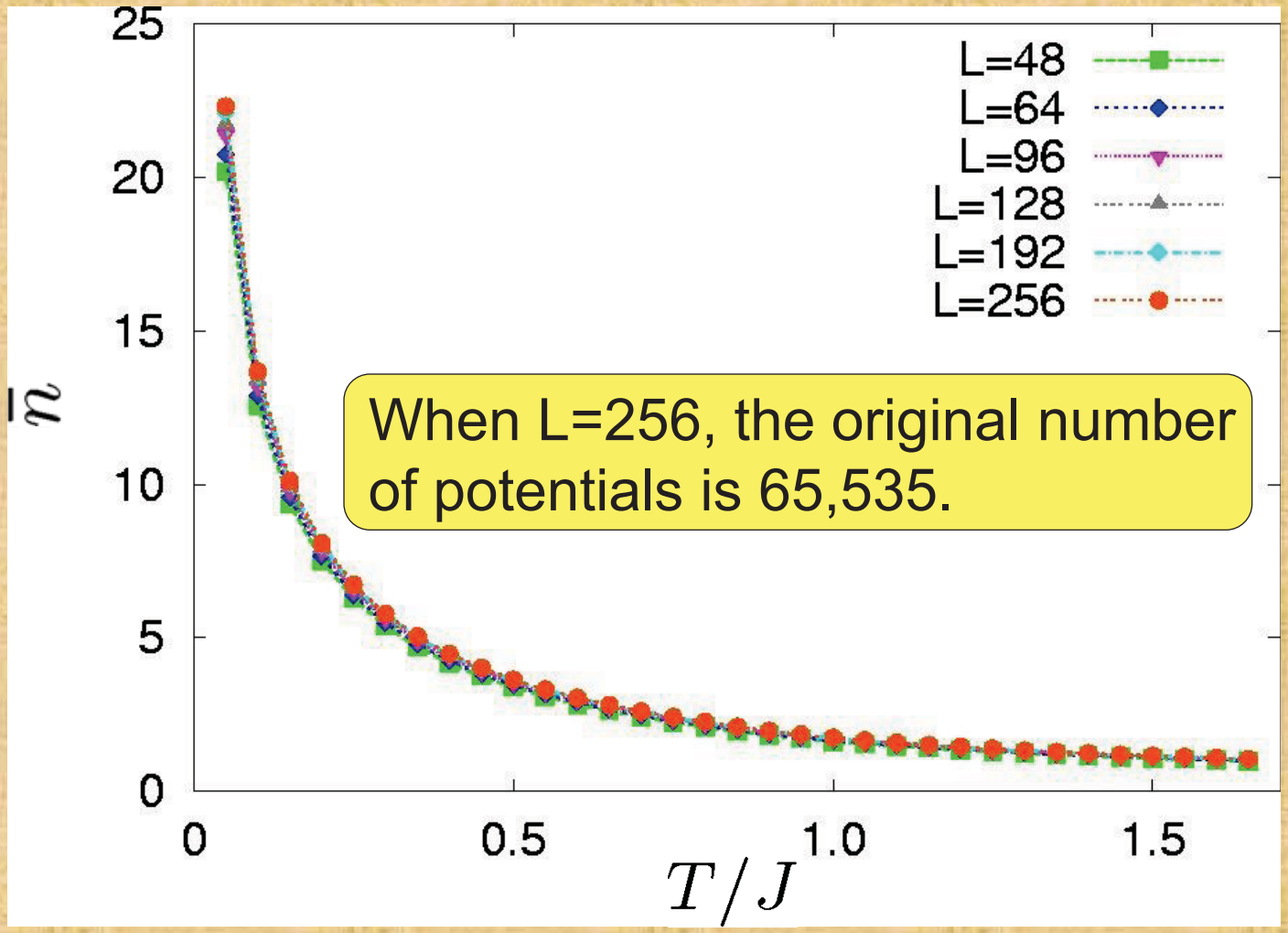

Computational time is reduced greatly.

5. Improvements in the SCO method

5.1 Internal energy and heat capacity measurements

Problem

If we measure the internal energy and heat capacity naively, it costs $\mathcal{O}(N^2)$ computational time.

Solution

Derive new formulae for the measurements which can be estimated with much shorter computational time[1].

[1] M. Sasaki: arXiv:1001.1023.

Formulae

$$E = \langle \mathcal{H} \rangle = E_{\text{const}} + \left\langle A\{\boldsymbol{S}\} \right\rangle_{\text{MC}} \qquad \text{①}$$

$$C = \beta^2 \left\{ \left\langle \left[A\{\boldsymbol{S}\} \right]^2 \right\rangle_{\text{MC}} - \left\langle A\{\boldsymbol{S}\} \right\rangle_{\text{MC}}^2 - \left\langle B\{\boldsymbol{S}\} \right\rangle_{\text{MC}} \right\} \qquad \text{②}$$

$$E_{\text{const}} \equiv \sum_{i<j} V_{ij}^{\max}, \quad A\{\boldsymbol{S}\} \equiv \sum{}' \left(\frac{V_{ij}\{\boldsymbol{S}\} - V_{ij}^{\max}}{1 - P_{ij}(\{\boldsymbol{S}\})} \right), \quad B\{\boldsymbol{S}\} \equiv \sum{}' \left(\frac{V_{ij}\{\boldsymbol{S}\} - V_{ij}^{\max}}{1 - P_{ij}(\{\boldsymbol{S}\})} \right)^2 P_{ij}\{\boldsymbol{S}\}$$

The sum only runs over the pairs which are not cut off.

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Procedure for the measurements

1) Calculate E_{const} at the beginning of simulation.
2) Measure $A\{\boldsymbol{S}\}, \left[A\{\boldsymbol{S}\}\right]^2, B\{\boldsymbol{S}\}$ at each MC step.
3) Estimate $\left\langle A\{\boldsymbol{S}\} \right\rangle_{\text{MC}}, \left\langle \left[A\{\boldsymbol{S}\}\right]^2 \right\rangle_{\text{MC}}, \left\langle B\{\boldsymbol{S}\} \right\rangle_{\text{MC}}$.
4) Substitute the results into eqs. ① and ②.

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$A\{\boldsymbol{S}\}$ and $B\{\boldsymbol{S}\}$ consist of the terms which are not cut off.
⟹ We can reduce the computational time.

5.2 Combination with the replica exchange method[1]

[1] K. Hukushima and K. Nemoto: J. Phys. Soc. Jpn. **65**, 1604 (1996).

Problem

It costs $\mathcal{O}(N^2)$ computational time to calculate the replica exchange probability.

Solution

Derive a new formula for the replica exchange probability which can be estimated with much shorter computational time[2].

[2] M. Sasaki: arXiv:1001.1023.

Replica exchange probability

$$= W(\cdots;\{\boldsymbol{S}\}_{\mathrm{A}},T_{\mathrm{A}};\{\boldsymbol{S}\}_{\mathrm{B}},T_{\mathrm{B}};\cdots\rightarrow\cdots;\{\boldsymbol{S}\}_{\mathrm{B}},T_{\mathrm{A}};\{\boldsymbol{S}\}_{\mathrm{A}},T_{\mathrm{B}};\cdots)$$

$$= \min[1,X]$$

Original formula

$$X = \prod_{i<j}\exp[(\beta_{\mathrm{B}}-\beta_{\mathrm{A}})(V_{ij}\{\boldsymbol{S}_{\mathrm{B}}\}-V_{ij}\{\boldsymbol{S}_{\mathrm{A}}\})]$$

The product runs over all the pairs.

⇒ It costs $\mathcal{O}(N^2)$ computational time to calculate it.

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New formula

$$X = \prod_{\mathrm{A}}'\exp[-(\beta_{\mathrm{B}}-\beta_{\mathrm{A}})(V_{ij}\{\boldsymbol{S}_{\mathrm{A}}\}-V_{ij}^{\max})]\frac{1-P_{ij}(\{\boldsymbol{S}_{\mathrm{A}}\},T_{\mathrm{B}})}{1-P_{ij}(\{\boldsymbol{S}_{\mathrm{A}}\},T_{\mathrm{A}})}$$

$$\times\prod_{\mathrm{B}}'\exp[-(\beta_{\mathrm{A}}-\beta_{\mathrm{B}})(V_{ij}\{\boldsymbol{S}_{\mathrm{B}}\}-\Delta V_{ij}^{\max})]\frac{1-P_{ij}(\{\boldsymbol{S}_{\mathrm{B}}\},T_{\mathrm{A}})}{1-P_{ij}(\{\boldsymbol{S}_{\mathrm{B}}\},T_{\mathrm{B}})}$$

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5.3 Combination with the Wang-Landau method[1]

[1] F. Wang and D. P. Landau: Phys. Rev. Lett. **86**, 2050 (2001), Phys. Rev. E **64**, 056101 (2001).

Problem

In usual Wang-Landau (WL) method, we estimate density of state associated with the energy. In order to do that, we have to calculate the energy whenever the configuration changes.

Solution

Perform a WL method without estimating density of state associated with the energy.

⇒ An efficient method to calculate free-energy

Purpose: Estimate free-energy

$$\exp[-\beta f(M)] \equiv \mathrm{Tr}_{\{\boldsymbol{S}_i\}} \exp[-\beta \mathcal{H}\{\boldsymbol{S}_i\}] \delta\left(M - \sum_i \boldsymbol{S}_i^z\right),$$

① WL method without estimating density of state

Perform a MC simulation whose Hamiltonian is

$$\mathcal{H}_{\mathrm{WL}}\{\boldsymbol{S}_i\} = \mathcal{H}\{\boldsymbol{S}_i\} - G\left(\sum_i \boldsymbol{S}_i^z\right).$$

Adjust $G(M)$ so that

$$P_{\mathrm{MC}}(M) \propto \mathrm{Tr}_{\sum_i \boldsymbol{S}_i^z = M} \exp[-\beta \mathcal{H}_{\mathrm{WL}}\{\boldsymbol{S}_i\}] = \text{const.}$$

$$G(M) = F(M) + \text{const.}$$

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$$G(M) = F(M) + \text{const.}$$

② Combination of the WL method with the SCO method

Just use the Hamiltonian

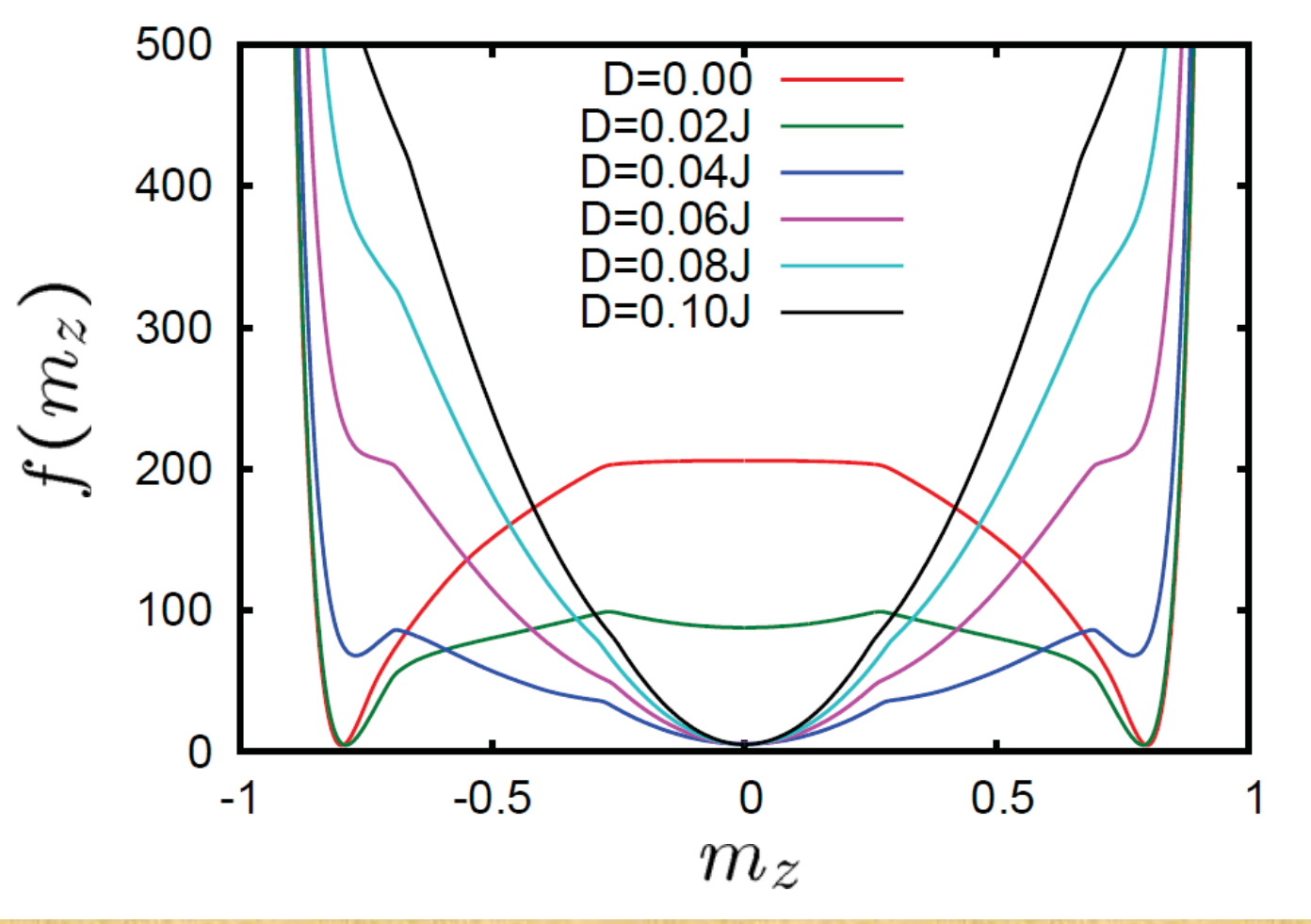
$$\mathcal{H}'_{\mathrm{WL}}\{\boldsymbol{S}_i\} = \mathcal{H}'\{\boldsymbol{S}_i\} - G\left(\sum_i \boldsymbol{S}_i^z\right)$$ ($\mathcal{H}'$: switched Hamiltonian)

We can reduce the computational time.

An example: Free-energy as a function of magnetization

$$\mathcal{H} = -J \sum_{n.n.} \boldsymbol{S}_i \cdot \boldsymbol{S}_j + K \sum_i (S_i^z)^2 + D \sum_{i<j} \left(\frac{\boldsymbol{S}_i \cdot \boldsymbol{S}_j}{r_{ij}^3} - 3 \frac{(\boldsymbol{S}_i \cdot \boldsymbol{r}_{ij})(\boldsymbol{S}_j \cdot \boldsymbol{r}_{ij})}{r_{ij}^5} \right),$$

$$(J > 0, \; K = 0.1J, \; k_B T = 0.7J)$$



- N=20^3
- open BC

6. Summary

1) We have developed an efficient Monte Carlo method for long-range interacting systems. This method involves no approximation.

2) We have applied the method to dipolar systems. The results show the efficiency of the method.

3) We have made an improvement for efficient internal energy and heat capacity measurements.

4) We have also made improvements to combine the SCO method with other MC methods.