Application of two-dimensional simulated tempering (ST) to the two-dimensional Ising model

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Introduction

We performed two-dimensional simulated tempering (ST) simulations of the two-dimensional Ising model in different sizes in order to investigate the phase transitions and to study the cross over behavior. In this two-dimensional ST, not only the temperature but also the external field become dynamical variables updated by the Metropolis criteria. Thus, this method can be referred to as "Simulated Tempering and Magnetizing (STM)." We also performed the "Simulated Magnetizing (SM)" simulations, in which the external field was considered as a dynamic variable but temperature was not. It is shown that STM can go over first-order phase transition lines by making a two-dimensional random walk in temperature and external field. We also studied the crossover behavior of phase transitions with respect to temperature and external field.

Methods

We employed the two-dimensional ST method [1], in which the temperature and external field are also considered as dynamical variables updated by Metroplis criteria. Thus the Boltzmann factor $e^{-(E-hM)/T+a(T,h)}$, considered as a probability distribution in the product space of sampling space, temperature and external field. In this simulation, temperature and external field are changed little by little. Note that a(T,h) is a parameter for obtaining the same number of samples at each condition. A good choice for a(T,h) is the free energy. We calculate it by rewighting techniques such as WHAM and MBAR. By repeating preliminary simulation and reweighting techniques, we obtained the free energy. Then we performed production run.

WHAM

$$n(E,M) = \frac{\sum_{T_i,h_j} n_{T_i,h_j}(E,M)}{\sum_{T_i,h_j} n_{T_i,h_j} exp(f(T_i,h_j) - (E-h_jM)/T_i)}$$

$$f(T_i,h_j) = -\log \sum_{E,M} n(E,M) exp(-(E-h_j)/T_i).$$

MBAR

$$f(T_i,h_j) = -\log \sum_{i=1}^{N_T}\sum_{j=1}^{N_h}\sum_{n=1}^{N} \frac{exp(-(E_n-h_jM_n)/T_i)}{\sum_{k=1}^{N_T}\sum_{l=1}^{N_h} N_{kl} exp(f(T_k,h_l) - 1/T_k(E_n-h_lM_n))}$$

Results

Figs. 1 and 2 show the temperature and external field as a function of MC sweeps, respectively. Both of them realized random walks. Figs. 3 and 4 show the energy and magnetization as a function of MC sweeps. They show also the random walk. Note that the expected correlation exists bwteen temperature and energy , and external field and mangetization. (go to the right column)

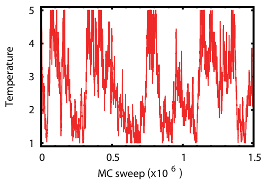


Fig.1 History of temperature .

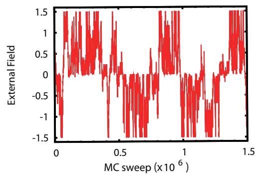


Fig. 2 History of external field.

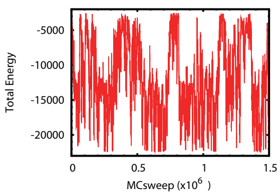


Fig. 3 History of total energy.

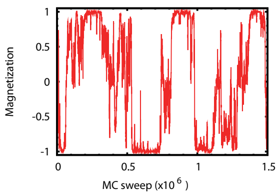


Fig. 4 History of magnetization.

To eveluate the effect of the dimensional generalization, we performed SM. Fig. 5 ilustrates the history of external field below Tc. In the small size system, the random walk happened as is in Fig. 5. However, in the larger size system, it did not happened.（Fig. 6(a)), while above Tc, random walk in external field happend（Fig. 6(b)). Thus the STM overcame the fisrt-order phase transition by going through the high temperature region (go back to the leftcolumn).

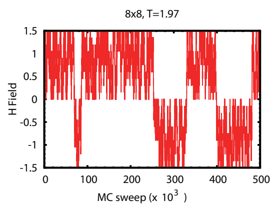
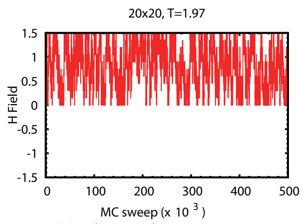
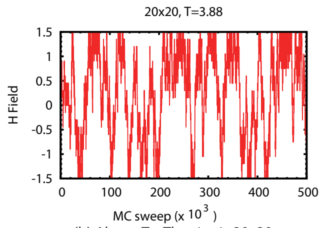


Fig. 5 History of external field below Tc of 8x8 simulation.



(a) Below Tc. The size is 20x20.



(b) Above Tc. The size is 20x20.

Fig. 6 History of external field.

We investigated the critical behavior. We employed the finte-size scaling approach. The scaling form of magnetization with respect to temperature T and external field h are given by

$$ML^{\beta/\nu} = \Psi(L^{1/\nu}t, L^{d+2-\eta}h)$$

$$t = |T-T_c|/T_c,$$

where L is linear lattice size. Note that in 2D ising model, d=2, β=1/8, ν =1, and η=1/4. Figure 7 shows the magnetization when external field is zero. The behivor follows M $\sim t^{\beta}$ when Lt is large enough. Figure 8 shows the magnetization when T=Tc. The behavior of M follows M $\sim |h|^{1/\delta}$ (δ=15) when $hL^{15/8}$ is large enough. Figrue 9 shows 3d plot of mangetizaiotn with respect to temperature and externl field. This suggests that M follows the larger one of $t^{1/8}$ or $|h|^{1/15}$. Figure 10 shows the difference bewteen magnetizaion and expected critical behavior. The black line shows $t^{1/8} = h^{1/15}$. From scaling theory, when $t^{1/8} h^{-1/15}$ is large enough the magnetization follows M $\sim t^{1/8}$, while when $t^{-1/8}h^{1/15}$ is large enough then M $\sim h^{1/15}$. Figure 10 illustrates that the line ($t^{1/8}h^{-1/15} = t^{-1/8} h^{1/15}$=1) is the boarder of critical phenomena. This is the behavor of corssover with respect to the temperature and external field.

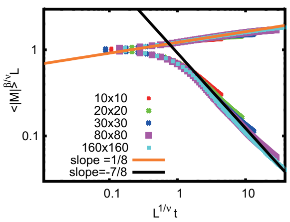


Fig. 7 Scaled M vs temperature.

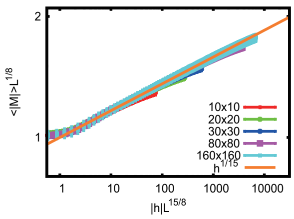


Fig. 8 Scaled M vs external field.

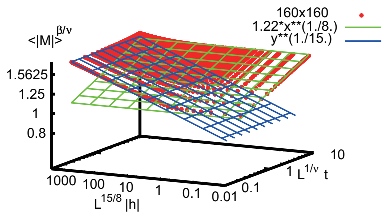


Fig. 9 Scaled M as afunction of h and t

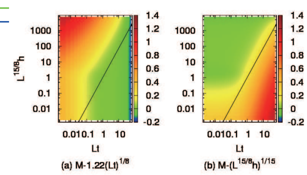


Fig. 10 Differemce between Scaled M and expected critical behivors

Conclusions

We peformed the two-dimensional ST simulations of two-dimensional Ising model. By realizing the random walk in the temperature and external feild, we overcame the first-order pahse transition difficulty, and obtained the information in large are of phase diagram by a single production run. We aslo studied the cross over behavior. The behavior was clearly depicted.

[1] A. Mitsutake and Y. Okamoto: Physical Review E 79 (2009) 047701; Journal of Chemical Physics 130 (2009) 214105. [2] D. P. Landau: Phys. Rev. B 13 (1976) 2997.