Randomness-induced evolution of the first-order to the second-order phase transition in two-dimensional six-state potts model[☆]

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Abstract

Employing Monte Carlo simulation method, we have studied randomness-induced evolution of the first-order to the second-order phase transition in two-dimensional six-state Potts model system. Biological applications of the Potts model are developed very much recently. We change the transition from first-order to second-order through tuning the bonds strength or the concentration of void bonds. The evolution of phase transition in two-dimensional six-state Potts system is examined with energy histogram and the Binder cumulant analysis. [Life Science Journal. 2009; 6(2): 29 – 32] (ISSN: 1097 – 8135).

Keywords: Monte Carlo; randomness; Potts model; phase transition

1 Introduction

It has attracted much interest that randomness influences cellular phase transition behavior both in theoretical and experimental studies. The disorder produced by porous media reveals experimental evidence of randomness affecting phase transition of a system. For a system exhibiting continuous phase transition in pure case, the quenched bond randomness or field randomness can change the value of critical exponent and may even eliminate the phase transition[1–3]. The phenomenological renormalization-group arguments[4–5] suggest that addition of bond randomness can smoothen the first order phase transition and induce a continuous phase transition. This conjecture arises recent research interest to explore randomness effect upon the nature of phase transition with second-order system, which originally carried on the first-order phase transition in the pure case[4–8]. As for experimental work, extensive studies of the isotropic to nematic phase transition of nCB liquid crystals in aerogel shows that the transition temperature is lowered compared with the pure situation[9–12].

It is well known that the Potts model possesses fruitfully critical behavior. The q-state Potts model on two-dimensional cellular lattices exhibits temperature-driven phase transition both in first-order and second-order[14]. The phase transition is first-order for $q > 4$ and is continuous for $q \leq 4$. So it could be a good candidate for testing the emergence of randomness-induced evolution of the first-order to second-order phase transition. Chen S *et al*[6–7] and Janke W[15] have performed Monte Carlo simulation study for the random bond Potts model in two-dimensional system with strong first-order region ($q = 8$). Yet some debated contradiction appears between the works of Chen S *et al* and Janke W demonstrates that quenched random-bond induces the second-order phase transition in two-dimensional eight-state Potts model. On the contrary, Janke W *et al* ascertain that the phase transition remains the first-order on random lattices in the same model. Paredesv R *et al*[13] study the five-state-Potts model with weak first-order region, and Yang CS *et al*[8] study the three-state Potts anti-ferromagnetic model

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on triangular lattice. Both models appear variation of the nature in phase transition induced by randomness.

In order to illustrate the randomness-induced change of the nature in phase transition, we investigate the six-state Potts model with various random by means of Monte Carlo simulation. Because the system has first-order phase transition in pure case, we may alter the nature of phase transition to the second-order through diluting the system, randomly introducing certain concentration of blank bonds or weakening strength of partial bonds. Applying field on the system, random effect also induce the change of nature in phase transition. We examine the evolution of phase transition in two-dimensional six-state Potts system with energy histogram and the Binder cumulant analysis in this study.

2 Model

The Hamiltonian of a six-state Potts model with quenched random interaction can be written as follows:

$H = \sum_{<i,j>} K_{ij}\delta\sigma_i\sigma_j$

Where δ is a Kronecker delta function; the spin σ_i can take on the values 1, 2, 3 ... 6; < i, j > indicates summation over all nearest-neighbor pairs of sites. The coefficient K_{ij} is the nearest-neighbor (< i, j >) random bond coupling constant, which can be randomly selected according to the following distribution.

$P(K_{ij}) = f\delta(K_{ij} - K_\alpha) + (1 - f)\delta(K_{ij} - K_\beta)$

Where f is a positive real number smaller than or equal to 1. Two differently prescribed random cases are studied. (1) The self-dual system (SD system): we randomly assign half of the total bonds to be the coupling K_1, and the rest bonds are the coupling K_2. The strength ratio is $r = K_a/K_b$. (2) The random dilution system (RD system): partial bonds is void, i.e. $r \rightarrow 0$. In order to investigate the evolution of phase transition, we tune the strength and the concentration of blank bonds systematically. In SD system we set the normal bond coupling (K_b) to be one, and then decrease the strength ratio to make the pure system uneven. In RD system we gradually increase the concentration of blank bonds from zero.

3 Simulation and Analysis

Consider a two-dimensional square lattice with fraction f as quenched bonds and fraction $(1 - f)$ as normal bonds. We perform extensive simulation on 90 × 90 lattices with periodic boundary conditions. The Monte Carlo steps are up to 10^6 typically. The first 20% of the steps are discarded, and we accumulate the remaining data at equilibrium states in our simulation. The temperature of the heat capacity peak corresponds to the transition temperature. We explore transition properties by analyzing energy histogram near the transition temperature. Usually the energy distribution displays a Gaussian type around some central energy due to fluctuation at thermal equilibrium states in a finite size system. As the first-order phase transition occurs, there may co-exist two states at the transition temperature. The energy histogram would display two distinct humps. By analyzing the histogram, one may be able to identify the presence of the first-order phase transition[15–17].

We study the phase transition of pure system first. The behavior of specific heat indicates that the transition temperature is $T = 0.808$. Thus, we explore the energy distribution around this temperature extensively. Figure 1 shows the energy histograms of pure case. The diagram displaying energy histogram near the transition temperature is sensitively dependent on temperature. At $T = 0.807$, the system start to melt, and the energy histogram displays a double-hump structure – a large right hump and a small left one. Then at $T = 0.808$, the energy histogram demonstrates a distinct double-hump structure, which has two humps of almost equal size. Just beyond the transition temperature, at $T = 0.809$, the energy histogram shows an inverse double-hump structure comparing to $T = 0.807$, with large left hump and a small right one. At a slight temperature difference away from the transition, $T = 0.812$, the energy histogram falls back Gaussian structure. Our simulation result reveals that the six-state pure Potts model proceeds a first-order phase transition at $T = 0.808$.

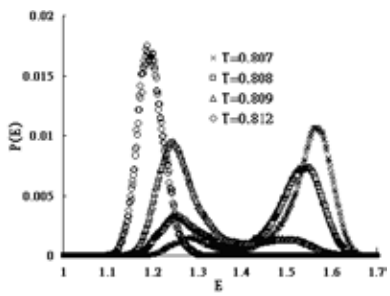

Figure 1. The energy histograms of pure case.

We then conduct the systematic study for the effect of randomness. The RD system is studied with randomly putting blank bonds. Figure 2 displays energy histograms of various blank bond fraction $f = 0.1$, 0.15, and 0.2, respectively. The transition temperature decreases with increasing the blank bond concentration, $T = 0.715$, 0.664, and 0.614, respectively. They display different

types of state distribution at transition temperature. The distribution of $f = 0.1$ still demonstrates a distinct two-hump structure. The histogram of $f = 0.15$ smears out to be a broad single hump. Yet, it is hard to find distinct dip. The distribution of $f = 0.2$ changes into nearly Gaussian type. In this case, the nature of phase transition may evolve into second-order behavior.

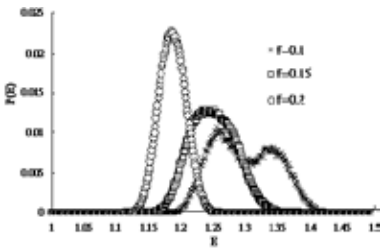

Figure 2. The energy histograms of various empty bond fraction $f = 0.1$, 0.15, and 0.2 in RD system, at transition temperature, $T = 0.715$, 0.664, and 0.614, respectively.

In the SD system with randomly selected half of the total bonds quenched, we vary the coupling strength ratio. Figure 3 displays energy histogram of various strength ration $r = 0.5$, 0.4, and 0.3. The phase transition temperature decreases with decreasing strength ratio, $T = 0.588$, 0.540 and 0.484, respectively. The evolution of the diagram is similar to that in Figure 2. The energy histogram of $r = 0.5$ and 0.4 displays an unsymmetrical broad hump. The distribution of $r = 0.3$ changes into nearly Gaussian type, which shows second-order phase transition behavior due to larger bond strength variation.

As for applying field on the system, we see systematic variation of the energy histogram with increasing the randomness. Simulation reveals that the nature of first-order phase transition will change into the second-order induced by randomness.

Furthermore we inspect the quantity of the Binder's fourth cumulant of energy defined as $V_L = 1 - (E^4)_L/3(E^2)^2$, which is used to distinguish numerically between first-order and continuous transitions. The concept is as the following: The energy distribution $P_L(E)$ for lattice $L \times L$ is described by a single Gaussian. It will reduce to δ-function singularity in thermally dynamical limit, while the system is away from the transition. The fourth-order being reduced cumulant of energy yields the value of $V_L = 2/3$, while $L \to \infty$, at $T \neq T_c$. And the quantity holds at T_c for second-order transition due to Gaussian energy distribution. On the other hand, the energy distribution $P_L(E)$ in finite lattice is considered to be a double Gaussian over a small range around T_c. The corresponding order and disorder states will yield a nontrivial value of V_L. There will be a minimum value of V_L at T_c.

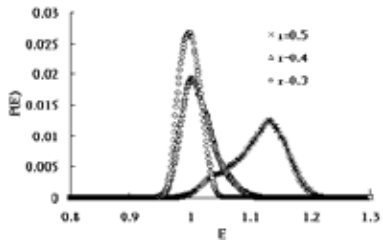

Figure 3. The energy histograms of various strength ratio $r = 0.5$, 0.4, and 0.3 in SD system, at transition temperature, $T = 0.588$, 0.540 and 0.484, respectively.

Figure 4 displays the Binder's cumulant V_L near the transition temperature in RD system. We can find the minimum dip of V_L at T_c in the pure system and in the case of empty bond fraction $f = 0.15$. Comparatively for the case of empty bond fraction $f = 0.2$, we find the V_L is very close to 2/3.

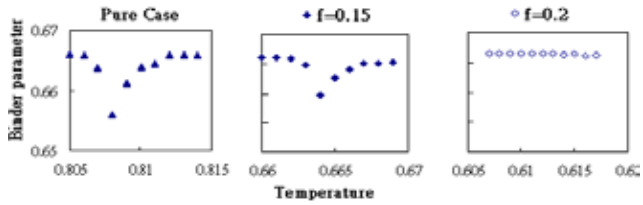

Figure 4. The Binder's cumulant V_L near the transition temperature in RD system.

Figure 5 displays the Binder's cumulant V_L near the transition temperature in SD system. We can also find that in the case of strength ratio $r = 0.3$, V_L is very close to 2/3. Therefore, we can ascertain the phase transition is changed by randomness from first-order to second-order.

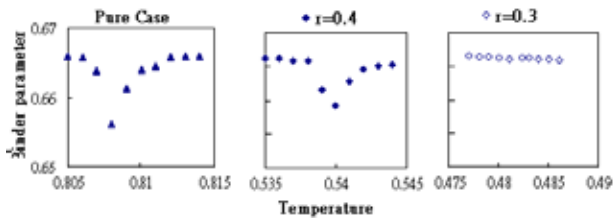

Figure 5. The Binder's cumulant V_L near the transition temperature in SD system.

4 Conclusion

We have conducted Monte Carlo simulation of two-di-

mensional six-state Potts model with constant couplings and random couplings. With thorough analysis, we have found that strength ratio $r = 0.3$ in SD system and blank bond ratio $f = 0.2$ in RD system will induce the variation of phase transition from the first-order to the second-order.

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