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Monte Carlo Study of the Order of the Phase Transition in Ising Systems with Multispin Interactions

By

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By analyzing the finite-size behavior of the maxima of the specific heat near the phase transition temperature, the order of phase transition of two-dimensional Ising systems with multispin interactions in the horizontal direction and two-body interactions in the vertical direction are determined. The results strongly support the Turban conjectures.

1. Introduction

There is considerable interest in the study of multispin interactions in Ising models [1, 2], because these models are not only relevant in many physical situations [3, 4], but can also serve as purely theoretical models to study phase transitions and critical phenomena, which might be very different from those of two-spin interactions in Ising models. For example, the Baxter-Wu model [5], an Ising model with three-spin interactions on every face of the triangular lattice which belongs to the same class of universality as the four-state Potts model [6, 7] according to the den Nijs conjecture [8], and the exactly solved eight-vertex model [9] which may be formulated as an Ising model with two- and four-body interactions, has a continuous dependence of the critical exponents on a parameter ("field" or "coupling constant") in the Hamiltonian. A few years ago, Debierre and Turban [10] generalized the two-dimensional Ising model with m-spin interactions in the horizontal direction and the usual two-spin interactions in the vertical direction on the rectangular lattice, the Hamiltonian of the system being

$$-\beta H = \sum_{\langle ij \rangle} \left\{ K_r S_{i,j} S_{i+1,j} + K_x \prod_{l=0}^{m-1} S_{i,j+l} \right\}.$$

As shown by Debierre and Turban [10], the above Hamiltonian is self-dual for any m, and as long as it has a single transition, the transition point will be located at the self-dual point, which is given by the known relation $\sinh 2K_r \sinh 2K_x = 1$, independent of the value of m. From the fact that the ground state is 2^{m-1} times degenerate, Turban conjectured that these models will be on the same universality class as the q-state Potts model whenever $q = 2^{m-1}$, so that $m = 3$ and the $q = 4$ Potts model should be on the same universality class, as well as the Baxter-Wu model. The mean field theory [10] stated that for $m \geqq m_c = 3$, the transition is of first order, which is certainly incorrect. Alcaraz [11] employed the heat-bath Monte Carlo algorithm for the isotropic case $K_r = K_x$ to determine the order

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of phase transitions by comparing at the critical temperature simulations of an initially ordered state and an initially totally disordered state. This method, however, is limited by many factors, e.g. the influence of the initial configurations [12]. When the lattice size is too small, it is not so easy to watch the discontinuity of the energies [13], so the lattice size must be chosen very large which is a forbidden task to obtain better statistics even for supercomputers. What is worse is that when the transition is of weakly first order, it is very hard [14] to watch the energy discontinuity which might mislead one to the conclusion that the transition is of second order. So Caticha et al. [2] used the fourth-order cumulant technique to study the order of phase transitions of the two models in the $m = 3$ and 4 cases, respectively. Although their results confirmed that for $m = 3$ ($m = 4$) the model undergoes a second-order (first-order) transition, in the $m = 3$ case they cannot confirm whether the model is on the same universality class as the $q = 4$ Potts model. The purpose of this paper is an attempt to fill this gap. We start from the different finite-size scaling theories of the maxima of the specific heat of first- and second-order phase transitions near the transition temperatures. Our results do not only agree with the previous conclusions, we also confirm that in the $m = 3$ case the critical exponents $\alpha = \nu$, which is not pointed out in previous papers [2, 11].

The outline of this paper is as follows. In Section 2, we briefly present the finite-size scaling theories of the maxima of the specific heat of first- and second-order phase transitions and the Monte Carlo method we have used. The simulation results and a finite-size behavior study are given in Section 3. Finally we summarize our conclusions.

2. Finite-Size Scaling Theory and Monte Carlo Method

Finite-size scaling theory has become a powerful and well-established tool for the studies of second-order phase transitions [15 to 18]. According to the standard theory of finite-size scaling, for sufficiently large lattice sizes L, the maxima of the specific heat in the critical region should diverge as $L^{\alpha/\nu}$, where α and ν are the infinite-lattice exponents.

For first-order phase transitions, finite-size scaling theory [12, 13, 19, 20] predicted that the maxima of the specific heat near the transition temperature should scale with L as follows:

$$C_{\max} - C_0 = L^d,$$

where d is the dimension of the system and C_0 is a constant which is a function of the internal energies and specific heats at the transition temperature of the two phases [12]. Note that the first-order finite-size scaling of the form of L^d will be possible only for systems of size $L \gg \xi$, where ξ is the correlation length of the system at the transition temperature.

We can see from the above that first- and second-order phase transitions will have different finite-size scaling forms of the maxima of the specific heat for sufficiently large lattice sizes L. So if we can calculate the specific heats near the transition point and locate the value of the maximum of the specific heat for different sizes L in the $m = 3$ and 4 cases, respectively, and make a careful analysis of the scaling forms of the maxima of the specific heat, we can determine the order of phase transitions in the two models.

Because we do not know a-priori for which L the asymptotic finite-size scaling of the form $L^{\alpha/\nu}$ for second-order and L^d for first-order transitions will set in, we choose lattice sizes $9 \leqq L \leqq 45$ ($m = 3$), $12 \leqq L \leqq 48$ ($m = 4$) to see whether these lattice sizes are

sufficiently large to reach the finite-size scaling regime. We will see below that the lattice sizes chosen are already in the finite-size scaling regime for some large lattice sizes L.

We employed the standard single-spin-flip Monte-Carlo algorithm of Metropolis et al. [21] and studied a system with dimension $L \times L$ and periodic boundary conditions applied in all directions. We performed the simulations at the self-dual symmetrical point for the isotropic case $K_c = K_r = K_x$. In order to locate the value of the maximum of the specific heat near the transition temperature quickly and accurately, we used the histogram method of Ferrenberg and Swendsen [22 to 25] for calculating the probability distribution of the internal energy at values of the coupling shifted from that of the actual value used in the simulation. Once in possession of the histograms the average of the total energy $\langle E \rangle_L$ and the average of the total squared energy $\langle E^2 \rangle_L$ for the size L can be calculated easily, so the specific heat C per spin at temperature T can be calculated from the fluctuations,

$$C(L) = \langle E^2 \rangle_L - \langle E \rangle_L^2)/(K_B T^2 L^d) .$$

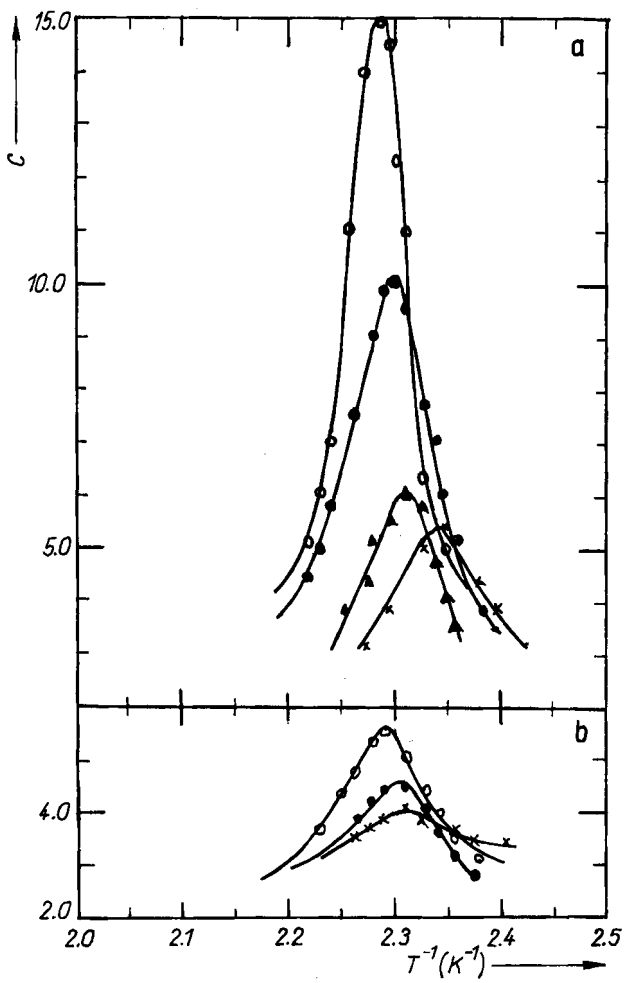

Fig. 1. Temperature variation of the specific heat for various lattice sizes. Data for some lattice sizes have been omitted in order to preserve the clarity of the figure. a) $m = 4$: ○ 48×48, ● 36×36, ▲ 28×28, × 24×24. b) $m = 3$: ○ 39×39, ● 30×30, × 18×18

With this method, it is possible to obtain complete thermodynamic information over the entire scaling region from a single run and, thereby to accurately locate the value of the maximum of specific heat. The typical runs comprised (5.0 to 7.0) $\times 10^5$ Monte Carlo steps (MCS). Thermalization was assumed after looking at the correlation times, and that leads to discarding the initial (1 to 5) $\times 10^4$ MCS. All the simulations were performed on Taiji 2230 at the Computer Center of Suzhou University, one of our longest series of measurements on a 48×48 lattice for $m = 4$, MCS = 600000 took about 56 h of CPU time.

3. Simulation Results

The temperature variation of the specific heat for various lattice sizes is shown in Fig. 1 for the $m = 3$ and 4 cases. For both cases, as the lattice size increases, the peaks grow while the width of the peak decreases. We also note that for $m = 4$ the peaks grow more rapidly than for $m = 3$. It is hard to judge just from these pictures if there is any difference at all between the phase transitions in the two models. However, this difference can be established by looking at the sequence of maxima of the specific heats C_{max} as a function of L. This method has been successfully used in [17]. Fig. 2 shows results of the finite-size scaling study of the maxima of the specific heat for $m = 3$ and 4. For $m = 3$ in Fig. 2a, we find a slope of 1.03 ± 0.01 with $B_0 = 1.6$, where B_0 is the nondivergent "background" contribution to the specific heat. The slope of the best linear fit to the data on log–log plot was obtained using a standard least-squares fitting routine. The values of B_0 used in Fig. 2a were the smallest ones for which the variation over the entire size range (except $L \leqq 12$) appeared linear. We also see from Fig. 2a that for $L \leqq 12$ corrections to finite-size scaling cannot be ignored, which gradually disappear as L becomes larger and larger. From the fitting procedure we obtained the value of the exponent ratio $\alpha/\nu = 1.03$, which implied the critical exponents $\alpha = \nu$, which leads to the conclusion that for $m = 3$ the model is on the same universality class as the $q = 4$ Potts model (note that for the $q = 4$ Potts model, the critical exponents $\alpha = \nu$). So our results strongly support the Turban conjectures. For $m = 4$, the finite-size scaling study is shown in Fig. 2b. The slope was obtained by excluding the lattice sizes $L \leqq 24$. The constant $C_0 = 3.8$ is the value for

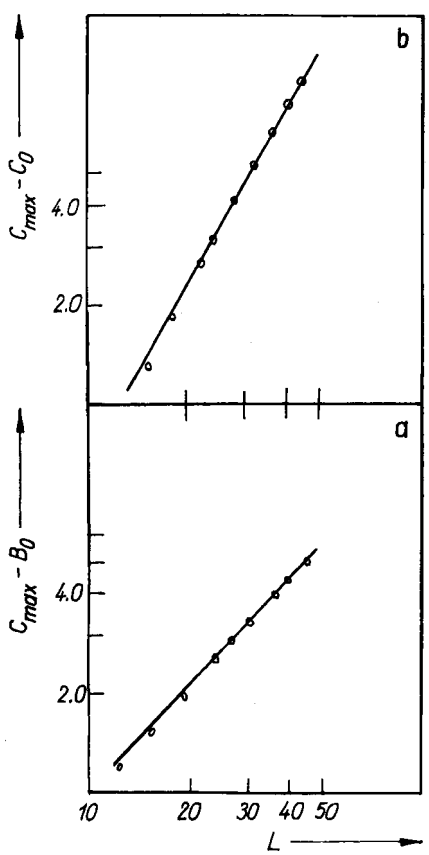

Fig. 2. Log–log plots of $C_{max} - B_0(C_0)$ vs. L for a) $m = 3$ and b) $m = 4$

which the variation over the size range $28 \leqq L \leqq 48$ appears linear. Because the correlation length ξ at the transition temperature may be larger than the small lattice size, one cannot reach the finite-size scaling regime. The slope is 2.01 ± 0.02 which is very close to the dimension $d = 2$ and leads us to the conclusion that the transition is of first order.

4. Conclusion

The multispin interaction Ising systems studied in this paper will undergo second-order phase transitions for $m = 3$ with the critical exponents $\alpha = \nu$, which strongly supports the Turban conjecture that for $m = 3$ the model will be on the same universality class as the $q = 4$ Potts model. For $m = 4$ the model will undergo a first-order phase transition. We emphasize here that using finite-size scaling theory to study phase transitions, one must make a careful analysis of the finite-size behavior of the model, especially pay attention to the corrections to finite-size scaling for second-order transitions. For first-order transitions one must choose large lattice sizes, larger than the correlation length at the transition temperature. Fortunately for $m = 3$ the corrections to finite-size scaling may be ignored for $L \geqq 15$ and the strongly first-order finite-size scaling regime is realized already at $L \geqq 28$ for $m = 4$. However, if one cannot reach the finite-size regime, one may obtain wrong results.

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