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NEW TYPE OF PHASE TRANSITION IN THE 2-*d* ISING MODEL WITH REGULARLY DISPOSED FRUSTRATION

H. Betsuyaku

Japan Atomic Energy Research Institute, Tokai, Ibaraki 319-11, JAPAN

Numerically exact spin-spin correlation functions were calculated by using a transfer-matrix method for two 2-*d* Ising models with regular disposition of the frustrated squares: (1) Villain's odd model with fully frustrated squares and (2) Bray's model with the chessboard arrangement of the frustrated squares. It has been found that the behavior of correlations of the odd model changes from the power-law decay to the exponential decay. On the other hand, the correlations of the chessboard model decay exponentially at all temperatures.

1. Introduction

The nature of spin glasses has recently been studied intensively, but the presence of a phase transition in spin glasses is still a very puzzling matter [1,2]. The simplest model of the spin glass system studied so far [3,4] is the two-dimensional (2-*d*) random-bond Ising model:

$$H=-\sum_{\langle i,j\rangle} J_{ij}\sigma_i\sigma_j \quad , \tag{1}$$

with nearest-neighbor interactions J_{ij} chosen randomly out of ± 1. Toulouse [5] pointed out that the frustration effect is the most genuine and interesting feature in such model. According to him the frustration function is defined by

$$\Phi_{[ijkl]}=J_{ij}J_{jk}J_{kl}J_{li} \quad , \tag{2}$$

which is the product of the interactions around an elementary square (*plaquette*) denoted by $[ijkl]$; Φ provides a local measure of frustration since whenever $\Phi=-1$ there is no way of choosing the orientation of the Ising spins around the plaquette without frustrating at least one bond.

Villain [6] remarked that regular-bond models with J_{ij} distributed by a certain rule exhibits some peculiarites of spin glasses. He considered a 2-*d* regular-bond Ising model in which all the plaquettes are frustrated with the odd rule $\Phi=-1$; this odd model is obtained if the bonds on every second line in the vertical direction are negative whereas all other bonds are positive as shown in Fig. 1(*a*). Bray *et al.* [4] considered another regular-bond model with the chessboard arrangement of the frustrated squares in which half of the total number of plaquettes is frustrated as shown in Fig. 1(*b*). It is known that both the models have very similar properties: the presence of freely rotating spins, a high ground-state degeneracy, a broad peak of the specific heat, and no phase transition at finite temperature [7].

The purpose of the present study is to investigate the nature of these two models by studing the temperature and distance dependences of the spin-

spin correlation functions. For this purposé a new scheme is developed to obtain numerically exact spin-spin correlation functions by using a transfer-matrix method [8,9]. It was found that the correlations of the two models behave very differently. The correlations of the odd model are long ranged and decay as $r^{-\eta}$ in the low temperature region, and decay exponentially in the high temperature region. The model apparently undergoes a new type of phase transition as Kosterlitz and Thouless [10] proposed for the 2-d planar model. However, detailed analysis of the data proved that the correlation has a form $e^{-r/\xi}/r^{1/2}$ with the correlation length $\xi \propto e^{(2.3\pm0.3)J/kT}$ in accordance with the theoretical result of Forgacs [11]. On the other hand, the correlations of the chessboard model exihibit an exponential decay at all temperatures. Its correlation length is constant in the low temperature region and decreases gradually with increasing temperature.

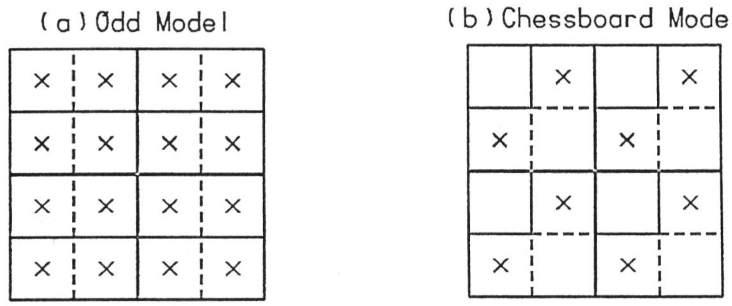

Fig. 1. The disposition of the bonds for the odd model (a) and the chessboard model (b). The ferromagnetic bonds are denoted by the solid lines, and the antiferromagnetic bonds are denoted by the dashed lines. The frustrated squares are marked by the crosses.

2. Method of Computation

The transfer-matrix method [8,9] was used to obtain numerically exact correlations between spins. Consider a square lattice of spins with M columns and N rows. Two types of the nth reduced density metrices:

$$\rho_n^+(\sigma_1,\sigma_2,\ldots,\sigma_M) \text{ and } \rho_n^-(\sigma_1,\sigma_2,\ldots,\sigma_M) \tag{3}$$

are defined by the traces taken over all the spins up to the $(n-1)$th row and down to the $(n+1)$th row, respectively, with all the spins $(\sigma_1,\sigma_2,\ldots,\sigma_M)$ on the nth row fixed. ρ_n^+ and ρ_n^- fulfil the following recursive relations:

$$\rho_n^+(\sigma_1,\sigma_2,\ldots,\sigma_M)=\exp(\beta\sum_i J_i\sigma_i\sigma_{i+1})\sum_{\{\sigma_i'\}}\exp(\beta\sum_i J_i'\sigma_i\sigma_i')\rho_{n-1}^+(\sigma_1',\sigma_2',\ldots,\sigma_M'),$$

$$\rho_n^-(\sigma_1,\sigma_2,\ldots,\sigma_M)=\sum_{\{\sigma_i''\}}\exp(\beta\sum_i J_i'''\sigma_i\sigma_i'')\exp(\beta\sum_i J_i''\sigma_i''\sigma_{i+1}'')\rho_{n+1}^-(\sigma_1'',\sigma_2'',\ldots,\sigma_M''), \tag{4}$$

where $\{J_i\}$ ($\{J_i''\}$) is the set of horizontal bonds in the nth ($(n+1)$th) row, and $\{J_i'\}$ ($\{J_i'''\}$) is the set of bonds connecting nth and $(n-1)$th ($(n+1)$th) rows. The partition functin Z is obtained from the trace of $\rho_n^+\rho_n^-$ taken over all the spins on the nth row:

$$Z=\sum_{\{\sigma_i\}}\rho_n^+(\sigma_1,\sigma_2,\ldots,\sigma_M)\rho_n^-(\sigma_1,\sigma_2,\ldots,\sigma_M) \; . \tag{5}$$

The correlation between spins on the nth row is given by

$$\langle\sigma_i\sigma_j\rangle = Z^{-1}\sum_{\{\sigma_i\}}\sigma_i\sigma_j\rho_n^+(\sigma_1,\sigma_2,\ldots,\sigma_M)\rho_n^-(\sigma_1,\sigma_2,\ldots,\sigma_M)\ . \tag{6}$$

This method is numerically exact and much simpler and faster than the method previously reported by Morgenstern and Binder [8] which involves cumbersome numerical differentiations. Only limitation of this method is that practical considerrations do not allow the application to large system; M is at most 20 and because of periodic boundary condition meaningful correlations are limited for $r \leqq M/2$. The sizes of M were 10, 12, 14, 16, and 18 with $N=M$.

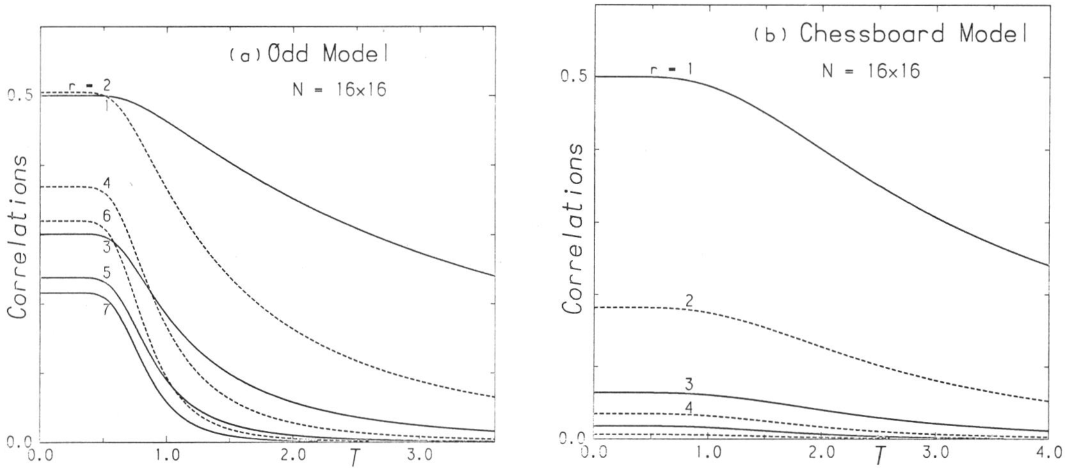

Fig. 2. The horizontal correlations of the odd model (a) and the chessboard model (b) as a function of temperature; $g(r)\equiv\langle\sigma_{0,0}\sigma_{r,0}\rangle$. The odd-order correlations are indicated by solid curves, and the even-order correlations by dashed curves.

3. Results

3.1 Odd model

The horizontal correlation of the odd model for 16×16 spins is shown in Fig. 2(a) as a function of temperature. The feature of the odd model is that the odd- and even-order correlations behave differently. By plotting the data in log-log form it was found that the odd- and even-order correlations independently fit well with a power-law decay:

$$g(r)\equiv\langle\sigma_{0,0}\sigma_{r,0}\rangle \propto r^{-\eta} \text{ with } \eta=0.47. \tag{7}$$

The correlations at high temperatures $(T>3.0)$ fit well with the simple exponential decay:

$$g(r)\propto e^{-r/\xi}. \tag{8}$$

The different behavior at high and low temperatures could indicate that a phase transition from exponential-decay to power-law decay occurs at some temperatue as in the 2-d planar model [10]. This possibility was found to be unlikely after the detailed study of the behavior of the correlations. The correlations begin to deviate from the simple exponential decay at $T<3.0$; the deviation increases markedly with decreasing temperature. However, the modified correlations $r^{1/2}g(r)$ fit well with the exponential decay:

$$g(r) \propto e^{-r/\xi}/r^{1/2}. \tag{9}$$

The correlation length ξ varies with temperature in a singular form:

$$\xi \propto e^{\alpha J/kT} \text{ with } \alpha = 2.3 \pm 0.3 \tag{10}$$

over the temperature range $0.9 < T < 3.0$. This behavior of ξ is not in agreement with the theory of Kosterlitz and Thouless [10], but in good agreement with the theory of Forgacs [11].

3.2 *Chessboard model*

The horizontal correlations of the chessboard model for 16×16 spins is shown in Fig. 2(*b*) as a function of temperature. By plotting the data in semilog form it was found that the even-order correlations fit well with a simple exponential decay; $g(r) \propto e^{-r/\xi}$ at all temperatures. The odd-order correlations deviate slightly from the simple exponential decay. The correlation length ξ is constant at low temperatures and decreases gradually with increasing temperature in the same way as the nearest correlation $g(1)$. The following relation holds over the wide temperature range:

$$\xi/\xi_0 = 1.75 \times g(1) + 0.125, \tag{11}$$

where $\xi_0 = 1.18$ is the correlation length at $T=0$.

4. Discussion and Conclusions

Forgacs [11] studied the spin-spin correlation function in the ground state of the odd model. He obtained the result that the correlations decay as $r^{-\eta}$ with $\eta = 0.5$ at large distance. The value of $\eta = 0.47$ obtained in the present study is slightly smaller than his value. This may be due to the fact that the lattice size of 18×18 is still small to obtain η at large distance. He also showed that for T close to zero the correlation length diverges exponentially fast as in 1-*d* Ising model. The present study showed that the correlation has the form $e^{-r/\xi}/r^{1/2}$ with the correlation length $\xi \propto e^{(2.3 \pm 0.3)J/kT}$ in accordance with the theory. This relation was found to hold well at $T \geq T_g$; T_g is the temperature where the specific heat has a broad peak. The low temperature behavior can be explained by assuming that the relation holds equally at low temperatures. On the other hand, the chessboard model provides a perfect paramagnet in which the correlation decay exponentially at all temperatures.

It is to be hoped that the study of numerically exact spin spin correlation functions of the 2-*d* Ising model with regularly disposed frustration will contribute to a better understanding of spin glasses.

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