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Defect energy with conjugate boundary conditions in spin-glass models in two dimensions

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We calculate the naive defect energy ΔE of Ising spin glass (SG) models in two dimensions using conjugate boundary conditions. We predict that, in the $\pm J$ model, the averaged value $\overline{\Delta E}$ converges to some nonzero value in the thermodynamic limit in contrast with $\overline{\Delta E}=0$ in the Gaussian model. This prediction supports a recent Monte Carlo prediction of the presence of the SG phase at finite temperatures in the $\pm J$ Ising model. We also calculate the interface free energy to confirm it. [S0163-1829(98)50842-9]

Spin glasses have attracted great challenge for computational physics in these two decades. It is widely believed that in two dimensions the spin glass (SG) transition occurs at zero temperature $T_c=0$. This belief arises from the study of the stiffness exponent θ_S which has a positive or negative value when the phase transition occurs at a finite, nonzero temperature $T_c\neq 0$ or $T_c=0$, respectively. McMillan,[1] and Bray and Moore[2] estimated a value of $\theta_S\sim -0.28$ for the Ising model with Gaussian distribution of bonds (Gaussian model) by calculating the defect energy ΔE of finite lattices and predicted that the model exhibits the SG transition at $T_c=0$ with the correlation exponent of $\nu=-1/\theta_S\sim 3.5$. This value of θ_S was confirmed by a recent estimation using larger lattices.[3] It should be noted, however, that the value of ν is significantly different from direct estimations of $\nu\sim 2.0$.[4–6] The problem is subtle in a discrete model with $+J$ and $-J$ bonds ($\pm J$ model) for which the value of θ_S was first estimated as $\theta_S\sim 0$.[7–9] However, a recent estimation gave a small negative value of $\theta_S\sim -0.05$.[10] From these results and an idea that the nature of the phase transition at a finite temperature would not depend on details of the bond distribution, one believes that $T_c=0$ *in any two-dimensional SG model*, although no direct evidence of $T_c=0$ has yet been obtained for every model, especially for the $\pm J$ model.[11] Recently, Shirakura and Matsubara made a Monte Carlo (MC) simulation of the $\pm J$ model at low temperatures[12] and that of an asymmetric discrete model with $+J$ and $-aJ(a\neq 1)$ bonds at very low temperatures[13] and predicted $T_c\neq 0$. Obviously, their prediction and the belief are incompatible.

In this paper, we carefully reexamine the defect energy of Ising SG models in two dimensions and find that the results support the prediction of $T_c\neq 0$. Our findings are as follows. (i) The conventional boundary conditions used for estimating the defect energy ΔE are inadequate in some cases, especially in delicate problems such as the phase transition of the $\pm J$ model. *A naive defect energy is calculated for the first time in the SG problem using conjugate boundary conditions.* (ii) The distribution of ΔE, $P(\Delta E)$, is highly asymmetric for small systems and *the conventional estimation of* θ_S *by means of the size dependence of the average value* $\overline{\Delta E}$ *could take the risk for misleading the conclusion.* (iii) $\overline{\Delta E}$'s are estimated for both Gaussian model and discrete models for different sizes of the lattice and the following predictions are given for large systems. In the Gaussian model, $P(\Delta E)$ shrinks to a sharp one at $\Delta E=0$. Therefore $\overline{\Delta E}=0$ and θ_S is negative as predicted previously but its value is larger than that of the previous estimations. In the discrete models, $P(\Delta E)$ exhibits discrete peaks whose weights at $\Delta E\sim 0$ as well as those at large ΔE never increase with increasing the size of the lattice. Therefore $\overline{\Delta E}$ converges to some nonzero value, i.e., $\theta_S=0$, in contrast with the recent prediction. (iv) Thus *the prediction of* $T_c\neq 0$ *for the discrete models is not incompatible with the results of the defect energy analysis.* The interface free energy is also calculated to confirm the presence of the SG phase at finite temperatures.

We start with an Ising model on a square lattice $L\times(L+1)$ described by the Hamiltonian

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

where $\sigma_i(=\pm 1)$ are Ising spins and $\langle ij\rangle$ runs all nearest-neighbor pairs. We consider the following two bond distributions:

$$P(J_{ij})=\frac{1}{\sqrt{2\pi}}\exp(-J_{ij}^2/2), \tag{2}$$

$$P(J_{ij})=\frac{1}{2}[\delta(J_{ij}-J)+\delta(J_{ij}+aJ)]. \tag{3}$$

The model (1) with the distribution (2) is the Gaussian model and that with Eq. (3) is a discrete model. Hereafter we refer to the direction for $(L+1)$ spins as the x direction and the other as the y direction. The defect energy ΔE has been conventionally defined by $\Delta E=E_{ap}-E_p$, where E_p and E_{ap}

are the ground-state energies for the periodic and antiperiodic boundary conditions in the y direction. The boundary condition in the x direction is chosen to be either periodic[1] or free.[3,10] Note that the defect energy calculated in this way is either positive or negative and one considers the absolute value $|\Delta E|$. Bray and Moore[2] applied somewhat different boundary conditions. They considered the lattice with the periodic boundary condition in the y direction. The spin configurations on the surfaces in the x direction, which are denoted as $\{S_a\}$ for $x=1$ and $\{S_b\}$ for $x=(L+1)$, are put at random. They defined E_p as the ground-state energy of the lattice with $\{S_a\}$ and $\{S_b\}$, and E_{ap} as that with $\{S_a\}$ and $\{-S_b\}$, where $\{-S_b\}$ is the spin configuration obtained reversing all the spins of $\{S_b\}$. These different sets of boundary conditions would be essentially the same for evaluating ΔE. In fact, the same value of $\theta_S \sim -0.28$ has been obtained in the Gaussian model.[1–3] However, it is not obvious whether these sets give the true defect energy or not.[14] For example, we consider the boundary conditions by Bray and Moore. For neither boundary condition will the system have its ground-state spin configuration of the lattice without any restriction. That is, some defect lines (or defect points) already exist in those ground states. Therefore, it is doubtful whether ΔE gives true defect energy or not. This problem would not be so serious when ΔE has a strong dependence on L as in the ferromagnetic case. However, in the two dimensional SG model, the size dependence is slight, e.g., $\Delta E \sim J$ even for $L \sim 30$.[3,10] That is, the value would considerably change even when only one position of the defect line changes. To relieve this difficulty, Ozeki[9] used a replica boundary condition for one end but still used the random boundary condition for the other end. It should be noted that he obtained a value of θ_S slightly larger than that of the conventional method.[7,9]

We consider the lattice treated by Bray and Moore. It is obvious that the spin configuration without any defect is the ground state without any restriction. Then it is quite natural to choose the spin configurations $\{S_a\}$ and $\{S_b\}$ as ones in the ground state for the free boundaries. We call this boundary condition a conjugate boundary condition, because it gives the true ground-state energy. By the use of the boundary conditions of $\{S_a\}$ and $\{-S_b\}$, we may certainly construct one defect line, if it could occur. The defect energy ΔE obtained using these sets of boundary conditions is, of course, non-negative in contrast to the conventional one. The problem is how to get $\{S_a\}$ and $\{S_b\}$. We can readily get them by using a cluster heat bath (CHB) method[13,15,16] for both $T=0$ and $T\neq 0$. Some comments should be given. For the Gaussian model, the ground state can be uniquely determined. Then ΔE for each sample can be uniquely determined. On the other hand, in the discrete models, there are many different sets of $\{S_a\}$ and $\{S_b\}$. Then we choose one of them for $\{S_a\}$, and $\{S_b\}$ is chosen so as to give the minimum value of ΔE.[17] These calculations may be readily done by using the transfer matrix method.[7,18]

We make the simulation using these conjugate boundary conditions. The lattices treated here are $L\times(L+1)$ for $L \leqslant 24$ and the numbers of the samples are $N_s = 10\,000 \sim 50\,000$. For every size of the lattice with L, the defect energy ΔE is calculated for every sample and the distribution function $P_L(\Delta E)$ is obtained. The defect energy $W(L)(\equiv \overline{\Delta E})$ for the lattice with L is obtained from $W(L) = \int \Delta E P_L(\Delta E) d\Delta E$.

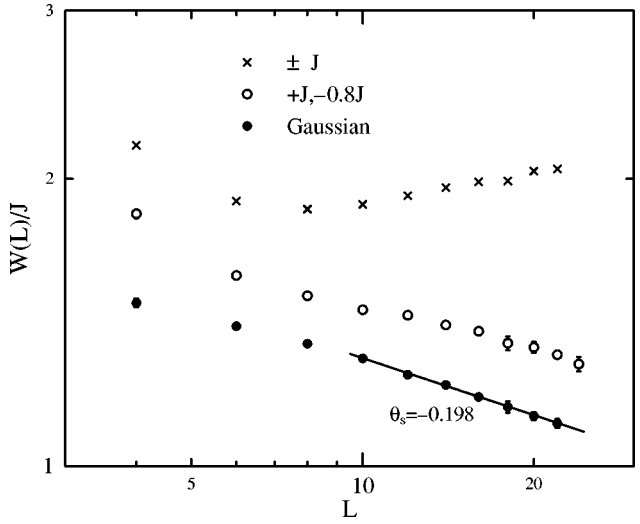

FIG. 1. The defect energies $W(L)$ as functions of the lattice size L.

The results of $W(L)$ are shown in Fig. 1 in a log-log scale. These size dependences of $W(L)$ are quite different. In the Gaussian model, log $W(L)$ decreases almost linearly with log L suggesting $W(L) \sim L^{\theta_S}$ with $\theta_S < 0$ as predicted previously. However, the value of $\theta_S \sim -0.20$ is larger than that of the previous estimations of $\theta_S \sim -0.28$.[1–3] In the $\pm J$ model, $W(L)$ slightly increases in contrast with the recent prediction based on the conventional boundary conditions.[10] On the other hand, in the asymmetric model with $+J$ and $-0.8J$ bonds, $W(L)$ decreases. These results in the discrete models are quite mysterious, because the MC studies[12,13] suggested $T_c \neq 0$ for both the models.

To examine this problem, we consider $P_L(\Delta E)$ itself. In Fig. 2, we present $P_L(\Delta E)$ of the Gaussian model. $P_L(\Delta E)$ has a continuous weight in a finite range of ΔE. As L is increased, the weight at $\Delta E \sim 0$ increases, while that at larger ΔE decreases. This fact implies that it collapses to $P_L(\Delta E) \sim \delta(\Delta E)$. On the other hand, in the $\pm J$ model, ΔE

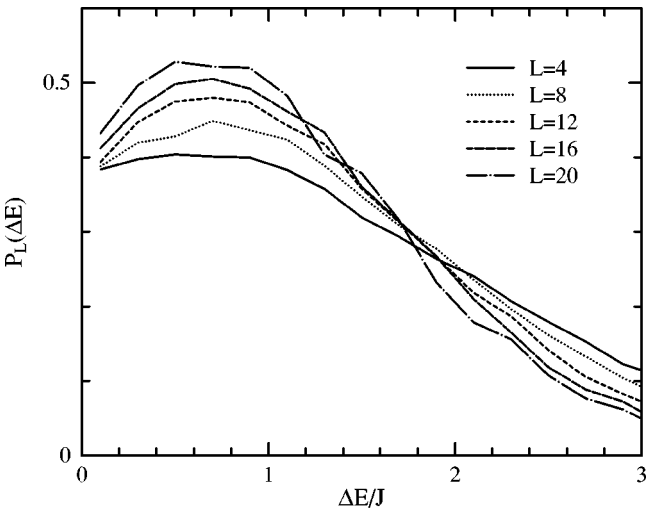

FIG. 2. Distribution of ΔE of the Gaussian model.

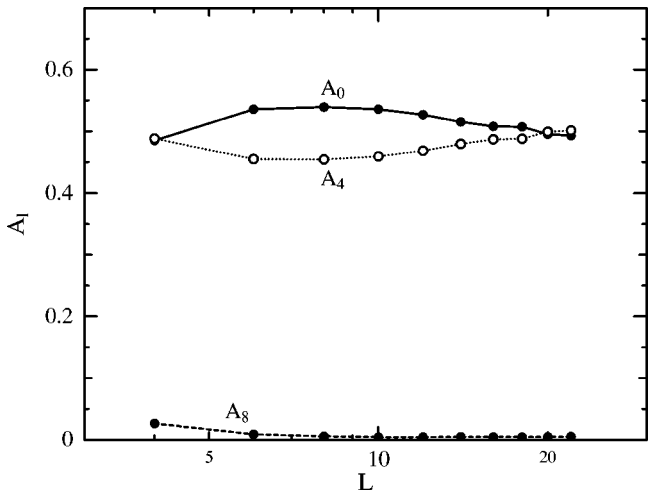

FIG. 3. The weights A_l of discrete peaks at $\Delta E = lJ$ of the $\pm J$ model.

takes values for every $4J$, i.e., $P_L(\Delta E) = \Sigma_{l=0,4,\ldots} A_l \delta(\Delta E - lJ)$. The size dependences of the coefficients of A_l are plotted in Fig. 3. Only A_0 and A_4 have considerable weights. The most important point is that A_0 and A_{4n} with $n \geq 2$ never increase with L. This means that $W(L)$ never vanishes nor diverges for $L \to \infty$, i.e., $W(L)$ converges to some nonzero value. In the asymmetric model, $P_L(\Delta E)$ also has discrete peaks at every $2(1-a)J$. In Fig. 4, we show $P_L(\Delta E)$ in a line graph. For small L, it has a double peak at $\Delta E \sim 0.4J$ and $3J$. As L is increased, the peak at $\Delta E \sim 3J$ rapidly diminishes and $P_L(\Delta E)$ becomes of the single peak. The weights of $\Delta E = 0$ and $0.4J$ components seem to converge and those at $\Delta E \sim J$ increase. Thus we think that, for $L \to \infty$, $P_L(\Delta E)$ has a single peak at $\Delta E \sim J$. That is, $W(L)$ also converges to some nonzero value. The distribution functions $P(\Delta E)$ for $L \to \infty$ suggested above and from the MC studies[12,13] are schematically shown in Fig. 5.

We conclude, hence, that whether the SG phase transition occurs or not in two dimensions depends on the model. In the Gaussian model, $T_c = 0$ as predicted previously. It should

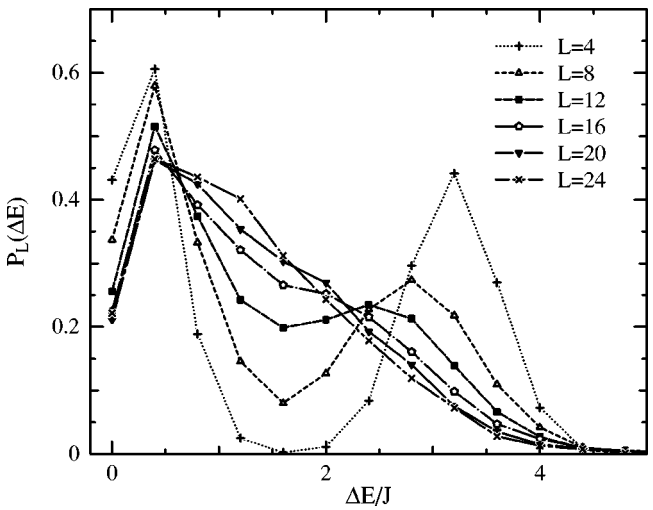

FIG. 4. Distribution of ΔE of the $+J$ and $-0.8J$ model. Lines are guide to the eye.

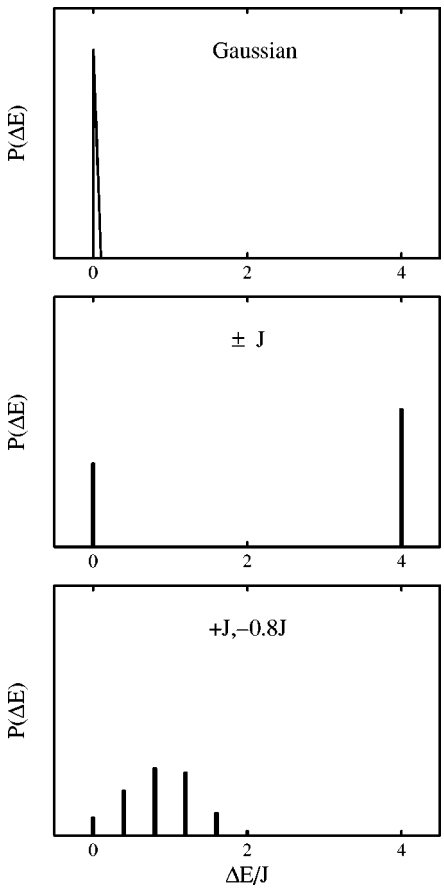

FIG. 5. Schematic pictures of distribution of ΔE for $L \to \infty$.

be emphasized again that the value of θ_S is different from that of the previous estimation. The value seems to have no relation with that of the correlation exponent ν.[4] In the discrete models, the problem is very delicate, because $W(\infty)$ has a finite, nonzero value like that in the two-dimensional

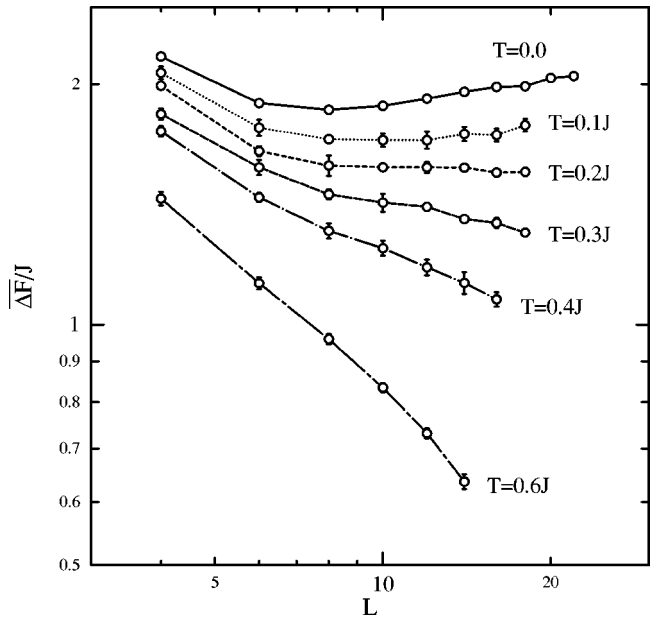

FIG. 6. The interface free energies $\overline{\Delta F}$ of the $\pm J$ model at different temperatures. Note that $\overline{\Delta F}$ at $T = 0$ is $W(L)$.

xy ferromagnet. This result suggests that $T=0$ is marginally stable. The SG order will exist at $T=0$ which is characterized by a power-law decay of the spin correlation.[7,18] Whether $T_c \neq 0$ or not should be examined separately. We have also made it by evaluating the interface free energy $\Delta F = F_{ap} - F_p$,[1,9] where F_p and F_{ap} are the free energies calculated using conjugate boundary conditions $\{S_a\}$ and $\{S_b\}$ at finite temperatures.[19] The result for the $\pm J$ model is presented in Fig. 6. In fact, the average value $\overline{\Delta F}$ for $T \leqslant 0.1J$ seems to increase with lattice size L, while that for $T \geqslant 0.3J$ decreases. Thus we believe that the phase at $T=0$ persists up to some finite temperature. That is, T_c is nonzero and exists between $0.1J$ and $0.3J$, probably $T_c \sim 0.2J$. This result is quite interesting, because the value of $T_c \sim 0.2J$ is compatible with the previous estimation of $T_c \sim 0.24J$ using the MC method.[12] Thus we believe that the defect energy analysis gives results which are not incompatible with the MC result.

Finally, we should note that the choice of the boundary condition will be crucially important also in three dimensions. Especially, studies of the defect energy in the three-dimensional vector SG models under the conjugate boundary conditions are desirable, because the possibility of the chiral SG ordering without any spin ordering is a current topic.[20–22]

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