Long-Range Order of the Site-Random Spin Glass Model*

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Abstract

The site-random Ising spin glass model is investigated. We find a rigorous symmetry for the SG correlation and the free energy, which provides some restrictions in the phase diagram. Using the defect energies calculated by the numerical transfer matrix method, we obtain evidence for the existence of the SG phase in the two-dimensional Ising system. We suggest that the transitions from the FM and the AF phases in the ground state in this model can be explained by the percolated-cluster picture, which is quite different from the frustration picture in the conventional $\pm J$ model.

KEYWORDS: site-random system, Ising spin glass, percolation, gauge transformation, transfer matrix method, defect energy

Since the pioneering work by Edwards and Anderson (EA), the spin glass (SG) problem has been investigated mainly in terms of bond-random models, which are generically called the EA models. Up to the mean-field level, the theoretical picture of the EA model has been established, and the system exhibits a typical many-valley structure in the phase space. Since the upper critical dimensions of these models are quite large, such a mean-field picture might be modified in a physical situation. Although the SG transition has been confirmed in the 3d Ising SG models, it has been denied in the 2d Ising and the 3d Heisenberg models. The real SG transitions are now interpreted theoretically as, for example, a crossover to the Ising SG or induced order from the Ising chiral SG.

Recently, Shirakura and Matsubara investigated the site-random Ising SG model numerically for $d = 2$ and $d = 3$, and found evidence for the existence of the SG phase even for $d = 2$. This behavior is quite different from that of the EA model. Since most of the SG materials can be described very well using site-random models, this model is more realistic than the EA-type models such as the $\pm J$ Ising model. In particular, an SG material, Fe$_x$Mn$_{1-x}$TiO$_3$ is closely related to it. Thus, this model is expected to clarify the problems and the difficulties in the conventional SG theory based on the

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bond randomness. In the present article, we show characteristic behavior of the site-random model not only numerically but also analytically. Although this model has no gauge symmetry in contrast to the $\pm J$ model,[12, 13, 14, 15] we find another type of symmetry which provides a restriction of the structure of the phase diagram. We also find numerically typical orderings of the ferromagnetic (FM) and the antiferromagnetic (AF) phases in $d = 2$. These results reveal a physical interpretation of the SG as well as the FM (AF) orderings.

The present site-random model consists of two kinds of magnetic ions (A and B) randomly distributed on all lattice sites with a fixed concentration, $c$, of the A-ion. Let us consider an Ising spin system $\mathcal{H} = -\sum_{ij} J_{ij} S_i S_j$ with nearest-neighbor interactions on a $d$-dimensional hypercubic lattice. The exchange interaction between $i$-th and $j$-th sites, $J_{ij}$, is determined by the species of the ions on these sites; $J_{ij} = -J$ if both are B-ions, and $J_{ij} = +J$ otherwise. Mathematically, we associate an independent quenched random variable $\omega_j$ with each site according to the species of ions; $\omega_i = 1$ and $\omega_i = -1$ represent the A-ion and the B-ion, respectively. Then, the exchange interaction is expressed as $J_{ij} = \frac{\omega_i + \omega_j - \omega_i \omega_j}{2}$. The average of the ion configuration is denoted as $\langle \cdots \rangle_c = \sum_{\{\omega_i = \pm 1\}} \cdots \prod_i P_c(\omega_i)$, where the distribution function of $\omega_i$ is given by $P_c(\omega_i) = c\delta(\omega_i - 1) + (1 - c)\delta(\omega_i + 1)$.

When the concentration $c$ is close to unity (zero), the FM (AF) phase appears in the low-temperature region for $d \geq 2$. At intermediate concentrations, $c \sim 1/2$, the SG phase is expected to appear for sufficiently high dimensions.

The probability $p_{FR}$ that one particular plaquette is frustrated is given by $p_{FR} = 4c^2(1 - c)^2$. Although the positions of frustrations are correlated with each other, we numerically find that this is a good approximation for the concentration of frustrations, at least in two dimensions. Similarly, the probability $p$ that one particular bond takes $J_{ij} = +J$ is given by $p = 2c - c^2$. We also find that this is a good approximation of the concentration of $+J$ bonds. Note that $p$ is greater than $1/2$ at $c = 1/2$, and becomes $1/2$ when $c = 1 - 1/\sqrt{2} \approx 0.293$. This is related to the absence of explicit symmetry with respect to $c = 1/2$.

In the $\pm J$ Ising model, the phase diagram is symmetric with respect to $p = 1/2$ when the FM and AF phases are identified. This is due to the invariance of the Hamiltonian in terms of the successive transformations $S_i \rightarrow (-1)^i S_i$ and $J_{ij} \rightarrow -J_{ij}$ for all sites and bonds. Here $(-1)^i$ gives a negative sign when the $i$-th site is located in one of the sublattices. This invariance means that the FM correlation function at $p$ is identical with the AF correlation function at $1 - p$, and the SG correlation function is invariant under the transformation $p \leftrightarrow 1 - p$.

In the present model, the Hamiltonian is invariant under the successive transformations $S_i \rightarrow (-1)^i S_i$, $S_i \rightarrow \omega_i S_i$ and $\omega_i \rightarrow -\omega_i$ for all sites (the order of operations is arbitrary). The first one represents the sublattice flip, the second one flips all spins on B-ions, and the last one switches the labels of the A-ion and the B-ion. Note that the last one changes the ion distribution $P_c(\omega)$ to $P_{1-c}(\omega)$. Then, the free energy as well as the SG correlation function, $\langle [S_i S_j]^2 \rangle_c$, is invariant under the transformation, $c \leftrightarrow 1 - c$, while the FM and the AF correlation functions, $\langle [S_i S_j] \rangle_c$ and $(-1)^{i-j} \langle [S_i S_j] \rangle_{1-c}$, have no such symmetry.
In fact, they satisfy \( [\langle S_i S_j \rangle]_c = (-1)^{i-j} [\langle S_i S_j \rangle \omega_i \omega_j]_{1-c} \). Since the SG order parameter does not vanish even in the FM and AF phases, the above symmetry rigorously shows that the SG phase must exist in the excess region when the FM and AF phases are not symmetric (see Fig. 1), and that the boundary of the paramagnetic phase, the onset of the SG order parameter, is symmetric with respect to \( c = 1/2 \).

When the bond concentration is close to zero or unity, one can approximate the present system by the \( \pm J \) model with the bond concentration \( p = 2c - c^2 \) (the \( \pm J \) mapping). The FM (AF) critical point has been obtained numerically as \( p \approx 0.89 \) (\( p \approx 0.11 \)) in the ground state in two dimensions.\(^{16,17,18}\) Using the above mapping, the corresponding critical concentrations of the present model are estimated as \( c_t \approx 0.668 \) for the FM critical point, and \( c_a \approx 0.057 \) for the AF critical point. Of course, this approximation is not good around the critical concentration, where we should take the correlation of bonds into account.

In order to estimate these critical concentrations precisely, we calculate the defect energy in the ground state in \( d = 2 \) using the numerical transfer matrix method introduced previously.\(^{17,18}\) Three kinds of boundary conditions (BCs) are applied; the (usual) uniform BC conjugate to the FM order, the staggered BC conjugate to the AF order, and the replica BC\(^{19}\) conjugate to all kinds of long-range order.\(^{19}\) At each concentration, the effective stiffness exponents, \( a_U(c), a_S(c) \) and \( a_R(c) \), are defined from the defect energies \( W_{U,L}(c), W_{S,L}(c) \) and \( W_{R,L}(c) \), respectively, as \( W_L(c) \sim L^{a(c)} \). Here suffixes U, S, R distinguish the BCs, and \( L \) indicates the linear size of the system. Since each stiffness exponent is expected\(^{17,18}\) to behave as \( a > 0 \) in the ordered phase, \( a = 0 \) at the critical point and \( a < 0 \) in the disordered phase, one can distinguish the phases according to the signs of \( a_U, a_S \) and \( a_R \).

Calculations are carried out at several concentrations for the square lattices of linear size \( L = 6, 8, 10, 12, 14, 16 \). At each concentration, \( W_L \) is estimated by averaging 10000–70000 randomly chosen samples of ion configurations. The concentration dependence of the stiffness exponents is shown in Fig. 2. Then, we estimate the critical concentrations as \( c_t \approx 0.63 \pm 0.01 \) and \( c_a \approx 0.41 \pm 0.01 \). Since \( a_R(c) \) is always positive for \( 0 \leq c \leq 1 \), we have evidence of the existence of the SG phase in \( 0.41 < c < 0.63 \).\(^2\)

As shown rigorously, \( a_R(c) \) is symmetric with respect to \( c = 1/2 \). On the other hand, the critical concentrations for the FM and the AF phases are slightly asymmetric. This indicates the existence of the SG phase at least in \( 0.59 < c < 0.63 \), which is consistent with the behavior of \( a_R \). Accordingly, we obtain evidence of the SG phase in a two-dimensional Ising system from both the conventional analysis and a new criterion. However, we should carefully conclude this point, because the concentration difference of widths of two phases (0.04 \( \pm 0.02 \)) is too narrow, and the system size is still small to confirm such a sensitive property.

Note that both regions of the FM and AF phases in the numerical results are larger than those in the \( \pm J \) mapping. In particular, the AF phase remains up to \( c_a \approx 0.41 \), where \( -J \) bonds are distributed less than \( +J \) bonds. Let us discuss the reason for this.

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1. The fixed spins on the boundary are modified from those in ref. 19, which were all up; the fixed spins are randomly chosen in the present calculation.

2. Although one should show some typical dynamical behaviors to confirm the SG phase, the above behaviors are sufficient in the static sense.
At the critical concentration, \( c \approx 0.41 \), the concentration of the B-ion \(( \approx 0.59 \) \) is close to the percolation threshold of the site process in 2d, \( 0.592745 \). Since the \(-J\) bonds are located only between B-ions, the infinite percolated cluster of B-ions is connected antiferromagnetically in the remnant FM bonds for \( c < 0.407255 = (1 - 0.592745) \). If the remnant bonds have no exchange interaction, i.e., the site-diluted system, the AF phase exists for \( 0 \leq c \leq 0.407255 \) in the ground state. However, there are two differences between the present system and the site-diluted system. One is the existence of frustrations, which usually inhibits the long-range order. Another is the fact that the clusters are not magnetically independent of each other in the present system. However, these two facts are not expected to change this “percolated-cluster picture” for the following reasons.

In the \( \pm J \) model, the FM order is destroyed at \( p = 0.89 \) much faster than the percolation threshold of the bond process — \( p = 1/2 \) on a 2d square lattice. The degree of frustration in the present system is weaker than that of the \( \pm J \) model: Since \( p_{\text{FR}} \approx 4c^2(1-c)^2 \), the maximum concentration of frustrated plaquettes is \( p_{\text{FR}} = 1/4 \) at \( c = 1/2 \), while \( p_{\text{FR}} = 1/2 \) at \( p = 1/2 \) in the \( \pm J \) model. Even at the critical concentration \( p = 0.89 \) or \( p = 0.11 \) in the \( \pm J \) model, \( p_{\text{FR}} = 0.317 \) is greater than the maximum value \( p_{\text{FR}} = 1/4 \) in the present model. Thus, the concentration of frustrated plaquettes is always lower than that at the FM (AF) critical point of the \( \pm J \) model, at which the frustration just destroys the uniform (FM) order.

In spite of the interactions between clusters, the effect through the boundaries of clusters is not expected to be strong. In the present site-random system, frustrations do not exist inside the clusters but among them. Typical connections of two adjacent FM and AF clusters are drawn in Fig. 3. If the boundary of the clusters is oblique to all the axes as in Fig. 3(a), no frustrations appear between the clusters and the magnetic orderings of two clusters do not compete. If it is parallel to one of the axes as in Fig. 3(b), all plaquettes between the clusters are frustrated, and each cluster can flip without changing the energy. If these two cases appear separately, the long-range order in an infinite cluster is stable. Although these two cases generally occur together, the effect of inhibition would be smaller than that in the \( \pm J \) model. In fact, the FM and AF phases are wider than those obtained by the \( \pm J \) mapping. Moreover, the AF ordering in the \(+J\)-bond-rich region comes from the percolated cluster of B-ions. The reason of the discrepancy between the FM and AF critical concentrations is not clear at present, and should be solved in future.

In two dimensions, the region of infinite percolation for the A-ion has no overlap with that for the B-ion. In three dimensions, the percolation threshold of the cubic lattice is \( 0.3117 \) and infinite clusters of both A-ions and B-ions exist for \( 0.3117 < c < 0.6883 \). In this region, the FM order on the A-ions and the AF order on the B-ions strongly compete, and consequently the SG phase would appear. Therefore, even if the SG phase exists in two dimensions, its origin may be qualitatively different from that of the SG phase in three dimensions.

In summary, we have studied the site-random Ising spin glass model. Although this model has no gauge symmetry in contrast to the \( \pm J \) model, we find a new rigorous symmetry for the SG correlation and the free energy. This symmetry provides restrictions on the structure of the phase diagram, and a criterion for the existence of the SG phase.
from a different point of view to that of conventional arguments. We calculate the defect energies with uniform, staggered and replica boundary conditions in the ground state in $d = 2$ using the numerical transfer matrix method, and obtain evidence of the SG phase from both the conventional scaling analysis and the new criterion. We propose the percolated-cluster picture in order to explain the transitions from the FM and the AF phases in the ground state, which are expected to be the origin of the SG ordering in $d \geq 3$. Thermodynamic properties and critical behaviors of the present site-random model are quite different from those of the bond-random models which have been investigated as the models of SG materials. Further studies in this direction are required.

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Figure 1: Schematic phase diagram of the site-random SG model. The asymmetry of the FM and the AF phases is assumed. The shaded area indicates the excess region out of the FM phase, in which the SG phase exists.

Figure 2: Stiffness exponents \( a_R \), \( a_U \) and \( a_S \) as a function of the A-ion concentration \( c \). These exponents are evaluated from the defect energies of \( L = 6 \sim 16 \) with the replica, uniform and staggered boundary conditions, respectively.

Figure 3: Schematic ion configurations at the boundary of the A-ion (closed circles) and the B-ion (open circles) clusters. Bold and dotted lines indicate \(+J\) and \(-J\) exchange interactions, respectively. Frustrated plaquettes are marked by crosses, while unfrustrated ones are unmarked.
