Spin Correlation Functions on Frustrated Lattices

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The spin correlation functions of the Ising systems on lattices with frustrated bond configurations are studied. Relations between structures of degeneracy and temperature dependences of spin correlation functions are investigated. Occurrence of phase transition is also discussed in connection with types of degeneracy.

§ 1. Introduction

There have been many works on spin glass phenomena. We could characterize spin glasses with the following two properties: One of them is non-uniformity of systems, which keeps us away from our traditional technique. Another one is competition between orders which are degenerated due to random bond configuration. The concept of "frustration" has been introduced for these competing situations. The importance of effects of frustrations has been suggested by many authors.

In this paper we concentrate ourselves on regularly disposed frustrated configurations on the Ising systems. Frustrated configurations produce degeneracies and result in weakening the spin correlation function. We have studied decay of ground state spin correlation functions due to the degeneracy and we have introduced a cluster picture of spin glasses. The cluster has been defined as a domain whose total inversion does not change the ground state energy. On the bond configuration shown in Fig. 1(a), both spin configurations, Figs. 1(b) and (c), are ground states. Bryksin et al. have obtained, however, a rigorous finite critical temperature for the lattice shown in Fig. 1(a). Their result suggests the importance of effects of degeneracy.

Fig. 1(a) A frustrated bond configuration. Bold and thin lines denote antiferromagnetic and ferromagnetic bonds, respectively. Symbols ▲ denote frustrated plaquettes. We maintain this notation throughout the paper.

(b) A parallel spin arrangement. Symbols □ and ● denote up and down spins, respectively. The lines with /// denote unsatisfied bonds. We also maintain this notation.

(c) An antiparallel spin arrangement.
finite critical temperature is one of the motivations of this paper.

Here we study the relation between structures of degeneracy and types of ordering process, in particular, temperature-dependence of spin correlation function and phase transition.

As has been widely pointed out, frustrated configurations are invariant under the following local gauge transformation:

\[ (\sigma_i, J_{ij}) \rightarrow (-\sigma_i, -J_{ij}) \quad \text{for all } j, \]  

which is shown in Fig. 2. Let us classify bond configurations according to an equivalence which identifies configurations if one of them can be transformed to another by the local gauge transformations. Then configuration of frustrated plaquettes characterizes each class and ordering processes in each class are the same because the local gauge transformation does not change the partition function

\[ Z = \text{Tr} \exp(\beta \sum_{\langle ij \rangle} J_{ij} \sigma_i \sigma_j). \]  

For example, the pure ferromagnetic, pure antiferromagnetic and Mattis configurations (site random configurations) belong to the same class which we may call a “pure class”. This classification is very similar to the topological classification of line defects. Thus we may say that configurations with frustrations are in a sense, topologically different from the pure one. One may expect that many trivial properties for the pure lattice are violated in “topologically different” lattices.

We study various types of temperature dependence of spin correlation functions and the relations between the types and structures of degeneracy in § 2. The relation between phase transitions and types of spin correlation functions is discussed in § 3.

§ 2. Spin correlation functions

On the frustrated lattice the lowest energy state may be degenerate. In the ordering process, these degenerate states compete with each other, and very peculiar behavior can be expected in the temperature-dependence of spin correla-
Fig. 3. Frustrated bond configurations. In the vertical direction, the periodic boundary condition is imposed. The spins \( \sigma \) and \( s \) are denoted by \( \bigcirc \) and \( \triangle \) in each figure and the spin \( s' \) is denoted by \( \square \).

Fig. 4. Spin correlation functions, \( \langle \sigma s \rangle \). Dotted lines denote that of the non-frustrated one. (a), (b), (c) and (d) correspond to those of Fig. 3.

It is interesting to classify the types of temperature-dependence of the spin correlation function \( \langle \sigma s \rangle \) and study the relations between these types and the structure of the degeneracy. We present here five types of temperature-dependence. The typical frustrated configurations corresponding to each type are shown in Fig. 3 where we denote spins \( \sigma \) and \( s \) by \( \bigcirc \) and \( \triangle \), respectively.

First we consider the configuration shown in Fig. 3(a). In this case the ground state spin configuration function is unique and frustrated configurations weaken the correlation only quantitatively at finite temperatures. The temperature-dependence of the spin correlation function is given in Fig. 4(a). Excitation levels when we fix \( \sigma = s \) and \( \sigma = -s \) are given in Table I. In this table the excitation levels of pure ferromagnetic case are given by Type 0. For the lattice shown in Fig. 3(a) the levels are given by Type 1, where only the case \( \sigma = s \) gives the lowest level, i.e., the ground state. Thus in this case the situation is essentially the same as the pure case and frustrations produce only a quantitative effect. Hereafter we consider cases where the ground state is degenerate for \( \sigma s = \pm 1 \).
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Table 1. Degrees of degeneracy of energy levels of the Ising systems shown in Fig. 3. Levels are symmetric with respect to the sign. See the text for definitions of types.

<table>
<thead>
<tr>
<th>TYPE</th>
<th>$\sigma s$</th>
<th>$-E/J$</th>
</tr>
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<tbody>
<tr>
<td></td>
<td>18 16 14 12 10 8 6 4 2 0</td>
<td></td>
</tr>
<tr>
<td>0 (pure)</td>
<td>+1</td>
<td>1 0 0 2 12 8 18 30 32 48</td>
</tr>
<tr>
<td></td>
<td>-1</td>
<td>0 0 4 2 6 8 22 30 32 48</td>
</tr>
<tr>
<td>1 (Fig. 3a)</td>
<td>+1</td>
<td>0 1 0 2 18 18 22 44 42</td>
</tr>
<tr>
<td></td>
<td>-1</td>
<td>0 0 0 6 12 18 26 44 40</td>
</tr>
<tr>
<td>2 (Fig. 3b&lt;as&gt;)</td>
<td>+1</td>
<td>0 0 2 0 8 9 20 28 54</td>
</tr>
<tr>
<td></td>
<td>-1</td>
<td>0 0 2 0 8 9 20 28 54</td>
</tr>
<tr>
<td>2' (Fig. 3b&lt;as&gt;)</td>
<td>+1</td>
<td>0 0 2 0 8 8 20 32 48</td>
</tr>
<tr>
<td></td>
<td>-1</td>
<td>0 0 2 0 8 12 22 32 40</td>
</tr>
<tr>
<td>3 (Fig. 3c)</td>
<td>+1</td>
<td>0 0 3 0 8 12 16 32 40</td>
</tr>
<tr>
<td></td>
<td>-1</td>
<td>0 0 2 0 12 12 16 32 40</td>
</tr>
</tbody>
</table>

We denote the degree of the ground state degeneracy by $D_{g}$ for $\sigma s = +1$ and by $D_{g}^{-}$ for $\sigma s = -1$, and we also denote the number of excitation levels for $\sigma s = \pm 1$ by $D_{i}^{\pm}$, $i=1, 2, \cdots$, respectively.

Next let us consider the configuration shown in Fig. 3(b). If we see the spin correlation function $\langle \sigma s \rangle$ ($s'$ is denoted by $\square$), we found $\langle \sigma s \rangle$ vanishes exactly at all temperatures, that is, the frustrated configuration separates these spins completely. The excitation levels for $\sigma = s$ and $\sigma = -s$ are completely identical, $D_{i}^{s} = D_{i}^{-}$, $i=0, 1, 2, \cdots$, as shown by Type 2 in Table 1. On the other hand, if we see the spin correlation function $\langle \sigma s \rangle$, it has a finite correlation at $T \neq 0$ although it vanishes at $T=0$, as we see in Fig. 4(b). The excitation spectrum of this case is given by Type 2' in Table 1, where we can see the fact that the degeneracy of both cases is the same for the lowest level, $D_{g}^{+} = D_{g}^{-}$, but differs at higher excited levels, $D_{i}^{+} \neq D_{i}^{-}$ for some $i$. At very low temperatures only the lowest level is relevant and the spin correlation is vanishing as,

$$
\langle \sigma s \rangle \propto \exp \left( (E_{0} - E_{i}) / k_{B} T \right),
$$

where $E_{i}$ is the minimum energy for which the numbers of degeneracy for $\sigma s = \pm 1$ are different. Figure 4(b) suggests that systems with this type of structure of degeneracy may have a low temperature phase in a region of finite temperatures and may show reentrance to the paramagnetic phase at a lower temperature. For a liquid crystal system\cite{12} this kind of reentrance phenomenon has been proposed. If we use a decorated bond shown in Fig. 5, it is easy to realize a reentrance phenomenon. An effective coupling constant and critical tempera-
As will be discussed in the next section, lattices with this type of frustrated configuration have a finite transition temperature.

Finally we present one more type which is difficult to realize on small size square lattice with nearest neighbor interaction. A simple bond structure of the final type is given in Fig. 3(d) and the spin correlation function in Fig. 4(d). This final type suggests that a relative spin orientation can be changed in temperatures. We can understand this correlation as follows: At high temperatures the entropy is relevant and the indirect interactions, $\sigma - \sigma_2 - s$ and $\sigma - \sigma_3 - s$, are irrelevant and the correlation $<\sigma s>$ follows the direct interaction $\sigma - s$ while at low temperatures energetically favorable configurations become relevant. When we perform Monte Carlo simulations of bond random systems on small lattices, we are often confronted with the situation that an order parameter $<\sigma_i \sigma_j>$, where $\{\sigma_i\}$ is a ground state spin configuration, scatters very largely with temperature. If the frustrated configuration has the final type of configuration for a large scale, the local order parameters referred to a ground state $<\sigma_i \sigma_j>$, change the sign at temperatures and total order parameter $\Sigma_i <\sigma_i \sigma_j>$ seems to scatter very largely. Thus this final configuration may be one of the origins of large scattering.

§ 3. Phase transitions and degeneracy

There are many papers on phase transitions on frustrated lattices. Bryksin et al. studied regularly-frustrated lattices and presented three types; phase transitions with a finite critical temperature (on the lattice shown in Fig. 1), phase transition at $T = 0$ (on the fully-frustrated lattice) and no phase transition at all (on the checkerboard type frustrated lattice). Recently Hoever et al. have
investigated a layered frustration model extensively and presented a beautiful relation between critical temperature and layer structure. In this section we study the relation between phase transitions and types of spin correlation function discussed in §2.

First we follow the method of Bryksin et al., which is an extension of Kac and Ward's method, and obtain singular points of the free energy or zero points of the partition function (see the Appendix).

In Table II, critical temperatures of various lattices whose unit bond structures are shown in Figs. 6(a)~(d) are given. We find there two types of phase transitions, that is, $T_c \neq 0$ and $T_c = 0$. We also find the tendency that lattices constituted with the first (Fig. 3(a)) and third (Fig. 3(c)) types of configuration discussed in §2 give phase transitions with $T_c \neq 0$ and lattices with second type (Fig. 3(b)) of configurations in §2 result in $T_c = 0$. Now let us consider the

<table>
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<th>Figures</th>
<th>6(a)</th>
<th>6(b)</th>
<th>6(c)</th>
<th>6(d)</th>
<th>8(a),(b),(c)</th>
<th>9</th>
<th>10(a)</th>
<th>10(b)</th>
</tr>
</thead>
<tbody>
<tr>
<td>$k_BT_c/J$</td>
<td>2.03</td>
<td>1.93</td>
<td>0.0</td>
<td>0.0</td>
<td>1.54</td>
<td>0.0</td>
<td>0.0</td>
<td>1.25</td>
</tr>
</tbody>
</table>

Fig. 6. Frustrated bond configurations. Lattices are constructed by repeating the configurations shown.

Fig. 7. Configurations of unsatisfied bonds for the parallel and antiparallel spin arrangements are illustrated by (a) and (b), respectively in the lattice shown in Fig. 6(b). (c) and (d) are those in the lattice shown in Fig. 6(d).
The relation between degeneracy studied in § 2 and phase transition. First we discuss the ground state degeneracy.

For the bond configuration shown in Fig. 6(a), the ground state spin configuration on the finite lattice is not degenerate as we see in Fig. 3(a) in § 2. Thus the clusterization discussed in § 1 does not occur and we easily expect a finite critical temperature.

For the bond configuration shown in Fig. 6(b), the ground state spin configuration on the finite lattice is degenerate but the degrees of degeneracy for parallel and antiparallel spin configurations are different, \( D_0^+ \neq D_0^- \), as we see in Fig. 3(c) in § 2. Let us consider the degeneracy for the lattice constructed by the configuration shown in Fig. 6(b). We denote the degree of degeneracy by \( \tilde{D}_0^+ \) for parallel arrangements of clusters, e.g., Fig. 1(b), and by \( \tilde{D}_0^- \) for antiparallel arrangements, e.g., Fig. 1(c). As illustrated in Figs. 7(a) and (b), the degree of ground state degeneracy is given by the number of the way of putting unsatisfied bonds:

\[
\tilde{D}_0^+ = \sum_{0}^{2m} \frac{(2m-2k)!}{k!(2m-2k)} \left(1 + \frac{(2m-2k)(2m-2k-1)}{(2m-k)(2m-k+1)}\right) + 1 \approx 2^m \quad (3\cdot1)
\]

and

\[
\tilde{D}_0^- = 2
\]

for a \( 5 \times 2m \) lattice. The ground state spin correlation function takes the following value and approaches unity for large \( m \),

\[
\langle \sigma_s \rangle = \frac{\tilde{D}_0^+ - \tilde{D}_0^-}{\tilde{D}_0^+ + \tilde{D}_0^-} = 1 - 0(2^{-m}) \rightarrow 1. \quad (3\cdot2)
\]

Thus we again expect a finite critical temperature for this lattice. In general, for lattices constituted with configurations which have the type of spin correlation in Fig. 4(c), where \( D_0^+ \) and \( D_0^- \) are different, the situation of degeneracy is similar to the above case and we expect finite critical temperatures.

Next let us consider lattices with the type of spin correlation in Fig. 4(b), e.g., lattices with bond configurations shown in Figs. 6(c) and (d). In these bond configurations the degree of ground state degeneracy is the same, \( D_0^+ = D_0^- \) as we see in Fig. 3(b) in § 2. For lattices constituted with these configurations, the degree of ground state degeneracy for parallel and antiparallel arrangements are the same:

\[
\tilde{D}_0^+ = \tilde{D}_0^- \quad (3\cdot3)
\]

as illustrated in Figs. 7(c) and (d). Then it follows that

\[
\langle \sigma_s \rangle = 0 \quad \text{at} \quad T = 0. \quad (3\cdot4)
\]
The above argument implies that the spin correlation vanishes at the ground state and the phase transition can be suppressed for this type as we actually see in Table II.

So far we have seen that types of frustration structure which are classified in § 2 have a close connection to the existence of a phase transition through the ground state degeneracy.

Roever et al.\(^{10}\) have obtained an exact estimate of the critical temperature for a layered frustration model, where frustrated plaquettes are in lines, and they have shown that vanishing of the critical temperature is a very rare case and that almost all distributions of layers give finite critical temperatures. Actually critical temperatures of the lattices shown in Fig. 8 are identical as they have predicted, although Figs. 8(a) and (b) belong to the third type in § 2 and Fig. 8(c) belongs to the second type in § 2. Thus the correspondence between types of bond configuration and the existence of a phase transition through the degree of ground state degeneracy discussed in this section does not work in the cases of Fig. 8. In these cases the excitation levels should have an essential role even at very low temperatures. For a more precise criterion for vanishing critical temperature, we have to study degeneracy of higher excitation levels which will be done in the future. If we study, however, layered chessboard configurations shown in Fig. 9, we find \(T_c=0\) as we expect from the correspondence discussed above through the ground state degeneracy. For two-dimensional dispositions of frustrated configurations shown in Fig. 10, we also find vanishing and non-vanishing critical temperatures as we expect from the correspondence. Thus we
find many cases where our primitive correspondence works and we conclude that vanishing critical temperature is not a very rare phenomenon in frustrated lattices and clusterization due to frustration can still give a picture of the spin glasses. 3)

§ 4. Discussion and summary

In this paper we study the effects of degeneracy on the spin correlation function and phase transition. As we see in § 2, spin correlation functions behave in a very interesting way, that is, they are not necessarily monotonic function with respect to the temperature and vary in space according to frustrated configurations. This fact suggests that it is very difficult to define a uniform order parameter in randomly frustrated lattices such as models of spin glasses. For the study of spin glasses, in particular for insulator spin glasses such as those modeled by the $±J$ model, it is very important to take the non-uniformity and temperature-dependence of symmetry breaking fields into account. This non-uniformity can be taken into account by the cluster picture of spin glasses the details of which will be presented in the future. The temperature dependence of symmetry breaking field is rather difficult to investigate, but some phenomenological arguments are possible.14,15)

In § 3 we have studied the relation between ground state degeneracy and the existence of a phase transition. A general criterion for the existence of phase transition is a difficult problem because excitation levels can have important roles as suggested by Hoever et al. For more detailed description of the existence of a phase transition a qualitative difference between Figs. 8(c) and 9 must be investigated. This will be studied in the future.

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Appendix

The partition function of the Ising model on the square lattice is written in the form
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Fig. A.1. Arrows with the number \( m, m=1, 2, 3 \) and 4.

\[
Z = \text{Tr} \exp(\sum_{\langle ij \rangle} K_{ij} \sigma_i \sigma_j) = (2 \cosh K)^{2N} \text{Tr} \prod_{\langle ij \rangle} \left( \frac{1 + x_{ij} \sigma_i \sigma_j}{2} \right),
\]

where \( N \) is the number of sites, \( x_{ij} = \tanh K_{ij} \) and \( \langle ij \rangle \) denote all bonds. As is well known, we can obtain \( \text{Tr} \prod_{\langle ij \rangle} (1 + x_{ij} \sigma_i \sigma_j) \) by using the transition probability of a weighted random walk from point \( r \) to \( r' \):

\[
\Lambda(r, m | r', m') = x_{rr} \omega(m | m'),
\]

where \( m \) and \( m' \) denote the directions shown in Fig. A-1.\(^\text{13} \) We use the weight \( \omega \), following a previous work,\(^\text{9} \) as

\[
\{ \omega(m | m') \} = \begin{pmatrix}
1 & 1 & 0 & 1 \\
1 & 1 & 1 & 0 \\
0 & 1 & 1 & -1 \\
1 & 0 & -1 & 1
\end{pmatrix}.
\]

If frustrations are disposed regularly, we can use the Fourier transformation over unit cells and reduce the matrix \( \Lambda \) to a finite matrix \( \Lambda_p \).

\[
\Lambda_p = \sum_{\mathbf{R}} e^{-i \mathbf{R} \cdot \mathbf{p}} \Lambda,
\]

where \( \mathbf{R} \) is the position of a unit cell and \( \mathbf{r} = \mathbf{R} + \delta_i \) and \( \delta_i \) denotes the position in a unit cell. Using this \( \Lambda_p \) the free energy can be written

\[
\frac{F}{kTN} = (-\ln 2 + \ln \cosh^2 K) - \frac{1}{2N} \sum_{\mathbf{p}} \ln \det(1 - \Lambda_p).
\]

Thus the zeros of \( \det(1 - \Lambda_p) \) give the singularity of the free energy corresponding to an instability of a spin density wave with \( \mathbf{p} \). In general, \( \det(1 - \Lambda_p) \) takes the following form with an integer \( k \)

\[
\det(1 - \Lambda_p) = (\cosh K)^k f(\mathbf{p}, K).
\]

In this paper we construct \( 1 - \Lambda_p \) and estimate the determinant numerically. The
lattices in this paper are ferromagnetic bond dominant, so that we expect that the instability should occur for \( p = 0 \). In order to exclude a trivial zero at \( x = 1 \) due to \((\cosh K)^4\) we calculate \( f((0, 0), K)/f((\pi, \pi), K)\). In Tables \( T_c = 0 \) means \( f(k, \infty) = 0 \) and 'None' means \( f(k, K) \neq 0 \) for all \( K \) including \( K = \infty \). In this paper we do not have the case 'None'.

References