A new method to calculate the spin-glass order parameter of the two-dimensional $\pm J$ Ising model

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Abstract. A new method to numerically calculate the $n$th moment of the spin overlap of the two-dimensional $\pm J$ Ising model is developed using the identity derived by one of the authors (HK) several years ago. By using the method, the $n$th moment of the spin overlap can be calculated as a simple average of the $n$th moment of the total spins with a modified bond probability distribution. The values of the Binder parameter etc have been extensively calculated with the linear size, $L$, up to $L = 23$. The accuracy of the calculations in the present method is similar to that in the conventional transfer matrix method with about $10^5$ bond samples. The simple scaling plots of the Binder parameter and the spin-glass susceptibility indicate the existence of a finite-temperature spin-glass phase transition. We find, however, that the estimation of $T_c$ is strongly affected by the corrections to scaling within the present data ($L \leq 23$). Thus, there still remains the possibility that $T_c = 0$, contrary to the recent results which suggest the existence of a finite-temperature spin-glass phase transition.

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1. Introduction

Over the last two decades, investigations of spin-glass problems have been extensively performed[1-20]. It is now widely believed that the three-dimensional $\pm J$ Ising model shows a finite-temperature spin-glass phase transition [1-6], while the critical temperature of the two-dimensional $\pm J$ Ising model is zero [5-11]. Most of these studies have been done using Monte Carlo simulations, where the thermal relaxation time in the simulations becomes very large in the low-temperature region. This makes the investigations of the two-dimensional models rather difficult, since the calculations of the physical quantities have to be performed at very low temperature. In previous studies, the data in the finite-size scaling analysis were in good agreement with a scaling function with the critical temperature, $T_c = 0$. The results, however, have not completely excluded the possibility of a finite-temperature spin-glass phase transition. Recently, Shirakura et al[12-15] have deduced the existence of a finite-temperature spin-glass phase transition of the two-dimensional models using extensive Monte Carlo simulations. To clarify the critical properties of the two-dimensional $\pm J$ Ising model, more precise results in the low-temperature region are necessary.

The transfer matrix method is free from the problem of thermal equilibration, and has been very successfully used to determine the ferromagnetic-nonferromagnetic

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phase boundary of the two-dimensional $\pm J$ Ising model in the $p - T$ plane \cite{16, 17} ($p$ is the concentration of the ferromagnetic bond). But, for the problem of the spin-glass phase transition, the transfer matrix method has only been used for the calculations of defect energies and correlation functions \cite{3, 10}, and has not been widely used for direct calculations of the $n$th moment of the spin overlap (the spin-glass susceptibility, the Binder parameter, etc) since, when we use real replicas in the calculations, the maximum linear size applicable is one-half of that in the calculations of the $n$th moment of the total spins. Thus, so far, no extensive result for the spin-glass phase transition with direct calculation of the spin-glass susceptibility etc has been given by the transfer matrix method.

In this paper, we present a new method to numerically calculate the $n$th moment of the spin overlap of the two-dimensional $\pm J$ Ising model, using the identity derived by one of the present authors several years ago \cite{19}. In this identity, the $n$th moment of the spin overlap is transformed as a simple average of the $n$th moment of the total spins with a modified bond probability distribution. Following a newly developed process, explained in section 2, we successively make the bond configurations according to the modified bond probability distribution using the Monte Carlo technique. In each bond configuration, we calculate the $n$th moment of the total spins by the transfer matrix method.

We have performed extensive calculations of the $n$th moment of the spin overlap up to the linear size, $L = 23$. The accuracy of the calculations in the present method is similar to that in the conventional transfer matrix method with about $10^5$ bond samples. Thus, the statistical errors in the present study are about an order of magnitude smaller than those in previous studies. Therefore, we can analyse the obtained data in detail using finite-size scaling analysis including the corrections to scaling. Our results show that the estimation of $T_c$ is strongly affected by the corrections to scaling in the two-dimensional $\pm J$ Ising model. Thus, there still remains the possibility that $T_c = 0$, contrary to the recent results by Shirakura et al \cite{12, 13, 15} which suggest the existence of a finite-temperature spin-glass phase transition.

2. New calculation method for the spin-glass order parameter

We consider the two-dimensional $\pm J$ Ising model on an $L \times L$ square lattice with only nearest neighbour interactions. The Hamiltonian is written as follows:

$$\mathcal{H} = - \sum_{(ij)} \tau_{ij} S_i S_j,$$

where $S_i = \pm 1$, and the summation of $(ij)$ runs over all the nearest neighbours. We take the skew boundary condition in one direction, and the free boundary condition in the other direction. Each $\tau_{ij}$ is determined according to the following probability distribution:

$$P(\tau_{ij}) = p\delta(\tau_{ij} - 1) + (1 - p)\delta(\tau_{ij} + 1).$$

In this paper, we make $J = 1$. We define the spin overlap, $Q$, between two replicas in each bond configuration as

$$Q = \sum_{i=1}^{N} S_i^\alpha S_i^\beta,$$
where $\alpha$ and $\beta$ denote the two replicas, and $N$ is the total number of spins. When we define $K_p$ as

$$\exp(2K_p) = \frac{p}{1-p},$$

the 2nd moment of the spin overlap is written as

$$< Q^{2n} >_{T,\{\alpha,\beta\}} = \frac{1}{(2\cosh(K_p))^N} \sum_{\tau_{ij}=\pm 1} \exp(K_p \sum_{(ij)} \tau_{ij}) < M^{2n} >_{\tau,\{\alpha,\beta\}},$$

where $< \cdots >_{T,\{\alpha,\beta\}}$ denotes the thermal average both for the $\alpha$- and $\beta$-spins in a bond configuration, $\{\tau\}$ at temperature, $T$. $\cdots_p$ denotes the configurational average at the ferromagnetic bond concentration, $p$, and $N_B$ is the number of bonds. By the use of a local gauge transformation, an identity has been derived:

$$< Q^{2n} >_{T,\{\alpha,\beta\}} = \frac{1}{(2\cosh(K_p))^N} \sum_{\tau_{ij}=\pm 1} \exp(K_p \sum_{(ij)} \tau_{ij}) \frac{Z(K_p,\{\tau\})}{Z(K,\{\tau\})} < M^{2n} >_{T,\{S\}},$$

where $M$ denotes the total spins,

$$M = \sum_{i=1}^{n} S_i,$$

$< \cdots >_{T,\{S\}}$ denotes the thermal average for the $S$-spins at temperature, $T$, and $Z(K,\{\tau\})$ is the partition function at the inverse temperature, $K(=1/T)$, with the bond configuration, $\{\tau\}$. We show the summary of the derivation of equation (6) in the appendix. (For the details of the derivation, see [19].) When we define the modified probability distribution, $P_2(K, K_p, \{\tau\})$, for the bond configuration, $\{\tau\}$, as

$$P_2(K, K_p, \{\tau\}) = \frac{1}{(2\cosh(K_p))^N} \exp(K_p \sum_{(ij)} \tau_{ij}) \frac{Z(K_p,\{\tau\})}{Z(K,\{\tau\})},$$

we can then write

$$< Q^{2n} >_{T,\{\alpha,\beta\}} = < M^{2n} >_{T,\{S\}}_{K,K_p},$$

where $\{\cdot\}_{K,K_p}$ denotes the configurational average by the modified bond probability distribution. That is, $< Q^{2n} >_{T,\{\alpha,\beta\}}$ at temperature, $T$, with the ferromagnetic bond concentration, $p$, is transformed into the configurational average of $< M^{2n} >_{T,\{S\}}$ by the modified bond probability distribution, $P_2(K, K_p, \{\tau\})$. Similarly, we can get the following identity [19]:

$$< M^{2n} >_{T,\{S\}}_p = < M^{2n} >_{T_p,\{S\}}_{K,K_p},$$

where $T_p = 1/K_p$. (Note that the above argument applies to any dimension.)

Hereafter, we explain a new approach to numerically calculate the values of $< Q^{2n} >_{T,\{\alpha,\beta\}}_p$, using equation (9). To realize the bond configuration with the modified bond probability distribution, $P_2(K, K_p, \{\tau\})$, we use the conventional Monte Carlo technique. We define $W(\tau_{ij} \rightarrow -\tau_{ij}, \{\tau\}')$ as the transition probability by which the value of the bond, $\tau_{ij}$, changes. To guarantee that the stationary probability distribution becomes $P_2(K, K_p, \{\tau\})$, the following detailed balance must be satisfied:

$$P_2(K, K_p, \tau_{ij}, \{\tau\}') W(\tau_{ij} \rightarrow -\tau_{ij}, \{\tau\}') = P_2(K, K_p, -\tau_{ij}, \{\tau\}') W(-\tau_{ij} \rightarrow \tau_{ij}, \{\tau\}')$$

(11)
Using equation (8), we obtain

\[
W(\tau_{ij} \rightarrow -\tau_{ij}, \{\tau\}') = \exp(-2K\tau_{ij}) \frac{\cosh(2K_p) - \sinh(2K_p) < S_iS_j >_{T,\{s\}}}{\cosh(2K) - \sinh(2K) < S_iS_j >_{T,\{S\}}} \tag{12}
\]

Namely, when we can calculate \( < S_iS_j >_{T,\{S\}} \) in a particular bond configuration, we can estimate the transition probability.

The processes to calculate \( [< Q^{2n} >_{T,\{S_0,S_3\}}]_p \) are as follows:

1) We start from an arbitrary bond configuration.
2) Using the transfer matrix method, we exactly calculate the value of \( < S_iS_j >_{T,\{S\}} \), and successively flip the bond, \( \tau_{ij} \), according to the transition probability, \( W(\tau_{ij} \rightarrow -\tau_{ij}, \{\tau\}') \), using the conventional Monte Carlo technique.
3) We continue process 2) until the modified bond probability distribution, \( P_2(K, K_p, \{\tau\}) \) is realized.
4) We calculate the value of \( < M^{2n} >_{T,\{S\}} \) for each bond configuration using the transfer matrix method.
5) We repeat processes 2) and 4).
6) Finally, the simple average of \( < M^{2n} >_{T,\{S\}} \) gives the value of \( [< Q^{2n} >_{T,\{S_0,S_3\}}]_p \) with the bond probability distribution, \( P(\tau_{ij}) \).

We now show the efficiency of this method. We define \( n_a, n_b \) and \( n_c \) as the number of initial Monte Carlo skip steps, the number of Monte Carlo steps where we calculate \( < M^{2n} >_{T,\{S\}} \), and the number of independent Monte Carlo runs, respectively. In all the calculations, we have evaluated \( \{\tau_{ij}(0)\tau_{ij}(t)\}_{K,K_p} \) using the statistical dependence time method [22], and find that the relaxation time of \( \{\tau_{ij}(0)\tau_{ij}(t)\}_{K,K_p} \) is always very small even when compared with one Monte Carlo step time. That is, only several tens of initial skip steps are enough to realize the stationary bond probability distribution. For example, we have compared the values of the spin-glass susceptibility \( \chi_{SG} = [< Q^2 >_{T,\{S_0,S_3\}}]_p / N \) calculated by the present method and that by the conventional transfer matrix method using real replicas. Table 1 shows the results at \( T = 0.1 \) for \( L = 7 \). The calculations by the conventional transfer matrix method have been done with \( 10^5 \) independent bond configurations. The error bars of the present methods have been estimated in the same way as those of conventional Monte Carlo simulations. From table 1, we can see that all the data are consistent within the error bars, and the size of the error bars of all the calculations are of the same magnitude. Consequently, we find that only 20 steps are enough for the initial Monte Carlo skip steps. Furthermore, we have examined whether equation (9) holds or not at \( p = 0.5 - 0.95, T = 0.1 - 0.5 \) for \( L = 7 \). We have also examined whether equation (10) holds or not at \( p = 0.8 - 0.9, T = 0.1 - 0.4 \) for \( L = 15 \). All the results are consistent in a statistical sense, from which we conclude that the present method is usable and not affected by systematic errors.

3. The spin-glass phase transition of the two-dimensional \( \pm J \) Ising model

We have extensively investigated the two-dimensional \( \pm J \) Ising model for \( p = 0.5 \). The results of the asymmetric case (\( p > 0.5 \)) will be given in a subsequent paper [20]. For \( p = 0.5 \), we have calculated \( [< Q^{2n} >_{T,\{S_0,S_3\}}]_p \) at \( T = 0.1 - 0.5 \) with the linear size \( L = 7 - 23 \). The calculations have been performed with \( (n_a, n_b, n_c) = (200, 1000, 100) \) for \( L \leq 21 \) and \( (200, 200, 480) \) for \( L = 23 \).
Table 1. The values of $\chi_{SG}$ with various $(n_a, n_b, n_c)$ at $T = 0.1$ for $L = 7$. The value of $\ast$ is calculated by the conventional transfer matrix method using real replicas with $10^5$ bond samples.

| $(n_a, n_b, n_c)$ | $\chi_{SG}$ |
|------------------|-------------|
| (2000,10000,10)  | 29.076(24)  |
| (200,1000,100)   | 29.084(38)  |
| (20,100,1000)    | 29.094(35)  |
| (20,20,5000)     | 29.045(34)  |
| $\ast$           | 29.037(35)  |

The energy gap between the ground state and the first excitation state is two in the unit of the interaction strength. Thus, in finite systems, any physical quantity at a very low temperature must saturate to its value at $T = 0$. We show the temperature dependence of the spin-glass susceptibility, $\chi_{SG}$, in figure 1. We find, indeed, that the values of $\chi_{SG}$ for each $L$ show the strong saturation near $T = 0$, and the tendency becomes clearer as the system size becomes smaller, as has already been pointed out by several authors [8, 12, 14]. The Binder parameter [21]

$$g_L = \frac{1}{2} \left( 3 - \frac{\langle Q^4 \rangle_{T, \{S^\alpha, S^\beta\}}}{\langle Q^2 \rangle_{T, \{S^\alpha, S^\beta\}}^2} \right)$$  (13)

is widely used for the determination of the critical temperature. The value of the Binder parameter becomes asymptotically size independent for large systems at the critical temperature. Therefore, the point where this quantity becomes asymptotically size independent gives an estimation of the critical point. The simple plot of the Binder parameter versus temperature is shown in figure 2. We can clearly see that the data for different sizes intersect at almost the same temperature, $T = 0.3$, and the size dependence of the intersection points is very small. We cannot, however, immediately conclude that the spin-glass phase transition occurs at $T \approx 0.3$, since the intersection might be due to the strong saturation of the data near $T = 0$ [8, 12, 14]. Therefore, we perform scaling analyses for $g_L$ and $\chi_{SG}$. There is no general rule to avoid the disturbance from the saturation mentioned above in the scaling analyses. Here, we adopt a criterion that every data point is not used all through the scaling analyses, when the value of $\chi_{SG}$ increases less than 3% in the temperature interval, $\Delta T = 0.05$. Although the criterion, which we have determined from the observation in figure 1, seems rather artificial, we believe that this criterion systematically removes the saturation to $T = 0$ in a certain sense. Consequently, we use, for example, the data with $T \geq 0.35$ for $L = 7$, and with $T \geq 0.2$ for $L = 23$.

First, we perform the scaling analyses without including the corrections to scaling. In this case, the Binder parameter, $g_L$, has the scaling form

$$g_L = \bar{g}(L^{1/\nu}(T - T_c))$$  (14)

and that of the spin-glass susceptibility, $\chi_{SG}$, is

$$\chi_{SG} = L^{2-\eta\tilde{\chi}}(L^{1/\nu}(T - T_c))$$  (15)

where $\nu$ is the critical exponent of the spin-glass correlation length, and $\eta$ is the critical exponent which describes the decay of the correlation at the critical temperature. Figure 3 shows the best-fit scaling plot of the Binder parameter, which indicates that
$T_C \simeq 0.3$ and the critical exponent $\nu \simeq 1.3$. We can see that the data at $T < T_c = 0.3$ and $T \geq T_c$ fit rather well on one scaling function, which indicates that the spin-glass phase transition of the two-dimensional $\pm J$ Ising model is a conventional phase transition, and there exists a finite long range order at $T < T_c$. The best-fit scaling plot of the spin-glass susceptibility is also shown in figure 4, which indicates that the critical exponent $\eta \simeq 0.225$. The estimated values of $T_c$ and the critical exponents are similar to those determined by Shirakura et al.\cite{12}. Figures 5 and 6 show the scaling plots of the Binder parameter and the spin-glass susceptibility, assuming $T_c = 0$, $\nu = 2.6$ and $\eta = 0.2 \pm 0.05$, where we clearly see the systematic deviations. Namely, the scaling plots without including the corrections to scaling strongly indicate the existence of a finite-temperature spin-glass phase transition.

Next, we perform the scaling analyses including the corrections to scaling. We take the scaling forms of the Binder parameter and the spin-glass susceptibility as

$$g_L = \bar{g}(L^{1/\nu}(T - T_c))(1 + \frac{a}{L^\omega}),$$

and

$$\chi_{SG} = L^{2-\eta}\bar{\chi}(L^{1/\nu}(T - T_c))(1 + \frac{b}{L^\omega}).$$

There is little quantitative change in figures 3 and 4, even though we fit the data using equations (16) and (17). Thus, when we assume $T_c = 0.3$, the effect of the corrections to scaling is rather small. On the other hand, assuming that $T_c = 0$, $\nu = 2.6$ and $\eta = 0.17 \pm 0.05$, the data of the Binder parameter and the spin-glass susceptibility fit very well on one scaling function, respectively, as shown in figures 7 and 8 with $\omega = \omega' = 0.5$ and $a = b = -0.3$, although the data with a small linear size, $L = 7$, deviate from the scaling function. (To fit the data, we use $\eta = 0.17$, which is, for example, consistent with the result in \cite{8}, $\eta = 0.2 \pm 0.05$.) Thus, including the corrections to scaling, both $T_c = 0$ and $T_c \approx 0.3$ are consistent with the scaling analyses. Furthermore, we find that every temperature for $0 \leq T \leq 0.3$ might become the critical temperature, $T_c$, in this scaling form. Consequently, we find that the estimation of the value of $T_c$ is strongly affected by the corrections to scaling in the two-dimensional $\pm J$ Ising model within the present data ($L \leq 23$).

4. Conclusions

We have developed a new method to numerically calculate $\langle Q^{2n} \rangle_{T,\{S^x, S^z\}}^p$ of the two-dimensional $\pm J$ Ising model, where, using a local gauge transformation, $\langle Q^{2n} \rangle_{T,\{S^x, S^z\}}^p$ can be calculated as a simple average of $\langle M^{2n} \rangle_{T,\{S\}}$ with a modified bond probability distribution. By using the present method, we have extensively calculated the values of $\langle Q^{2n} \rangle_{T,\{S^x, S^z\}}^p$, where the statistical errors become about an order of magnitude smaller than in previous studies, and we have investigated the scaling analyses including the corrections to scaling. By using the scaling analyses without including the corrections to scaling, our data strongly indicate a finite-temperature spin-glass phase transition. We find, however, that the estimation of $T_c$ is strongly affected by the corrections to scaling within the data with $L \leq 23$, and that every temperature for $0 \leq T \leq 0.3$ might be able to become the critical temperature. Consequently, our results indicate that there still remains the possibility that $T_c = 0$, contrary to the recent results of Shirakura et al.\cite{12, 13, 15} which suggest the existence of a finite-temperature spin-glass phase transition.
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Appendix A.

In this appendix, we briefly explain the derivation of equation (6). We show that both sides of equation (6) coincide with each other.

Using equation (5), \[< Q^{2n} >_{T_1 (S^a, S^b)} \] is written as

\[< Q^{2n} >_{T_1 (S^a, S^b)} = \frac{1}{C} \sum_{\tau_{ij} = \pm 1} \exp(K_p \sum_{(ij)} \tau_{ij}) \] \[\times \left( \sum_{i=1}^N S^a_i S^b_i \right)^{2n} >_{T_1 (S^a, S^b)} \] \tag{A1}

and we abbreviate \((2 \cosh(K_p))^N\) as \(C\) from now on.

Here, we perform the following local gauge transformation:

\[\tau_{ij} \rightarrow \tau_{ij} \sigma_i \sigma_j, \quad S^a_i \rightarrow S^a_i \sigma_i, \quad S^b_i \rightarrow S^b_i \sigma_i, \quad (\sigma_i = \pm 1) \] \tag{A2}

where each \(\sigma_i\) arbitrarily takes +1 or -1. Since \(\left( \sum_{i=1}^N S^a_i S^b_i \right)^{2n} >_{T_1 (S^a, S^b)} \) is invariant under this transformation, we obtain

\[< Q^{2n} >_{T_1 (S^a, S^b)} = \frac{1}{C} \sum_{\tau_{ij} = \pm 1} \exp(K_p \sum_{(ij)} \tau_{ij} \sigma_i \sigma_j) \times \left( \sum_{i=1}^N S^a_i S^b_i \right)^{2n} >_{T_1 (S^a, S^b)} \] \tag{A3}

where we note that the summation over \(\tau_{ij} \sigma_i \sigma_j = \pm 1\) is equivalent to that over \(\tau_{ij} = \pm 1\). As each \(\sigma_i\) arbitrarily takes +1 or -1, therefore, we take all the summations of \(\sigma_i\) and divide by 2\(N\), namely

\[< Q^{2n} >_{T_1 (S^a, S^b)} = \frac{1}{C} \sum_{\tau_{ij} = \pm 1} \frac{Z(K_p, \{\tau\})}{2^N} \times \left( \sum_{i=1}^N S^a_i S^b_i \right)^{2n} >_{T_1 (S^a, S^b)} \] \tag{A4}

Next, we consider the r.h.s. (we denote it as \(A\)) of equation (6). The r.h.s. of equation (6) is written as

\[A = \frac{1}{C} \sum_{\tau_{ij} = \pm 1} \exp(K \sum_{(ij)} \tau_{ij}) \frac{Z(K_p, \{\tau\})}{Z(K, \{\tau\})} \times \left( \sum_{i=1}^N S_i \right)^{2n} >_{T_1 (S)} \] \tag{A5}

Here, we perform the same local gauge transformation. Then, we obtain

\[A = \frac{1}{C} \sum_{\tau_{ij} = \pm 1} \exp(K \sum_{(ij)} \tau_{ij} \sigma_i \sigma_j) \frac{Z(K_p, \{\tau\})}{Z(K, \{\tau\})} \times \left( \sum_{i=1}^N S_i \sigma_i \right)^{2n} >_{T_1 (S)} \]
Thus, from equations (A4) and (A6), we conclude that both sides of equation (6) coincide with each other.

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Figure 1. A plot of $\chi_{SG}$ versus $T$.

Figure 2. A plot of $g_L$ versus $T$.

Figure 3. A scaling plot for $g_L$.

Figure 4. A scaling plot for $\chi_{SG}$.

Figure 5. A scaling plot for $g_L$, assuming $T_c = 0$. 
Figure 6. A scaling plot for $\chi_{SG}$, assuming $T_c = 0$.

Figure 7. A scaling plot for $g_L$ including the corrections to scaling with $\omega' = 0.5$ and $a = -0.3$, assuming $T_c = 0$.

Figure 8. A scaling plot for $\chi_{SG}$ including the corrections to scaling with $\omega' = 0.5$ and $b = -0.3$, assuming $T_c = 0$. 

$T_c = 0$
$\nu = 2.6$
$\eta = 0.2$

$\eta = 0.17$

$(T - T_c)^L_{1/\nu}$

$(T - T_c)^L_{1/\nu}$