

## Replica-symmetry-breaking transition in finite-size simulations

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Finite-size effects in the mean-field Ising spin glass and the mean-field three-state Potts glass are investigated by Monte Carlo simulations. In the thermodynamic limit, each model is known to exhibit a continuous phase transition into the ordered state with a full and a one-step replica-symmetry breaking (RSB), respectively. In the Ising case, the Binder parameter  $g$  calculated for various finite sizes remains positive at any temperature and crosses at the transition point, while in the Potts case  $g$  develops a negative dip without showing a crossing in the  $g > 0$  region. By contrast, non-self-averaging parameters always remain positive and show a clear crossing at the transition temperature in both cases. Our finding suggests that care should be taken in interpreting the numerical data of the Binder parameter, particularly when the system exhibits a one-step-like RSB.

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### I. INTRODUCTION

The concept of replica-symmetry breaking (RSB) [1] gives us new insight into the character of the ordered state of complex systems such as spin glasses (SGs) [2] and real structural glasses [3]. Systems exhibiting RSB can roughly be divided into two categories depending on their breaking patterns: One is a full or hierarchical RSB and the other is a one-step RSB. In both cases, there are many different equilibrium states unrelated by the global symmetry of the Hamiltonian, and an overlap between these states plays an important role in describing the ordered state.

In the case of one-step RSB [1], the overlap  $q$  takes only two values in the thermodynamic limit, namely, either a self-overlap equal to the Edwards-Anderson order parameter,  $q = q_{EA}$ , or a non-self-overlap usually equal to zero,  $q = 0$ . The overlap distribution function  $P(q)$  consists of two distinct  $\delta$ -function peaks, one at  $q = q_{EA}$  and the other at  $q = 0$ . One-step RSB transitions could be either continuous or first order, either with or without a finite discontinuity in  $q_{EA}$  at the transition. Examples of the first-order one-step RSB transition may be the mean-field  $p$ -spin glass with  $p > 2$ , the random energy model, and the mean-field  $p$ -state Potts glass with  $p > 4$ , while those of the continuous one-step RSB transition may be the mean-field  $p$ -state Potts glass with  $2.8 < p \leq 4$ .

In the case of the full RSB, by contrast, possible values of the overlap are distributed continuously in a certain range, and the states are organized in a hierarchical manner. The overlap distribution function has a continuous plateau at  $q < q_{EA}$  in addition to the  $\delta$ -function peak at  $q = q_{EA}$ . A well-known example of this category is the standard mean-field Ising SG, namely, the Sherrington-Kirkpatrick (SK) model. In some special cases, the admixture of the above two, where the overlap distribution function has a continuous plateau together with the  $\delta$ -function peak at  $q = 0$  (and the one at  $q = q_{EA}$ ), is also possible. An example of this may be the mean-field  $p$ -state Potts glass with  $2 < p < 2.8$ .

Recent interest in SG studies has been focused largely on the validity of applying the RSB idea established in some

mean-field models to more realistic short-range SG models. In almost all such studies, the three-dimensional (3D) Ising SGs model has been employed. Indeed, some researchers have claimed that the full or hierarchical RSB as observed in the SK model [4] is also realized in realistic 3D SGs [5], while other researchers have claimed, based on an alternative droplet picture [6], that the ordered state of realistic 3D SGs is unique up to global symmetry of the Hamiltonian, without showing RSB of any kind [7,8]. Thus, intensive debate has continued between these two scenarios as to the true nature of the SG ordered state of 3D short-range systems.

Meanwhile, the one-step RSB has been discussed mainly with interest in its close connection to structural glasses rather than SG magnets [9,10]. Recently, however, one-step RSB features have been found unexpectedly by the present authors in the chiral-glass state of a 3D Heisenberg SGs [11]. According to the chirality mechanism of experimental SG transitions based on the spin-chirality decoupling-recoupling scenario [12], the SG ordered state and the SG phase transition of real Heisenberg-like SG magnets possessing weak but nonzero magnetic anisotropy are governed by the chirality ordering of the fully isotropic system which is "revealed" by the weak magnetic anisotropy, *not by the spin ordering* which has been "separated" in the fully isotropic case from the chirality ordering. Then, the observation of Ref. [11] means that the SG ordered state of most of real SG magnets should also exhibit such one-step RSB-like features. Note that such a picture of the SG ordered state contrasts with the standard pictures discussed so far, either the droplet picture without RSB or the SK picture with full RSB.

Under such circumstances, further studies of the nature of the possible RSB in 3D short-range SG models are clearly required. Since we are usually forced to employ numerical simulations to investigate 3D short-range models and since numerical simulations are often hampered by severe finite-size effects, we feel it worthwhile to further clarify by numerical simulations the finite-size effects in some *mean-field models* which are exactly known to exhibit RSB transitions in the thermodynamic limit. In particular, the question as to how the one-step and full RSB transitions look like in finite-

size simulations is of both fundamental and practical interest. Such information would be of much help as a reference in interpreting the numerical data obtained for finite-dimensional short-range SG models.

In the present paper, we choose two mean-field SG models exactly known to exhibit a *continuous* (second-order) phase transition in the thermodynamic limit: One is the SK model which shows full RSB, and the other is the mean-field three-state ( $p=3$ ) Potts-glass model which shows one-step RSB. We calculate by Monte Carlo simulations several quantities which have widely been used in identifying the phase transition, including the spin-glass order parameter and the Binder parameter, together with quantities recently introduced to represent the non-self-averaging character of the ordered state. By carefully examining the size dependence of these quantities, a comparison is made between the two types of RSB. Our results have revealed that the Binder parameter of the one-step RSB system shows a behavior very different from the standard behavior, giving warning about the interpretation of the numerical data for relevant short-range systems.

## II. MODELS

The mean-field  $p$ -state Potts-glass model is defined by the Hamiltonian,

$$\mathcal{H} = -p \sum_{i < j}^N J_{ij} \delta_{n_i, n_j}, \quad (1)$$

where  $n_i$  denotes a Potts-spin variable at the  $i$ th site which takes  $p$  distinct states, and  $N$  is the total number of Potts spins. The exchange interaction  $J_{ij}$  is an independent random Gaussian variable with zero mean and variance  $J^2/N$ . The model with  $p=2$  is equivalent to the SK model. In the present study, we focus our attention on the standard SK model corresponding to  $p=2$  and the three-state Potts-glass model corresponding to  $p=3$ . Although the thermodynamic properties of an infinite system have been rather well understood by the calculation based on a replica technique [1,4,13,14], its finite-size properties have been much less understood.

It is convenient to use an equivalent simplex spin representation where the Potts spin  $n_i$  is written in terms of a  $(p-1)$ -dimensional unit vector  $\vec{S}_i$ , which satisfies  $\vec{S}_i \cdot \vec{S}_j = (p \delta_{n_i n_j} - 1)/(p-1)$ ,

$$\mathcal{H} = -(p-1) \sum_{i < j}^N J_{ij} \vec{S}_i \cdot \vec{S}_j. \quad (2)$$

In the particular case of  $p=2$ ,  $\vec{S}_i$  simply reduces to the one-component Ising variable  $S_i = \pm 1$ , and the Hamiltonian (2) is equivalent to the standard SK Hamiltonian.

In terms of the simplex spin  $S_i^\mu$  ( $1 \leq \mu \leq p-1$ ), the parameter  $q$  may be defined by

$$q = \sqrt{\sum_{\mu, \nu}^{p-1} (q^{\mu\nu})^2}, \quad (3)$$

where  $q^{\mu\nu}$  denotes an overlap tensor between two replicas 1 and 2:

$$q^{\mu\nu} = \frac{1}{N} \sum_{i=1}^N S_{i,1}^\mu S_{i,2}^\nu. \quad (4)$$

The Binder parameter is then given by

$$g(T, N) = \frac{(p-1)^2}{2} \left( 1 + \frac{2}{(p-1)^2} - \frac{[\langle q^4 \rangle]}{[\langle q^2 \rangle]^2} \right), \quad (5)$$

where  $\langle \dots \rangle$  denotes the thermal average and  $[\dots]$  denotes the average over the quenched randomness  $\{J_{ij}\}$ . The Binder parameter is normalized so as to vanish above the transition temperature  $T_g$  in the thermodynamic limit. Recall that at  $T > T_g$  each component  $q_{\mu\nu}$  should behave as an independent Gaussian variable. Below  $T_g$ ,  $g$  is normalized to give unity in the thermodynamic limit for the nondegenerate ordered state where  $P(q)$  has only trivial peak at  $q = q_{EA}$ . Of course, this is not the case for SG models showing RSB including the present mean-field SG models, for which  $g$  takes nontrivial values different from unity even in the thermodynamic limit. Hence, at least in the case where a continuous phase transition occurs into the trivial ordered state,  $g$  for various finite sizes is expected to cross at  $T = T_g$ . Indeed, this aspect has widely been used for locating the transition temperature from the numerical data for finite systems.

## III. MONTE CARLO RESULTS

We perform Monte Carlo (MC) simulations based on a version of the extended ensemble method, called the exchange method [15]. As in other SG models, an extremely slow relaxation becomes a serious problem of MC simulations in the present mean-field SG models. Such difficulty could partly be overcome by using the exchange method, which has turned out to be quite efficient in thermalizing various hardly relaxing systems. The method enables us to study larger sizes and/or lower temperatures than those attained previously. Our MC simulations have been performed up to  $N=512$  at  $T/J=0.25$  for the SK model and  $N=256$  at  $T/J=0.4$  for the mean-field  $p=3$  Potts-glass model, where  $T_g/J=1$  in both models. Sample averages are taken over 200–1792 independent bond realizations depending on the size  $N$ . We note that the minimum temperature studied here are considerably lower than the previous ones: e.g.,  $N=512$  at  $T/J=0.75$  [16] for the SK model and  $N=120$  at  $T/J=0.98$  for the mean-field  $p=3$  Potts-glass model [17].

The temperature and size dependence of the calculated Binder parameter  $g$  is shown in Figs. 1 and 2 for the SK and the  $p=3$  Potts-glass models, respectively. As is evident from these figures, the Binder parameters of the two mean-field models show considerably different behaviors from each other.

In the SK model, as shown in Fig. 1, a clear crossing of  $g$  is observed at  $T = T_g$ , which looks similar to the ones seen in the standard continuous transitions. In fact, the behavior of  $g$  found here also resembles the ones observed in the short-range Ising SG models in 3D [18,19] and in 4D [20], though the crossing tendency is less pronounced in 3D than in 4D. As mentioned,  $g$  of the SK model takes a nontrivial value

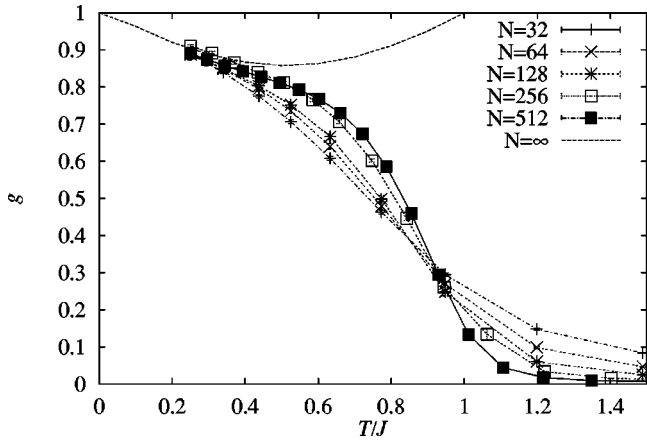


FIG. 1. Temperature and size dependence of the Binder parameter of the SK model. The bulk transition temperature is located at  $T/J=1$ . The dashed line represents the RSB solution derived by solving the Parisi equation.

below  $T_g$  even in the thermodynamic limit due to its RSB. We show in Fig. 1 the behavior of  $g(T, \infty)$  evaluated in the replica formalism by numerically solving the Parisi equation [Ref. 1(a)]. Note that, as the temperature approaches  $T_g$  from below, the limiting value  $g(T_g^-, \infty)$  goes to unity as in the case of ordinary continuous phase transitions. Hence, with increasing  $N$ ,  $g(T_g^-, N)$  just below  $T_g$  is expected to approach unity *from below* while  $g(T_g^+, N)$  just above  $T_g$  approaches zero *from above*, which entails a crossing of  $g$  at  $T=T_g$ . With lowering the temperature,  $g(T, \infty)$  first decreases, reaching a minimum around  $T/J=0.5$ , and increases again tending to unity at  $T=0$ . Here note that, for any model with a nondegenerate ground state,  $P(q)$  becomes trivial at  $T=0$  irrespective of the occurrence of RSB, and  $g$  tends to unity. As can be seen in Fig. 1, the present MC results for finite  $N$  gradually approach the  $g(T, \infty)$  curve of an infinite system.

In the mean-field  $p=3$  Potts glass, as shown in Fig. 2, no crossing of  $g$  is observed at  $T=T_g$  [21], at least of the type as observed in the SK model. Instead, unlike the case of the SK model, a shallow *negative* dip develops above  $T_g$  for larger  $N$  which becomes deeper as the system gets larger. Although

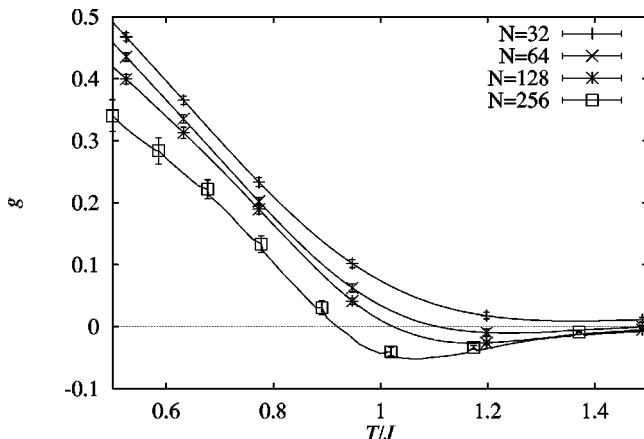


FIG. 2. Temperature and size dependence of the Binder parameter of the mean-field  $p=3$  Potts glass. The bulk transition temperature is located at  $T/J=1$ .

the existence of a negative dip was not reported in previous numerical works [21], we note that a negative dip appears only for larger  $N$  which accounts for the absence of a negative dip in the previous data. Perhaps, on looking at Fig. 2, one would hardly imagine that there occurs a continuous phase transition at  $T/J=1$ : Nevertheless, the occurrence of a continuous transition at  $T/J=1$  is an exactly established property of the model. We also note that, while the appearance of a growing negative dip in the Binder parameter is often related to the occurrence of a first-order transition [22], this is not always the case: Here, the transition is established to be continuous.

It might be instructive to examine here the behavior of  $g$  in the thermodynamic limit. As the temperature approaches  $T_g$  from below,  $g(T_g^-, \infty)$  tends to a *negative* value,  $-1$  in the present case. Such a negative value of  $g(T_g^-, \infty)$  is in sharp contrast to the system showing full RSB where  $g(T_g^-, \infty)=1$ . Indeed, this negativity is closely related to the occurrence of one-step RSB in the model [23].

Then, one expects that the negative dip of  $g(T, N)$  observed in Fig. 2 further deepens with increasing  $N$ , and eventually approaches  $-1$  *from above* at  $T=T_g^-$ , in sharp contrast to the SK case where  $g(T_g^-, N)$  approaches 1 *from below*. Therefore, the crossing of  $g$  in the  $g>0$  region as observed in the SK model hardly occurs in the  $p=3$  Potts-glass model. Rather, if one considers the fact that  $g(T, N)$  above  $T_g$  is negative for moderately large  $N$  approaching zero *from below*, the crossing of  $g$  is expected to occur *in the*  $g<0$  *region*, not in the  $g>0$  region as in the case of the SK model. The data of Fig. 2 are certainly consistent with such a behavior. Anyway, our present result of the mean-field  $p=3$  Potts glass has revealed that the data of the Binder parameter have to be interpreted with special care particularly when the ordered state has one-step RSB features.

Next, we study the so-called Guerra parameter which was originally introduced to detect the RSB transition [24]:

$$G(T, N) = \frac{[\langle q^2 \rangle^2] - [\langle q^2 \rangle]^2}{[\langle q^4 \rangle] - [\langle q^2 \rangle]^2}. \quad (6)$$

Since the numerator represents a sample-to-sample fluctuation of the overlap, a nonvanishing of  $G$  means a lack of self-averaging as long as the denominator remains nonzero. In the mean-field SG models studied here, their RSB indeed gives rise to the lack of self-averaging, i.e., the occurrence of a nontrivial probability distribution of the overlap over quenched disorder. It has been rigorously proved, without using the replica trick, that in the SG phase of the SK model the  $G$  parameter in the thermodynamic limit is equal to  $1/3$ , independent of the temperature [25]. Meanwhile, it has been pointed out in Ref. [26] that, even when  $P(q)$  is trivial and the ordered state is self-averaging, the  $G$  parameter can still take a nonzero value due to the possible vanishing of the denominator, leading to a crossing at  $T_g$  [26]. Hence, the crossing of  $G$  does not necessarily mean a lack of self-averaging, although it can still be used as an indicator of a phase transition. As an indicator of the non-self-averageness in the ordered state, one may use the  $A$  parameter defined by [27]

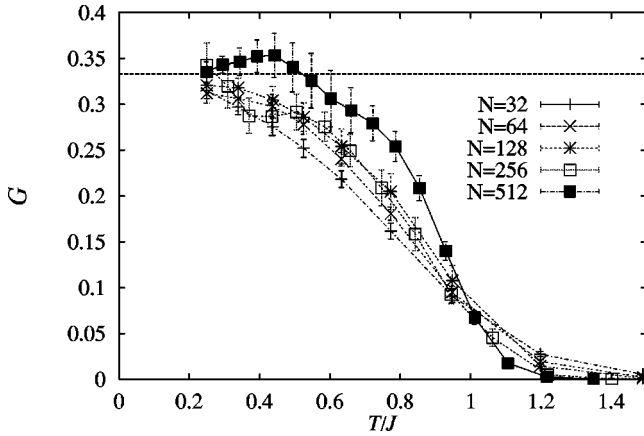


FIG. 3. Temperature and size dependence of the  $G$  parameter, defined by Eq. (6), of the SK model. The bulk transition temperature is located at  $T/J=1$ . The dashed horizontal line represents the line  $G=1/3$ .

$$A(T,N) = \frac{[\langle q^2 \rangle^2] - [\langle q^2 \rangle]^2}{[\langle q^2 \rangle]^2}. \quad (7)$$

We calculate these two parameters  $G$  and  $A$ , both for the SK and the mean-field  $p=3$  Potts-glass models. The temperature and size dependence of the  $G$  and  $A$  parameters of the SK model is shown in Figs. 3 and 4, respectively. Although the error bars are still large, both  $G$  and  $A$  show a clear crossing at  $T_g$ , remaining positive at any temperature. As expected, with increasing  $N$ , the  $G$  parameter approaches  $1/3$  independent of  $T$  below  $T_g$ . By contrast, the  $A$  parameter for various sizes merge into a curve below  $T_g$ , which clearly stays nonzero indicating the non-self-averageness of the ordered state. Here it should be noticed that, just at the transition point, non-self-averageness is expected to occur in any random system, even including the ones without showing RSB in the ordered state [28,29]. Hence, in the type of random systems which do not show RSB in the ordered state,  $A(T,\infty)$  stays nonzero only just at  $T=T_g$  and vanishes on both sides of  $T_g$ . By contrast, in the present SK model,  $A(T,\infty)$  should stay finite even below  $T_g$  due to its RSB, which explains the observed merging behavior seen in Fig. 4

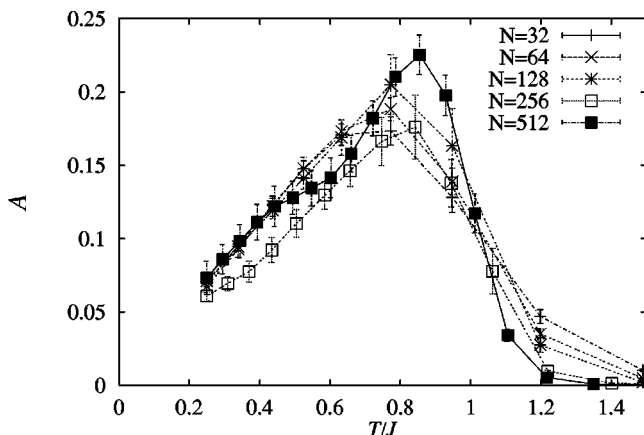


FIG. 4. Temperature and size dependence of the  $A$  parameter, defined by Eq. (7), of the SK model. The bulk transition temperature is located at  $T/J=1$ .

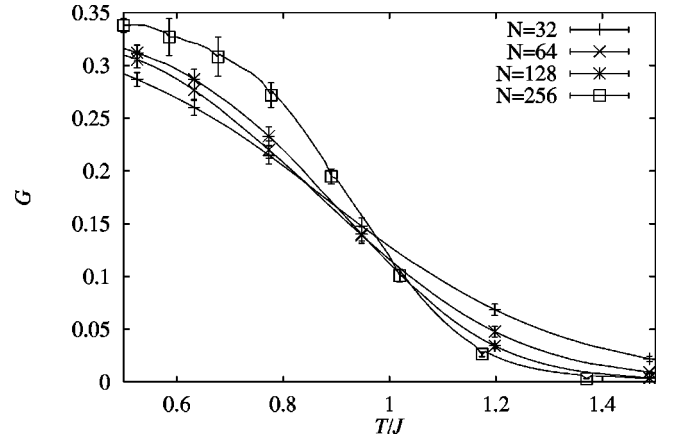


FIG. 5. Temperature and size dependence of  $G$  parameter, defined by Eq. (6), of the mean-field  $p=3$  Potts glass. The bulk transition temperature is located at  $T/J=1$ .

at  $T < T_g$ . As can be seen from Fig. 4, on further lowering the temperature toward  $T=0$ ,  $A(T,N)$  tends to vanish in contrast to the behavior of  $G(T,N)$ . This aspect is consistent with the fact that at  $T=0$  the overlap distribution becomes trivial and the self-averageness is recovered irrespective of the occurrence of RSB.

The  $G$  and  $A$  of the mean-field  $p=3$  Potts glass are presented in Figs. 5 and 6, respectively. Unlike the case of the Binder parameter  $g$  shown in Fig. 2, the  $G$  and  $A$  parameters remain positive at any  $T$  and show a clear crossing at  $T=T_g$ : They behave more like the Binder parameter of standard systems, e.g., like the one shown in Fig. 1. In fact, the behaviors of the  $G$  and  $A$  parameters shown in Figs. 5 and 6 are similar to those of the SK model shown in Figs. 3 and 4, suggesting that  $G$  and  $A$  are less sensitive to the kind of breaking pattern of replica symmetry. Hence, one could use the  $G$  and  $A$  parameters to identify the SG transition based on the standard crossing method even for systems showing a one-step RSB.

Once the transition temperature is established, the next task would be to determine critical exponents. Here we wish to examine a finite-size scaling hypothesis concerning the SG order parameter for the present mean-field models. A

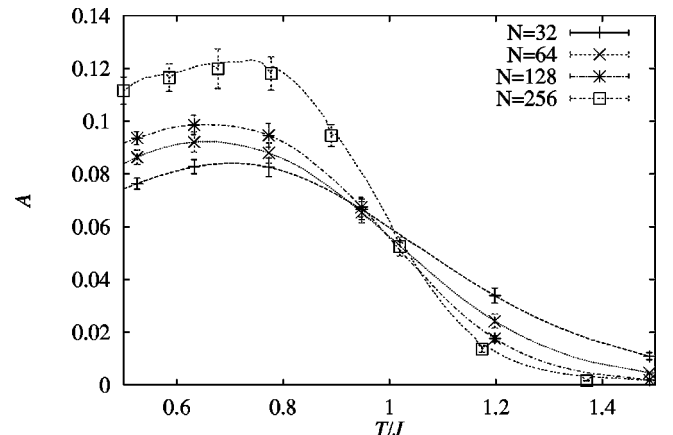


FIG. 6. Temperature and size dependence of  $A$  parameter, defined by Eq. (7), of the mean-field  $p=3$  Potts glass. The bulk transition temperature is located at  $T/J=1$ .

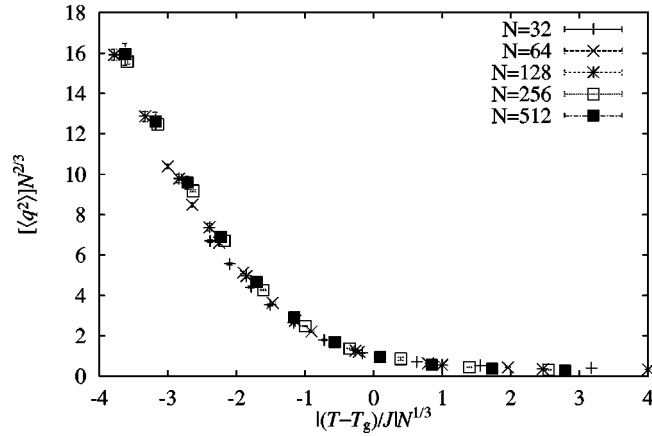


FIG. 7. Finite-size scaling plot of the squared order parameter of the SK model with the scaling form, Eq. (9), with  $T_g/J=1$ .

similar analysis has widely been used for extracting the critical exponents from the numerical data. According to Ref. [30], finite-size scaling of the mean-field models can be derived by assuming that the ‘‘coherence number’’ behaves as  $\xi^{d_u}$  where  $d_u$  is the upper critical dimension of the corresponding short-range model, while the ‘‘coherence length’’  $\xi$  diverges at  $T=T_g$  with the correlation-length exponent at the upper critical dimension  $\nu_{MF}$ ,  $\xi \sim |T-T_g|^{-\nu_{MF}}$ . Then, the squared order parameter can be written as

$$\begin{aligned} [\langle q^2 \rangle] &\sim |T-T_g|^{2\beta_{MF}} f(N|T-T_g|^{d_u \nu_{MF}}) \\ &\sim N^{-2\beta_{MF}/d_u \nu_{MF}} f'(|T-T_g|^{d_u \nu_{MF}}), \end{aligned} \quad (8)$$

where  $\beta_{MF}=1$  is the mean-field order-parameter exponent whereas  $f$  and  $f'$  are the scaling functions. Noting the fact that the upper critical dimension of the SG models is  $d_u=6$  and the correlation-length exponent at  $d=d_u=6$  is equal to  $\nu_{MF}=1/2$ , it follows that

$$[\langle q^2 \rangle] \sim N^{-2/3} f''(|T-T_g|N^{1/3}). \quad (9)$$

The resulting finite-size scaling plots are shown in Figs. 7 and 8 for the SK and the  $p=3$  Potts-glass models, respectively. In both models, the scaling of the form (9) turns out to work fairly well both *below* and *above*  $T_g$  as far as the tem-

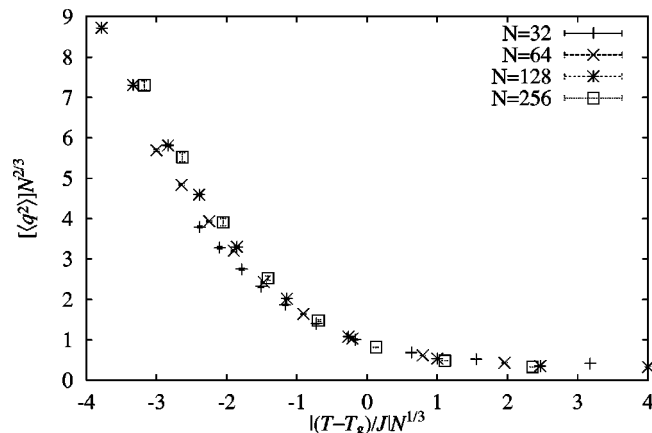


FIG. 8. Finite-size scaling plot of the squared order parameter of the  $p=3$  mean-field Potts glass with the scaling form, Eq. (9), with  $T_g/J=1$ .

perature is sufficiently close to  $T_g$ . We note that a similar finite-size-scaling analysis has already been reported for the SK model just at  $T_g$  [31] and for the  $p=3$  Potts-glass model above  $T_g$  [17]. In particular, the scaling turns out to be reasonably good even for the  $p=3$  Potts glass where the Binder parameter does not exhibit a clear crossing in the range of sizes studied. This implies that the standard finite-size scaling analysis of the order parameter could still be useful even in RSB systems including one-step RSB systems.

#### IV. DISCUSSION AND REMARKS

In this section, with our present results for the mean-field models in mind, we wish to comment on the possible RSB in some *short-range* SG models.

As mentioned, one-step RSB-like features were recently observed in the chiral-glass state of the 3D short-range Heisenberg SG [11]. There, the Binder parameter for the chirality, the order parameter of the chiral-glass transition, did not cross in the  $g>0$  region and developed a negative dip which deepened with the system size. Instead, a crossing of  $g$  was observed in the  $g<0$  region close to the negative dip (see Fig. 1 of Ref. [11]). Meanwhile, the  $G$  parameter always remained positive and showed a clear crossing at  $T=T_g$  (see Fig. 3 of Ref. [11]). All these features are similar to the ones observed here in the mean-field  $p=3$  Potts glass, suggesting that the chiral-glass state of the 3D Heisenberg SG has a one-step RSB-like character [32].

Another obvious interest is the nature of the possible phase transition of the short-range three-state ( $p=3$ ) Potts-glass model in 3D. It is widely believed that there is no finite-temperature phase transition in 3D  $p=3$  Potts glass which was investigated by MC simulations [33–35] and other numerical methods [36]. In particular, the MC results of Refs. [33,35] revealed that the Binder parameter decreased monotonically with system size without showing a crossing, which was taken as evidence of the absence of a finite-temperature transition. However, the behavior of  $g$  observed in Refs. [33,35] was not dissimilar to the one observed here in the mean-field  $p=3$  Potts glass, and we feel that the possibility of the occurrence of a one-step RSB-like transition at finite  $T_g$  still cannot be ruled out.

Recently, short-range  $p$ -spin glass models whose mean-field versions have been known to show one-step RSB were studied by MC simulations [37,38]. For example, according to the calculation of Ref. [38] for the 4D three-spin model, the Binder parameter did not exhibit a crossing of the standard type, while the  $G$  and  $A$  parameters showed a clear crossing at  $T=T_g>0$ , strongly suggesting the occurrence of a finite-temperature transition. Thus, from our present study, the possible occurrence of a one-step RSB transition at  $T=T_g>0$  is suspected. Meanwhile, closer inspection reveals that a negative dip observed in  $g$  becomes shallower with increasing system size [38], in contrast to the case of the mean-field  $p=3$  Potts glass studied here. Further studies seem to be required to clarify the nature of the RSB in the short-range  $p$ -spin glass.

In conclusion, we have investigated by MC simulations the finite-size effects of the two mean-field SG models whose replica-symmetry-breaking properties in the thermodynamic limit are well established. In the mean-field Ising

spin glass (the SK model), the Binder parameter  $g$  of various sizes always remains positive and crosses at  $T=T_g$ , while in the mean-field three-state Potts glass, it develops a negative dip which deepens as the system size increases, without a crossing in the  $g>0$  region as observed in the SK model. Instead, a crossing of  $g$  occurs in the  $g<0$  region near the negative dip. Such a difference in the behaviors of  $g$  reflects the different types of associated RSB of the two models, i.e., full versus one-step RSB. By contrast, the Guerra parameter  $G$  and the non-self-averaging parameter  $A$  always remain positive and show a crossing of the standard type at  $T=T_g$  for both the SK and  $p=3$  Potts-glass models. We have also discussed the implications of the present results to the

sible interpretation of the numerical results for some short-range SG models.

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