Domain-wall free energy of spin-glass models: Numerical method and boundary conditions

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An efficient Monte Carlo method is extended to evaluate directly domain-wall free energy for randomly frustrated spin systems. Using the method, critical phenomena of spin-glass phase transition are investigated in the $4d \pm J$ Ising model under the replica boundary condition. Our values of the critical temperature and exponent, obtained by finite-size scaling, are in good agreement with those of the standard Monte Carlo and the series expansion studies. In addition, two exponents, the stiffness exponent and the fractal dimension of the domain wall, which characterize the ordered phase, are obtained. The latter value is larger than $d-1$, indicating that the domain wall is really rough in the $4d$ Ising spin-glass phase. [S1063-651X(99)01810-3]

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I. INTRODUCTION

Numerical simulations, in particular, Monte Carlo (MC) methods, have played a quite important role in spin-glass (SG) studies [1]. For example, very large-scale MC simulations have strongly suggested the existence of a SG phase transition in three-dimensional Ising SG systems [2–4]. In these studies, a cumulant of SG overlap function q, so called the Binder parameter, has frequently been used in order to extract critical temperature T_c. However, the Binder parameter in $3d$ Edwards-Anderson (EA) Ising models [4,5] merely depends on system sizes below T_c as compared to that above T_c [6]. Moreover, unusual size dependence of the Binder parameter is observed in a short-ranged Ising EA model under the magnetic field [7]. Consequently, the existence of the SG phase transition under the field has still remained unclear. In order to settle the issue and make progress toward a good understanding of the SG picture, we consider other numerical analyses to be quite necessary.

In this direction, some promising ways have recently been proposed based on nonequilibrium dynamics [8,9] and the idea of non-self-averaging [10], but here we pay attention to the domain-wall renormalization-group (DWRG) method originally proposed by McMillan [11]. The DWRG estimates a singular part of free energy by calculating the domain-wall free energy, ΔF, which is defined as the free-energy difference between periodic and antiperiodic boundary conditions (BC's). In the scaling regime at low temperatures, ΔF follows a power law as a function of the system size L, $\Delta F \sim L^{\theta}$, where the stiffness exponent θ is related to the rigidity of the system. If the exponent θ takes a positive value at a temperature, then the system stays in an ordered phase. On the other hand, a negative exponent means a disordered phase. In this sense, the sign of the exponent θ is an indicator of the existence of long-range ordering. This exponent θ also characterizes a low-energy excitation in the SG phase and is predicted to be smaller than $(d-1)/2$, d being dimensionality, in the droplet scaling theory [12,13].

The DWRG approach relies on an accurate way for estimating the free-energy difference between two BC's. It is a difficult task in general for a MC method to estimate free energy or entropy. Except for the numerical transfer-matrix method for Ising models, it is therefore usual to integrate over the free-energy derivative, measured by MC simulations, along a parameter path between a reference system and the one of interest. As for zero-temperature calculations, various optimization techniques have been demonstrated to be useful for Ising [14,15] and vector spin systems [16]. These facts restrict so far to rather small sizes and/or at zero temperature. In this paper we have developed a boundary-flip MC method proposed by Hasenbusch [17], which allows us to estimate the free-energy difference at a *finite temperature* directly from a MC simulation. In applying a naive boundary-flip MC method to large systems and/or at low temperatures, one may encounter a hardly relaxing problem even in simple models without many metastable states, namely, the system is trapped into a local area in the phase space. The original work [17] has successfully overcome the relaxational problem by combining the method with the cluster MC dynamics.

In the present paper, we have proposed an alternative strategy, which is the boundary-flip method with exchange MC (EMC) method [18], in order to make the relaxation faster. This combined method is found to be quite efficient for randomly frustrated spin systems such as spin glasses, while the original method based on the cluster MC method is restricted to nonfrustrated systems. The present method is applicable to a wide class of spin systems. Moreover, the direct measurements have an advantage over the thermodynamic integration method from a numerical standpoint, because statistical error is controlled within MC scheme in the former. Consequently, we have succeeded to estimate the free-energy difference in a SG model, accurately enough to observe systematic correction to finite-size scaling.

For applying DWRG to SG systems, we need to choose the relevant boundary conditions to the ordered phase. The standard approach has often used a randomly fixed spin-boundary condition [19]. Instead, we employ the replica boundary condition proposed by Ozeki [25], in which two real replicas are coupled with each other through a boundary surface. The replica boundary condition provides that the domain-wall free energy becomes positive at any bond disorder, implying that it conjugates to the SG ordering. This positivity is of benefit to us for estimating the domain-wall free energy accurately from a numerical point of view.

Here we study the $4d \pm J$ Ising SG model under the rep-

lica BC by the MC method. We obtain the critical temperature and the exponent by a finite-size-scaling analysis of the domain-wall free energy, in agreement with the previous works. In addition, we estimate two exponents, the stiffness exponent θ and the fractal dimension d_s of the domain wall. We find that d_s is larger than $d-1$ in the SG phase.

This paper is organized as follows: In the next section, we explain the method for calculating the domain-wall free energy. Section III is mainly devoted to discussion about the replica boundary conditions. We give an interpretation of the domain wall appearing in the replica boundary condition and propose a way to measure the morphology of the domain wall. We show results for application of the method to $4d$ $\pm J$ Ising SG model in Sec. IV. In the last section, possible extensions of the method and nature of the low-temperature phase are discussed. The Appendix contains a way for setting temperature points, which is needed before simulation in the exchange MC method.

II. BOUNDARY-FLIP MC METHOD WITH EXCHANGE PROCESS

In this section we describe a method that allows us to evaluate directly the domain-wall free energy using MC simulations. For the sake of simplicity, we restrict ourselves to Ising spin systems and fixed spin-boundary conditions. Let us consider a total model Hamiltonian defined by

$$\mathcal{H}_{\rm tot}(\sigma,S_1,S_2)=\mathcal{H}_{\rm model}(\sigma)+\alpha\mathcal{H}_{\rm BC}(\sigma,S_1,S_2), \qquad (1)$$

where σ denotes Ising spin variable defined on a d-dimensional hypercubic lattice V of L^d and two additional spins, S_1 and S_2, represent boundary spins. The second term gives a coupling between the model system and the boundary spins along one direction as

$$\mathcal{H}_{\rm BC}(\sigma,S_1,S_2)=-\sum_{i\in\partial_1 V} J_{i,1}\sigma_i S_1-\sum_{i\epsilon\partial_2 V} J_{i,2}\sigma_i S_2, \qquad (2)$$

where the summation runs over one surface $\partial_1 V$ of the lattice V and its opposite surface $\partial_2 V$. A standard periodic boundary condition for σ is used along the remaining directions. Then, the total partition function $Z_{\rm tot}$ and the free energy $F_{\rm tot}$ of this whole system are defined by

$$\begin{aligned} Z_{\rm tot}(T) &= {\rm Tr}_{\{\sigma,S_1,S_2\}}\exp[-H_{\rm tot}(\sigma,S_1,S_2)/T] \\ &= \exp[-F_{\rm tot}(T)/T], \end{aligned} \qquad (3)$$

where T is temperature and we set the Boltzmann constant to unity. The phase space of the total Hamiltonian is enlarged by adding the degree of freedom of the boundary spins S_1 and S_2. When these spins are parallel, the boundary condition is regarded as *periodic* and similarly the *antiperiodic* boundary condition corresponds to antiparallel boundary spins. For a given temperature the probability for finding the periodic boundary condition is given by

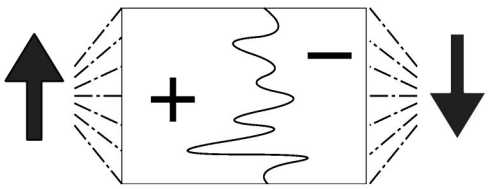

FIG. 1. Typical example for metastable configuration in a ferromagnetic model.

$$\begin{aligned} P_{\rm P}(T) &\equiv \frac{{\rm Tr}_{\{\sigma,S_1,S_2\}}\delta_{S_1,S_2}\exp[-\mathcal{H}_{\rm tot}(\sigma,S_1,S_2)/T]}{Z_{\rm tot}(T)} \\ &= \frac{Z_{\rm P}(T)}{Z_{\rm tot}(T)}, \end{aligned} \qquad (4)$$

where δ is the Kroneker delta function. This quantity is accessible from a MC simulation, namely, it is nothing but the probability for realizing the periodic BC during MC simulation in which the boundary spins as well as the bulk spins are updated according to a standard MC procedure. In terms of the probability and the corresponding one to the antiperiodic BC, the domain-wall free energy ΔF we want to investigate is given by

$$\exp[\beta\Delta F(T)]=e^{-\beta(F_{\rm P}-F_{\rm AP})}=\frac{Z_{\rm P}}{Z_{\rm AP}}=\frac{P_{\rm P}(T)}{P_{\rm AP}(T)}. \qquad (5)$$

This is the basic idea of the boundary-flip MC method proposed by Hasenbusch [17]. When we adopt a naive local updating process for the boundary spins in the boundary-flip MC method, however, we are at once faced with a hardly relaxing problem. For example, once the antiperiodic boundary conditions and the domain-wall structure in the system are realized in the simulation at low temperatures, as shown in Fig. 1, the boundary spins are kept to be fixed in the sense that the probability for flipping these spins is vanishing in practice. This fact makes statistical error of ΔF significantly large. The original work [17] has overcome this difficulty by utilizing the modified cluster flip. We can also practically solve this so-called hardly relaxing problem using recently proposed extended ensemble methods such as the multicanonical MC method [20], the simulated tempering [21], and the exchange MC method [18]. In fact, a similar difficulty has been overcome using the multicanonical idea in the lattice-switch MC method [22], which has been proposed to estimate the free-energy difference between two different crystalline structures in a hard-sphere system.

In the present paper, we employ the EMC method in order to obtain an efficient path between two boundary-condition states. In the EMC method, we simulate a combined system, which consists of a noninteracting M-replicated system. The mth replica is simulated independently with its own external variable such as temperature. We introduce an exchange process between configurations of two of the M replicas with the whole combined system remaining in equilibrium. One possible way for obtaining the path is that we distribute various values of the coupling α in Eq. (1) ranging from 0 to 1 to M replicas. A target system we are physically interested in is the replica with $\alpha=1$. For a replica with null coupling of α, which we call a source system, the boundary spins can be

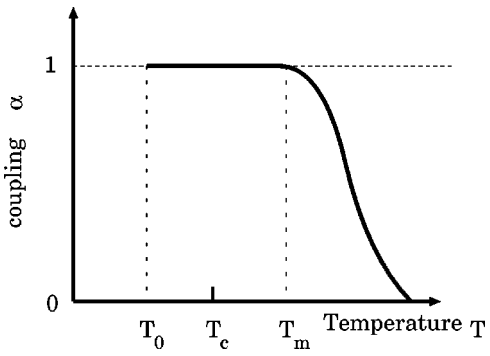

FIG. 2. Schematic picture of the exchange line in parameter space.

flipped freely. Therefore, the path between different boundary-condition states in the target system would be recovered by the exchange process through the source system.

In randomly frustrated spin systems such as SG models, there is another serious relaxation problem arising from bulk spins in the model system itself. This problem can be overcome also by the EMC method. [18] When we distribute M temperature points widely including high enough temperature in a disordered phase, configurations at low temperatures are expected to be refreshed through the exchange process. The EMC method has turned out to work efficiently in the SG systems [18,23]. Therefore, for the boundary-flip MC method on SG models, we need to construct the EMC method in two-dimensional parameter space of the coupling α and the temperature T. It is possible to introduce the exchange process in the two parameter space, but it is quite time consuming. In the present paper, therefore, we choose an exchange line in the two-dimensional space appropriately, namely, we set a system at high temperature with $\alpha=0$ as one end of the exchange line and systems at lower temperature with α being unity, as shown in Fig. 2. It is noted that the parameter region of the our final interest lies on the line with $\alpha=1$ around T_c and below. An efficient choice of the exchange line would depend on systems we want to investigate. Actual implementation to the Ising spin-glass model will be explained in detail in Sec. IV.

III. REPLICA BOUNDARY CONDITIONS FOR SG SYSTEMS

In this section, we discuss how to choose a boundary condition for SG systems in the DWRG study. We concentrate on a way of choice of a boundary condition along one direction while the remaining ones are considered to be given appropriately. In conventional DWRG studies [11,24] as well as the defect energy method, a boundary condition frequently used is a connected spin BC in which the corresponding boundary term in Eq. (1) is described by

$$\mathcal{H}_{\mathrm{BC}}=\sum_{i\in\partial_1 V, j\in\partial_2 V} J_{ij}\sigma_i\sigma_j . \tag{6}$$

The case with $\alpha/|\alpha|=1(-1)$ is regarded as the (anti-) periodic boundary condition. For the boundary condition defined by Eq. (6), the boundary-flip MC method can be applied by treating the sign of the coupling α as a MC dynamical variable. In SG systems, the free-energy difference between these BC's cannot be assured positive so that the width of distribution of the free-energy difference is examined as an effective coupling of the SG ordering, $F_{\mathrm{eff}}=\sqrt{(F_{\mathrm{AP}}-F_{\mathrm{P}})^2}$. To evaluate the mean width is rather difficult as compared with the average in numerical calculations. Further, it is less clear how the domain wall is created in a random spin system under these BC's.

In order to avoid the difficulty and make clear an idea of the domain wall, Ozeki [25] has proposed a replica boundary condition (RBC), in which two real replicas are prepared with the same bond realization. Its essential point is to introduce a uniform coupling between these two replicas only for one surface $\partial_0 V$ along a given direction. For the other directions periodic BC is employed as usual. We show explicitly an example expressed as the Ising Hamiltonian,

$$\mathcal{H}_{\mathrm{model}}(\sigma,\tau)=-\sum_{\langle ij\rangle} J_{ij}(\sigma_i\sigma_j+\tau_i\tau_j)-J_{\mathrm{int}}\sum_{i\in\partial_0 V}\sigma_i\tau_i , \tag{7}$$

where both σ and τ are Ising variables and the summation of the first term runs over nearest-neighbor bonds. The second term corresponds to the replica interaction mentioned above. When J_{int} is set to (anti-) ferromagnetic, the boundary condition is called replica (anti-) periodic BC(RAPBC). Spins on the opposite side of $\partial_0 V$ are kept randomly fixed with $\sigma_i=\tau_i$.

Ferromagnetic interactions between the replicas in the RPBC prefer a *self-overlap state*, even if the system has many local minima or pure states. Namely, one replica gives an effective conjugated field to the other replica through the interreplica interaction. It is convenient to consider the domain wall in terms of the replica overlap $q_i=\sigma_i\tau_i$. The self-overlap state is characterized by positive values of q_i at all the sites, meaning no domain wall in the system. At sites on the opposite surfaces of $\partial_0 V$, q_i take unity by definition, irrespective of RAPBC's. On the other hand, antiferromagnetic intercouplings between the replicas in the RAPBC would induce negative overlap at sites near the coupling. Therefore, at least one domain wall, characterized by a region where the sign of q_i changes, likely appears in the RAPBC, if the system has a rigid ordered state. From a mathematical point of view, non-negativity of the free-energy difference $\Delta F_{\mathrm{R}}=F_{\mathrm{RAPBC}}-F_{\mathrm{RPBC}}$ under the replica BC has been proven rigorously in any random Ising model at any finite temperature using the transfer-matrix formalism [25]. This non-negativity holds true irrespectively of a choice of spins on the surface opposite to $\partial_0 V$. As a result, only the average of the domain-wall free energy is needed for estimating a relevant effective coupling of the SG ordering. This is advantageous for reducing the statistical error of ΔF_{R} from which a transition point from paramagnetic to SG phase is detected.

An additional merit of the replica boundary condition is that we can discuss the morphology of the domain wall at finite temperatures. In terms of the local overlap q_i, the area of the domain boundary mentioned above is expressed as $W=\Sigma_{\langle ij\rangle}\frac{1}{2}(1-q_iq_j)$, where the summation is over nearest-

neighboring pairs. Then we can extract directly domain-wall properties such as its fractal dimension, from the difference $\Delta W(T)$ defined by

$$\Delta W(T)=\frac{1}{2}\sum_{\langle ij\rangle}(\langle\sigma_i\sigma_j\tau_i\tau_j\rangle_{\mathrm{RPBC}}-\langle\sigma_i\sigma_j\tau_i\tau_j\rangle_{\mathrm{RAPBC}}), \tag{8}$$

where $\langle\cdots\rangle_{\mathrm{RAPBC}}$ denotes the thermal average under the replica (anti-) periodic BC. This quantity is also regarded as a difference of link correlation [26] between two boundary conditions in $\pm J$ models. The correlation function as well as the replica overlap have been studied in a similar replicated system [26], which has a global coupling between the replicas. This coupled system is different from the present system under RBC. In particular, correlation function (8) is related to domain-wall properties only in the RBC. The domain-wall area ΔW has not been directly studied so far in SG systems, except for the zero-temperature calculation in a two-dimensional Ising SG model [32]. We will present new results for ΔW in the next section.

IV. RESULTS

In this section, we present results of an application of the MC method explained in the previous sections to the $4d$ $\pm J$ Ising SG model. The interactions $\{J_{ij}\}$ in Eq. (7) are random variables, which take values $\pm J$ with equal probability. The boundary-flip MC method can be applied to the replica BC by regarding the sign of the interaction J_{int} in Eq. (7) as a dynamical variable. Equivalently these boundary conditions are defined by relative direction of the boundary spins S_1 and S_2 added to Eq. (7) whose J_{int} are fixed to be positive. Then, the boundary part in Eq. (1) is given by

$$\mathcal{H}_{\mathrm{BC}}(\sigma,\tau,S_1,S_2)=-\sum_{i\in\partial V}J_i(\sigma_iS_1+\tau_iS_2), \tag{9}$$

where the interactions J_i are also distributed randomly. In the present paper we adopt this method with the boundary spins.

The number of replicas M in the EMC method is fixed at 32 irrespectively of the system sizes to utilize the multispin coding technique. Each replica with the parameters α and T tries to exchange configuration with the nearest replica in the parameter space. As we have explained in Sec. II, we choose in this two-parameter space, a line on which M replicas are prepared. The line chosen is such that the value of α is unity below a certain temperature T_m, but it decreases like a Gaussian formula as a function of $T-T_m$ above T_m. The onset T_m is set to be about two times the critical temperature. We distribute the set of the parameters to the 32 replicas such that the acceptance ratio for each exchange process becomes independent of the replicas. This can be succeeded by a simple iteration method using the energy function, which is estimated from a short preliminary run. Details of the iteration method is explained in the Appendix.

As an equilibration check, we study time evolution of ΔF_{R} starting from two initial conditions: periodic and antiperiodic boundary conditions imposed for the whole replicated systems in the EMC simulation. The initial conditions for the bulk spins are chosen at random. The free-energy difference ΔF_{R} is estimated as a function of a MC step t by averaging over short MC steps around time t. In the case of the whole antiperiodic BC, free-energy difference, starting from a large negative value at the initial time, evolves toward equilibrium. The other estimation with the periodic BC at the initial time reaches the equilibrium value from the opposite direction to that of the antiperiodic BC. In equilibrium, two curves coincide with each other. As expected, we see in Fig. 3 that the equilibration of ΔF_{R} is obtained after a certain time. It should be noted that the relaxational function approaching the equilibrium value follows an exponential law rather than a power law observed in the standard SG simulations. This implies the existence of a typical time scale for equilibration in the present method. We thus expect that the system really reaches equilibrium after a few times of such time scale. We estimated the time scale for other sizes and determined the MC steps (MCS) for thermalization and measurements. For example, in simulations of the $4d$ case with $L=8$, we take 9.6×10^4 MCS for the initial step and 2.0×10^5 MCS for measurement. We have also checked that the ergodic time [20,18] is about 3×10^2, 3.0×10^4, 5.8×10^4, and 1.7×10^5 MCS on average for $L=4$, 6, 8, and 10, respectively.

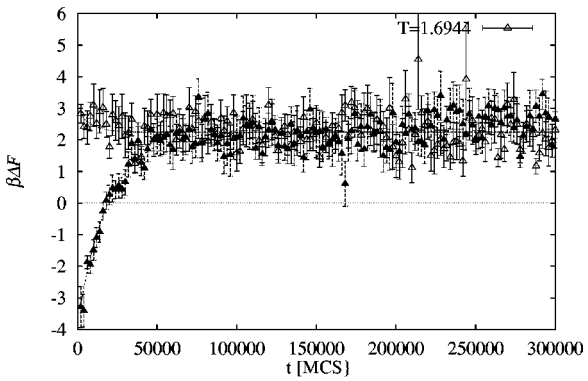

FIG. 3. The domain-wall free energy of the $4d\pm J$ Ising SG model with $L=8$ and $T=1.694$ well below the SG transition temperature as a function of MC steps. The upper data marked by open triangles are started from the periodic boundary condition for the whole system, while the lower one, from the antiperiodic one. Each point at time t is obtained by averaging over 2000 MCS around t, and error bars are estimated from statistical fluctuation over ten samples.

We show temperature dependence of ΔF_{R} for the $4d$ Ising SG model in Fig. 4. The lattice size studied are $L=4$, 6, 8, and 10 with samples 2197, 2060, 1332, and 892, respectively. According to the standard finite-size-scaling argument, the domain-wall free energy should be scaled as

$$\Delta F_{\mathrm{R}}(L,T)\sim F_0((T-T_{\mathrm{c}})L^{1/\nu}), \tag{10}$$

where the parameter ν denotes the critical exponent of the correlation length and F_0 is a scaling function. Therefore, the critical temperature can be located at the point where ΔF_{R} for different sizes as a function of T cross with each other. The crossing feature of ΔF_{R} at T_{c} is common to the Binder parameter. In fact, as shown in Fig. 4, crossing of ΔF_{R} of two different sizes is seen at a certain temperature. However, the crossing temperature is found to shift systematically to

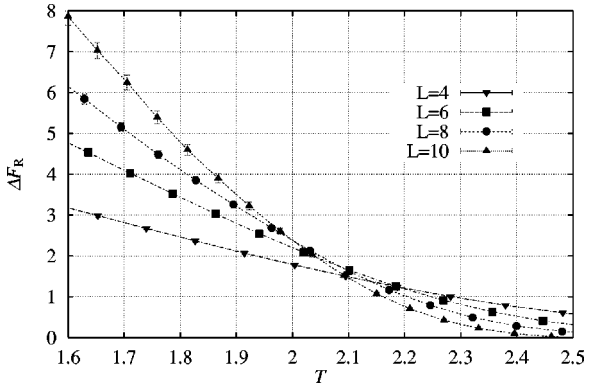

FIG. 4. Temperature dependence of the domain-wall free energy for the $4d$ $\pm J$ Ising SG model near the critical temperature. These lines are for a guide to the eyes.

the low-temperature side as the system size increases, implying that correction to the finite-size scaling is significant. We consider correction due to the leading irrelevant scaling variable whose scaling dimension is ω,

$$\Delta F_{\mathrm{R}}(L,T) \sim F_0((T-T_{\mathrm{c}})L^{1/\nu}) + L^{-\omega}F_1((T-T_{\mathrm{c}})L^{1/\nu}). \tag{11}$$

These exponents ν and ω and the critical temperature T_c are determined by fitting the simulated data to scaling formula (11), where the scaling functions F_0 and F_1 are assumed to be given by third-order polynomial functions. From the fitting, we estimate $T_{\mathrm{c}}=2.00(4)$, $\nu=0.92(6)$, and $\omega=1.5(9)$. The finite-size scaling of F_0 after subtraction of the leading correction is plotted in Fig. 5, where all the data points are found to collapse almost into a universal function. The scaling plot including the smallest size $L=4$ is obtained only when the leading term of the correction is taken into account. The estimated critical temperature is consistent with the previous results obtained by the MC method [27,28] and the high temperature expansion [29,30]. Our result for ν is also in agreement with these expansion studies, and not very different with that obtained by MC simulations for $\pm J$ [27] and

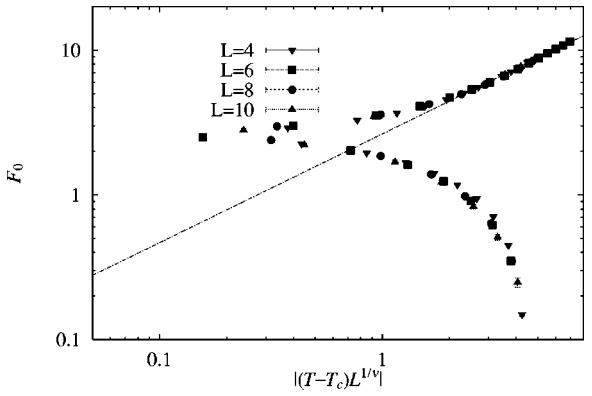

FIG. 5. Finite-size scaling plot of the domain-wall free energy in the $4d\pm J$ Ising SG model. The leading correction to the scaling is taken into account. The scaling plot after subtraction of the leading correction is shown. The estimated scaling parameters are $T_c=2.00(4)$, $\nu=0.92(6)$, and the irrelevant exponent $\omega=1.5(9)$. The slope of the scaling function is asymptotically close to 0.75(1), meaning that the stiffness exponent θ is 0.82(6).

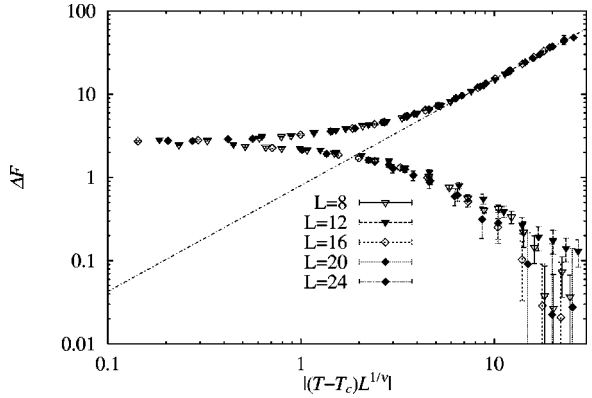

FIG. 6. Finite-size scaling plot of the domain-wall free energy in the $3d$ ferromagnetic Ising model. The parameters of the scaling are estimated as follows: $T_c=4.5117(4)$, $\nu=0.624(7)$. The asymptotic behavior of the scaling function follows a power law as a function of the scaling parameter $(T-T_c)L^{1/\nu}$ with slope 1.27(1). The value of the slope is compatible with the low-temperature behavior, namely, $\theta\nu$ being $\theta=d-1$.

Gaussian distribution [31]. Since the system sizes used in the present paper are larger than those in the previous MC simulations, we expect that our estimation is reliable. The irrelevant exponent ω is, to our knowledge, the first estimation for a $4d$ Ising SG model by MC simulation, but its value is slightly lower than that obtained from the series expansion [30], which quoted about 3.

At low enough temperature, the domain-wall free energy is expected to be scaled as

$$\Delta F_{\mathrm{R}}(L,T) \sim L^{\theta}, \tag{12}$$

where θ is an exponent, which gives the characteristic energy scale L^{θ} of low-energy excitations of typical size L. We cannot evaluate ΔF_{R} at low temperatures enough to distinguish the low-temperature properties from the critical behavior. Here we try to estimate the exponent θ from the scaling function of ΔF_{R}. We assume that the behavior of ΔF_{R} at a large length scale is also described by the scaling form of Eq. (11) near below T_{c}. This assumption implies that the asymptotic behavior of the scaling function F_0 is predicted as

$$F_0(x) \sim |x|^{\theta\nu}, \tag{13}$$

at $x \to -\infty$. We examine this scaling idea in the simple $3d$ Ising ferromagnetic model, where the stiffness exponent coincides with the surface dimensions $d-1$. We estimate the domain-wall free energy by the present MC method under the connected spin BC described in Eq. (6). In the $3d$ Ising model, we scale the data to the leading scaling formula (10) without the correction, because we have not observed a shift of the crossing temperature under our numerical accuracy. The finite-size scaling of the domain-wall free energy works well as observed in Fig. 6. The asymptotic behavior of the scaling function gives $\theta\nu \sim 1.27$, compatible with the well-known values of ν and $\theta=d-1$.

Let us turn to the $4d$ Ising SG model. The stiffness exponent θ in SG systems is expected to be much smaller than that of the ferromagnetic model. The droplet theory predicted

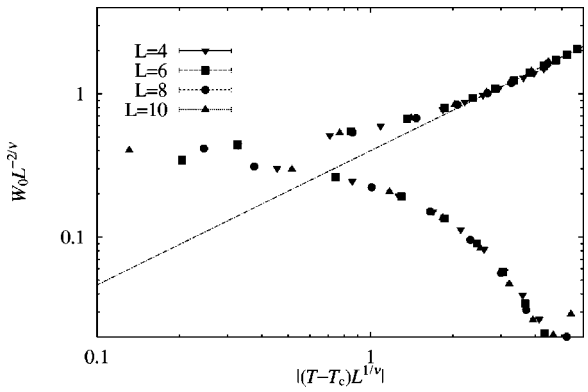

FIG. 7. Finite-size scaling plot of the domain-wall area in the $4d \pm J$ Ising SG model after subtraction of the leading correction to the scaling. The critical temperature is used as a result of the scaling analysis for the domain-wall free energy. The exponent ν is found to be 0.94(2), consistent with the previous estimation. The estimated irrelevant exponent $\omega = 1.86(77)$ agrees with that obtained from the ΔF_{R} scaling. The slope is estimated to be 0.94(2), suggesting $d_s = 3.13(2)$.

the upper bound of θ to be $(d-1)/2$ [13]. We extract value of θ from the scaling function obtained in Fig. 5. We fit the scaled data with the scaling variable x larger than 3 to a power law. The best fit is obtained with the exponent $\theta\nu = 0.75(1)$, which yields the stiffness exponent of $\theta = 0.82(6)$.

We also investigate the domain-wall area ΔW defined by Eq. (8) in this model, which is easily calculated in the present MC scheme. A scaling analysis similar to the one for ΔF_{R} is performed for ΔW, taking into account the leading correction to the scaling. It is noted that in contrast with the ΔF_{R} scaling, ΔW is proportional to $L^{2/\nu}$ near T_{c} because it has essentially the same scaling dimension as the energy-energy correlation function. The finite-size scaling plot for ΔW is shown in Fig. 7, where the critical temperature is used, which is estimated by the ΔF_{R} scaling. The scaling works nicely both above and below T_{c} and the estimated ν value is consistent with that from ΔF_{R}. We suppose that at low temperature the domain wall in the SG system is rather rough. Correspondingly, the domain-wall area ΔW is expected to follow a power law on size with a nontrivial fractal dimension d_s. We estimate d_s by extracting the asymptotic behavior of the scaling function of ΔW in the same way as in the analysis of ΔF_{R}. The asymptotic slope of the scaling function is $d_s\nu - 2$. The fractal dimension of this model is found to be 3.13(2). According to the Bray-Moore scaling law [32], the exponents θ and d_s are related to the chaos exponent ζ,

$$\zeta = \frac{d_s}{2} - \theta. \tag{14}$$

By this combined with the values of θ and d_s obtained here, our estimation of ζ is 0.75(6). This value is smaller than those of MC simulations for $4d$ Ising SG models [33,34], but rather close to that by the Migdal-Kadanoff renormalization-group analysis [35].

V. DISCUSSION AND SUMMARY

We have developed a numerical method, which enable us to estimate a free-energy difference directly from MC simulation. It is a boundary-flip MC method, in which the replica boundary conditions and the exchange MC technique are incorporated. The proposed method works well in the short-range Ising SG model. This method presented here can be applied to various spin systems including vector spin models because our argument does not depend on a model Hamiltonian. It should be noted that the EMC method, as well as other extended ensemble methods, is also applicable to randomly frustrated spin systems, while the cluster-flip-based method is restricted in nonfrustrated models. Another extension would be concerned with the choice of the boundary conditions. In this paper, we have described the case for the fixed spin BC, but it is straightforward to extend it to other types of BC's. It is only necessary for boundary conditions to be expressed by a countable variable, while the degree of freedom of the model system is not restricted.

We also discuss boundary conditions for SG systems. Let us comment on related studies. A similar coupled-replica system has been studied analytically by a mean-field variational method [36], where two replicas are coupled with each other by fixing the value of overlap between surface spins of these replicas. The system studied roughly corresponds to the present replica boundary model by choosing appropriate parameters. It is predicted that an excess free energy due to the effective coupling is proportional to $L^{d-5/2}$, which accidentally coincides with the upper limit of the droplet scaling theory in the four-dimensional case. Our estimation of the stiffness exponent is not compatible to that predicted from the variational calculation.

Recently a boundary condition, called the naive boundary condition, has been proposed in 2D Ising [37] and XY [38] spin-glass models, independently. In these studies, they minimize energy of a whole system under the free-boundary condition. Using the obtained boundary spin configuration as a reference system, a twisted boundary condition is prepared by flipping the sign of spins on one surface. The ground-state energy of such a system is always higher than that of the reference system. They claimed that this non-negativity is evidence of introducing correctly a domain wall into the system. It is doubtful whether such boundary conditions defined at zero temperature are also relevant to the ordering at finite temperatures. This is because many SG systems including both short-range [32] and mean-field models [39] are expected to exhibit chaotic nature; namely, spin configurations at finite temperatures differ from those at $T=0$ in larger scale than the so-called overlap length. Further, the replica boundary condition takes an advantage from the naive one in a practical sense, because the former does not need the ground-state calculations. This fact makes our investigations easier in three- or high-dimensional systems, where the ground states are hardly found for suitable large systems due to NP hardness.

The present method has successfully been applied to the $4d \pm J$ Ising SG model under the replica boundary conditions. The average of the domain-wall free energy ΔF_{R} over samples, not the variance as used in the standard DWRG study, exhibits very clear crossing at the critical temperature,

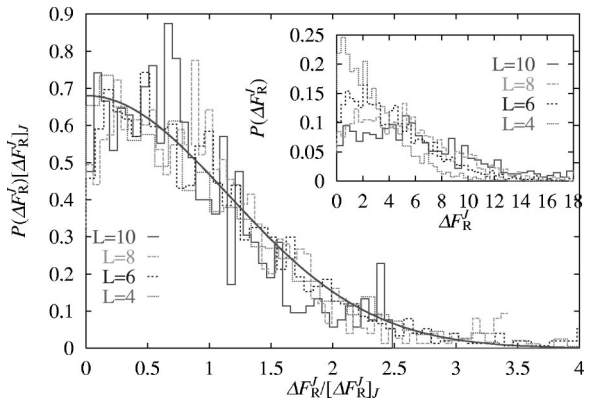

FIG. 8. Scaling plot of the distribution function of the domain-wall free energy with $T\sim 1.6$. Both axes are scaled by the first moment of the distribution. The solid curve is obtained by fitting the scaling function to a Gaussian formula. The raw data are shown in the inset.

implying that it is a good indicator of the SG transition. It is noted that the replica BC is crucial for providing the non-negativity of ΔF_{R}. We expect that, when the system has a well-defined rigidity in the ordered phase, the ΔF_{R} analysis works well even in the case where the Binder parameter does not show a crossing at T_{c}. In such systems, the short-range SG models with the field are one of the most attractive problems in the SG study. As a byproduct of the RBC, we can argue the domain-wall area in the SG phase. We have estimated the stiffness exponent θ and the surface dimension d_s of the domain wall in the $4d$ Ising SG phase independently. The latter value lies significantly above the trivial surface dimension $d-1$, meaning that the domain wall is rough, while both θ and d_s coincide with $d-1$ in the ferromagnetic Ising models.

Finally we make a comment on distribution of ΔF_{R} over samples $P(\Delta F_{\mathrm{R}})$, whose typical results are shown in Fig. 8. To our surprise, the distribution functions of different sizes, when scaled by their first moment, lie on top of each other in the SG phase. Another remarkable observation is that the scaling function is approximated by a Gaussian function; namely, it approaches a nonzero value as its argument goes to zero. These results, similar to those observed in $2d$ and $3d$ Ising SG models at zero temperature [24,40], are consistent with the droplet picture [12,13].

The question of whether many equilibrium pure states exist or not in the SG phase has still remained controversial. For the system of present interest, some MC studies [41,26] have supported the existence of the multiple pure states, namely, the mean-field picture, while the Migdal-Kadanoff approximation for the short-range SG model [42] has claimed that the asymptotic size scale to detect the correct thermodynamic properties is far from those investigated in the MC simulations. As mentioned in Sec. III, the replica BC used in the present paper prefers a self-overlap configuration in the two replicas. Correspondingly, under the replica anti-periodic BC, there likely appear such configurations with a domain wall, which lies in one of the two replicas and separates one configuration from its time-reversal one. Therefore, our results mentioned above strongly suggest that nature of low-lying excitations within one pure state is as expected in the droplet theory. Our data alone, however, cannot exclude the possibility that there are many pure states.

In conclusion, we have proposed a MC method that enables us to estimate the free-energy difference, and have successfully applied it to the $4d\pm J$ Ising SG model. Our value of T_{c} is in good agreement with the previous results obtained from the numerical simulations and the series expansions. We have presented estimates of two exponents, the stiffness exponent and the fractal dimension. We have also found that low-lying excitations as expected in the droplet theory are realized within one pure state in the SG phase, though we cannot rule out the possibility that there exist many pure states.

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APPENDIX: SETTING TEMPERATURE POINTS FOR THE EXCHANGE MC METHOD

In this appendix we propose a practical way to determine temperature set, which is needed in the exchange MC method. For simplicity, we consider a procedure for setting a temperature point β_n between two fixed ones, β_{n-1} and β_{n+1}. Our criterion is that acceptance probabilities for the exchange trial with both neighboring temperatures become equal:

$$(\beta_{n-1}-\beta_n)[E(\beta_{n-1})-E(\beta_n)]=C,$$
$$(\beta_n-\beta_{n+1})[E(\beta_n)-E(\beta_{n+1})]=C, \tag{A1}$$

where C and β_n are unknown constants. A formal solution for β_n is given by

$$\beta_n=g(\beta_n)$$
$$=\frac{1}{E(\beta_{n-1})-E(\beta_{n+1})}\times[\beta_{n-1}E(\beta_{n-1})$$
$$-\beta_{n+1}E(\beta_{n+1})-E(\beta_n)(\beta_{n-1}-\beta_{n+1})]. \tag{A2}$$

Regarding $\beta'=g(\beta)$ as a map of β to β', we find a fixed point of period 2 with $\beta_{n+1}=g(\beta_{n-1})$ and $\beta_{n-1}=g(\beta_{n+1})$. Therefore, we expect a repulsive fixed point between β_{n-1} and β_{n+1}. A new mapping to obtain the fixed point is given by

$$\beta_n(t+1)=\tfrac{1}{2}[\beta_n(t)+g(\beta_n(t))], \tag{A3}$$

where t is the iteration step. This iteration scheme can be extended straightforwardly to the case of multiple temperature points. The whole set of temperature is divided into two groups with even n and odd n. Using the iteration scheme, temperature points of the one group are updated with the

other group fixed, alternatively. In actual iterations, the initial temperature points $\{\beta_n\}$ are set in a suitable way, for example, equidistant β. The energy $E(\beta)$ at the initial set of β is roughly estimated by short MC simulation and the energy at any temperature between β_1 and β_M is assumed to be obtained from the MC data, for example, by interpolation technique. The convergence of the iteration is rapidly achieved in many systems we have investigated.

From our experiences so far, efficiency of the EMC method is rather insensitive for the choice of temperature points, when it is applied to systems such as spin glasses, with nondiverging specific heat at the phase transition. This fact that it is not necessary to specify any parameters before main simulation is, in fact, one of the big advantages of the EMC method against the other extended ensemble methods such as the multicanonical MC method and simulated tempering method. Nevertheless, we emphasize that little effort on preparing the temperature points by pre-MC runs following the prescription described above ensures the acceptance ratio almost independent of temperature and so is quite useful.

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