Numerical simulations of Ising spin glasses with free boundary conditions: The role of droplet excitations and domain walls

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The relative importance of the contributions of droplet excitations and domain walls on the ordering of short-range Edwards-Anderson spin glasses in three and four dimensions is studied. We compare the spin overlap distribution functions of periodic and free boundary conditions using population annealing Monte Carlo. For system sizes up to about 1000 spins, spin glasses show nontrivial spin overlap distributions. Periodic boundary conditions may trap diffusive domain walls which can contribute to small spin overlaps, and the other contribution is the existence of low-energy droplet excitations within the system. We use free boundary conditions to minimize domain-wall effects, and show that low-energy droplet excitations are the major contribution to small overlaps in numerical simulations. Free boundary conditions has stronger finite-size effects, and is likely to have the same thermodynamic limit with periodic boundary conditions.

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I. INTRODUCTION

The nature of the ordering of short-range Edwards-Anderson (EA) spin glasses [1] is a subject of long-standing controversy [2–26]. The infinite-range Sherrington-Kirkpatrick (SK) model [27] is known to have an infinite number of pure states, described by replica symmetry breaking [28–30]. In the context of short-range spin glasses, there are two similar and plausible ways to have many pairs of pure states, but in terms of metastates [31–33]. For a finite large volume of spins, there might be one pair of pure states present, the chaotic pairs picture [33,34], or many pairs of pure states, the nonstandard replica symmetry breaking (RSB) picture [33,35], both with chaotic size dependence and space-filling domain walls. The droplet picture on the other hand, developed by McMillan [36], Bray and Moore [37], as well as Fisher and Huse [38–40], is an example of the simple scenario that there is only a single pair of pure states and the thermodynamic limit is defined in the usual way. In the droplet picture, domain walls are fractal surfaces, not space filling.

Many numerical simulations have been conducted to study the ordering of the EA model [2–5,7–23,26] with a confusing mixture of results, in particular whether domain walls are space filling, and there is a finite weight near zero overlap in the spin overlap distribution function $P(q)$. According to the droplet picture, the free energy cost to flip a droplet of size ℓ scales as ℓ^{θ}, where $\theta > 0$ is the stiffness exponent, which is expected to be the same for domain-wall and droplet excitations. On the other hand, RSB predicts that $\theta = 0$ for droplet excitations. Consequently $P(0)$ scales as $\ell^{-\theta}$. Therefore, a finite $P(0)$ means there exist large-scale excitations in the system with $O(1)$ cost in free energy. Otherwise, there is a unique ordering of spins without system-size excitations. When a domain wall is created, there are ℓ^{d_s} spins on the surface of the domain wall, where d_s is the fractal dimension of the domain wall. In the droplet picture, the surface is a fractal with $D - 1 \leqslant d_s \leqslant D$, while in RSB the surface is space filling and $d_s = D$, in D dimensions. To leading order without finite-size corrections, domain walls appear to be fractals and the weights near zero overlap is finite [7,8,11,14] for the system sizes currently accessible. New statistics or finite-size corrections are therefore intensively developed, and pointing to different scenarios [20,23,41–43].

In this work, we focus on the weights near zero overlap $P(0)$. We are interested in the question if the droplet picture holds, could it be that $P(0)$ is a finite constant trivially because of trapped diffusive domain walls in the usually applied periodic boundary conditions (PBCs), or low-energy droplet excitations are the dominate contribution? Note that boundary conditions are only relevant to the EA model, not the SK model. The motivation of the idea of diffusive domain walls is from the consideration that the overlap distribution function of the ferromagnetic Ising model is flat if the antiperiodic boundary condition in the x axis is applied, where the system traps topologically protected domain walls. For disordered systems like spin glasses, one can generalize this term by comparing the interfaces [44] of the thermodynamic states of the system, where an interface is a bond that is satisfied in one state but unsatisfied in the other state, i.e., a negative link overlap. If the interfaces are two percolating domain-wall surfaces at different locations of the system, then we say the system has trapped diffusive domain walls, which may be inserted at different locations, but with similar free energy cost. It is not hard to see that PBCs may trap a diffusive domain wall that is topologically protected. On the other hand, such effects should be reduced for free boundary conditions (FBCs). In this work, we use $P(0)$ as our primary observable, which is also sufficient, to detect the domain-wall effects instead of studying the complex interfaces at finite temperatures. We propose to compare $P(0)$ of PBCs and FBCs to answer the question. Our strategy is as follows: (1) If domain-wall effects dominate, FBCs should have stronger ordering than PBCs as domain-wall effects are reduced, and (2) If droplet excitations dominate, FBCs should make the ordering weaker or not change for finite systems, as droplet excitations are easier at the surface of the system. In this context, a stronger ordering means a smaller $P(0)$ and a weaker ordering means a larger $P(0)$. To be more quantitative, if domain-wall effects dominate, we expect $P(0)$ to drop by a constant amount with little or no system size

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dependence as domain walls impact all system sizes in the same manner [26]. On the other hand, if droplet excitations dominate, the difference of $P(0)$ of PBCs and FBCs is expected to be a decreasing function of system size and converges to zero since the fraction of surface spins decreases to zero in the thermodynamic limit.

Thermal boundary conditions (TBCs) [23] were used to reduce domain-wall effects, answered this question to some extent, and indicated that the answer is perhaps negative. The answer however is not completely clear, because TBCs limit fluctuations only between periodic and antiperiodic boundary conditions according to the Boltzmann weights in each spatial direction, can still trap domain walls, and also overlaps between different boundary conditions are introduced. In this work, we minimize the domain-wall effects using FBCs. FBCs are probably the best boundary conditions one can work with to separate the two effects. Our results show that droplet excitations dominate $P(0)$, in line with that of TBCs.

It is also well known that FBCs introduce new finite-size effects as a substantial fraction of the spins are on the surface, which could be misleading when looking for a trend with limited system sizes. Therefore, it is crucial to compare FBCs with PBCs in interpreting the FBC data properly. FBCs were used in the early work of Ref. [14] in revealing the nature of ordering of short-range spin glasses, and results for small system sizes were reported. In this work, we conduct large-scale Monte Carlo simulations, focusing in particular on $P(0)$ as a function of the system size in both three and four dimensions. The comparison of the PBC and FBC overlap functions suggests that they are likely to have the same thermodynamic limit. The existence of low-energy droplet excitations and whether droplet excitations and domain walls have the same stiffness exponent have also been intensively studied. In Refs. [7,45], a small perturbation is added to the Hamiltonian such that the ground state energy increases more than the excited states to detect changes in the ground state, and hence the existence of low-energy droplet excitations. In Ref. [46], various forms of droplet excitations are generated and the stiffness exponents are measured in two dimensions.

The paper is organized as follows. We first discuss the model, simulation methods, and observables in Sec. II, followed by numerical results in Sec. III. Concluding remarks are stated in Sec. IV.

II. MODELS, METHODS, AND OBSERVABLES

We study the three-dimensional (3D) and four-dimensional (4D) Edwards-Anderson Ising spin-glass model [1] defined by the Hamiltonian

$$H = -\sum_{\langle ij\rangle} J_{ij} S_i S_j, \qquad (1)$$

where $S_i = \pm 1$ are Ising spins and the sum is over nearest neighbors on a hypercubic lattice of linear size L with number of spins $N = L^{\mathrm{D}}$. The random couplings J_{ij} are chosen from a Gaussian distribution with mean 0 and variance 1. A set of couplings $\{J_{ij}\}$ defines a disorder realization. We apply free boundary conditions, as well as periodic boundary conditions to each instance. The simulation is carried out using population annealing Monte Carlo [47–50]. The simulation parameters are summarized in Table I. Note that the transition temperatures are $T_C \approx 1$ in three dimensions [51] and $T_C \approx 1.8$ in four dimensions [52].

TABLE I. Simulation parameters for the 3D and 4D EA model using population annealing Monte Carlo. D is the dimension of the system, BC is the boundary condition, L is the linear system size, R_0 is the population size, T_0 is the lowest temperature simulated, N_T is the number of temperatures used in the annealing schedule, which is linear in β, and M is the number of disorder realizations studied. $N_S = 10$ sweeps are applied to each replica at each temperature.

D	BC	L	R_0	T_0	N_T	M
3	FBC	4	$5\,10^4$	0.20	101	5000
3	FBC	6	$2\,10^5$	0.20	101	5000
3	FBC	8	$5\,10^5$	0.20	201	5000
3	FBC	10	10^6	0.20	301	5000
3	FBC	12	10^6	0.33	301	5000
4	FBC	3	$2\,10^4$	0.36	101	5000
4	FBC	4	$5\,10^4$	0.36	101	5000
4	FBC	5	10^5	0.36	101	5000
4	FBC	6	$2\,10^5$	0.36	201	5000
4	FBC	7	$5\,10^5$	0.36	201	4400
4	FBC	8	$8\,10^5$	0.72	301	2000
4	PBC	3	$2\,10^4$	0.36	101	3000
4	PBC	4	$5\,10^4$	0.36	101	3000
4	PBC	5	10^5	0.36	101	3000
4	PBC	6	$2\,10^5$	0.36	201	3000
4	PBC	7	$5\,10^5$	0.36	201	3000
4	PBC	8	$8\,10^5$	0.72	301	3000

We study the spin overlap q defined as

$$q = \frac{1}{N}\sum_i S_i^{(1)} S_i^{(2)}, \qquad (2)$$

where spin configurations (1) and (2) are chosen independently from the Boltzmann distribution, and its statistic $I(q_0)$,

$$I(q_0) = \int_{-q_0}^{q_0} P(q)dq. \qquad (3)$$

We study $I(0.2)$ unless otherwise specified.

III. RESULTS

In this section, we present our numerical results. We discuss the 3D results in Sec. III A and the 4D results in Sec. III B.

A. Three dimensions

The disorder-averaged spin overlap distributions $P(q)$ for periodic and free boundary conditions are shown in Fig. 1. The data for PBCs are taken from a previous study of Ref. [23]. Both display peaks at finite-size values of $\pm q_{\mathrm{EA}}$, with the Edwards-Anderson order parameter q_{EA} decreasing with L. For PBCs at small q the distribution is nearly independent of L, consistent with many past studies [7,11,14,20].

The statistic I as a function of system sizes is shown in Fig. 2. We find that the FBC ordering gets *weaker* rather than stronger compared with PBCs, with noticeable size corrections. This suggests that trapped domain walls in PBCs

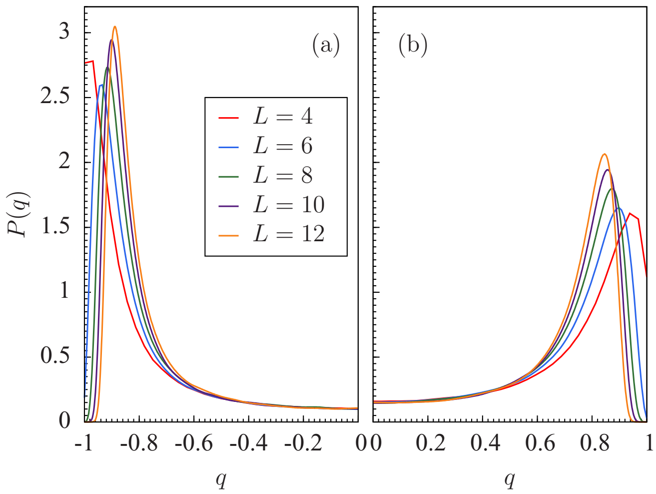

FIG. 1. Disorder-averaged spin overlap distributions $P(q)$ in three dimensions for sizes $L = 4,6,8,10$, and 12 at $T = 0.42$ with (a) periodic and (b) free boundary conditions. The finite-size values of $\pm q_{\mathrm{EA}}$ decrease with system size. Note that FBCs are less ordered than PBCs for the system sizes studied. (a) PBC; (b) FBC.

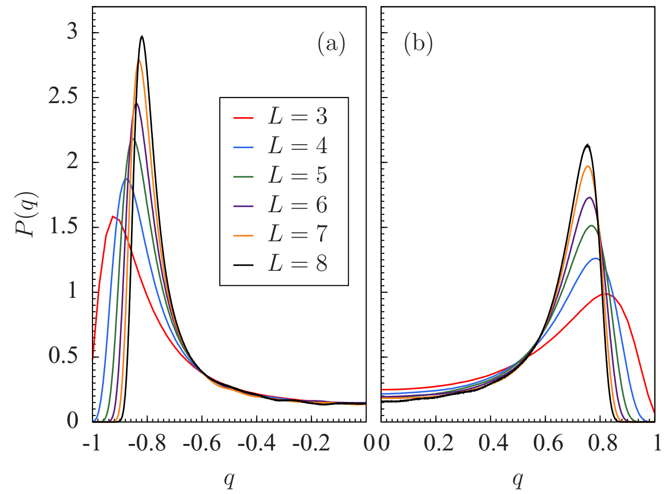

FIG. 3. Disorder-averaged spin overlap distributions $P(q)$ in four dimensions for sizes $L = 3$, 4, 5, 6, 7, and 8 at $T = 0.72$ with (a) periodic and (b) free boundary conditions. The finite-size values of $\pm q_{\mathrm{EA}}$ decrease with system size. Note that FBCs are less ordered than PBCs for the system sizes studied. (a) PBC; (b) FBC.

cannot be used to argue why $P(0)$ is finite, and droplet excitations are at work. For very small system sizes, I appears to decrease with system size, similar to what was found in Ref. [14]. However, as system size gets larger, this trend does not appear to hold, especially at the lower temperature $T = 0.2$, PBCs appear to provide a lower bound for FBCs. The same appears to hold in four dimensions, as shown in the next section.

It is easy to understand why I is larger for small system sizes in FBCs than PBCs if droplet excitations dominate. If droplet picture holds, larger droplets can be excited by taking advantage of the free bonds on the surface. But I would eventually become trivially the same and become zero when system size gets larger, as the free energy cost inside the system would dominate and diverge, the free bonds on the surface will not help. If on the other hand RSB is correct, we again expect the excitations can take advantage of the free bonds on the surface, and expect this effect to be increasingly less important for larger system sizes. This would naturally suggest the same thermodynamic limit for FBCs and PBCs. Furthermore, the insensitivity of metastates to boundary conditions in the nonstandard RSB [33,35] with chaotic size dependence also supports the scenario that FBCs and PBCs have the same thermodynamic limit. Therefore, we believe that the PBC I is not only a lower bound for FBCs, but the two would eventually become the same in the thermodynamic limit. Our numerical results appear to support this conjecture, especially in four dimensions and lower temperatures, where finite-size effects are smaller.

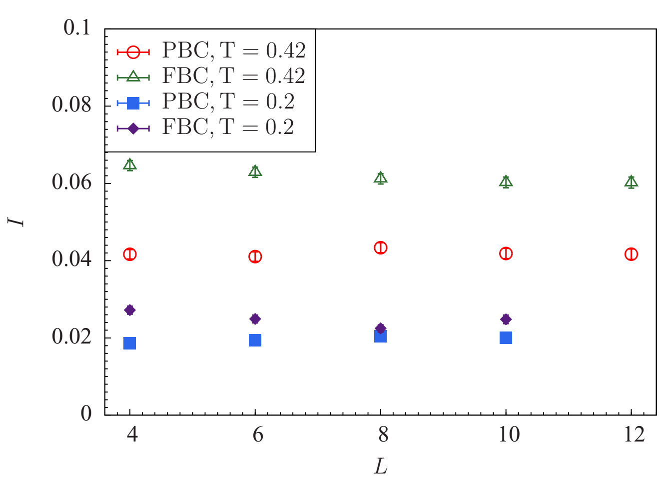

FIG. 2. I as a function of system size L in three dimensions for periodic and free boundary conditions. I is approximately a constant for PBCs, and is a fast decreasing function at small L for FBCs, but appears to level off and is bounded by the values of the PBCs when L increases.

B. Four dimensions

The overlap distribution $P(q)$ and the statistic I for PBCs and FBCs are shown in Figs. 3 and 4, respectively. Similar behaviors as in three dimensions are found except that the trend becomes more profound. By looking at I of FBCs alone, one may like to argue that I is a decreasing function of L. However, we believe this is due to the strong finite-size effects of FBCs. Note that in three dimensions, I is also a decreasing function of L up to around $L \approx 8$, and only appears to decrease more slowly or level off thereafter. We expect I of FBCs is still bounded and will converge to that of PBCs in four dimensions. It is easy to understand why the convergence is faster at lower temperatures, where thermal fluctuation is smaller. It is interesting that the convergence is faster in four dimensions than in three when the temperatures are similar (both are around $0.4T_C$ and $0.2T_C$). This could be intuitively understood from the number of neighbors. For example for a spin on the interior of a surface, it will lose one neighbor out of a total of eight neighbors in four dimensions but only six neighbors in three dimensions. Therefore, the effects

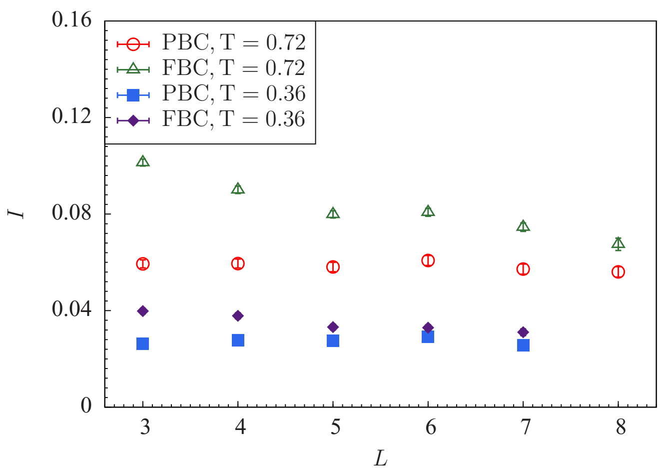

FIG. 4. I as a function of system size L in four dimensions for periodic and free boundary conditions. I is approximately a constant for PBCs, and is a fast decreasing function of L for FBCs, but appears to level off and is bounded by the values of the PBCs when L increases. The fluctuation at $L = 5$ and 6 is likely due to even-odd effects for small system sizes.

of FBCs will be a decreasing function of dimensionality, except for very small system sizes where the fraction of surface spins would dominate. This simple explanation is in agreement with the more quantitative or generic explanation that the correlation function decays faster in four dimensions or the sample stiffness exponent is much larger in four dimensions, as discussed in greater detail in the following text. This consideration gives more weight to our conjecture that the overlap distribution of FBCs and PBCs has the same thermodynamic limit, as finite-size effects are smaller in four dimensions than in three.

Finally we analyze quantitatively our data with curve fitting using ansatz scalings of both the RSB and the droplet pictures. The goal is to test if the asymptotic values of I of PBCs and FBCs are the same, and also which picture our data fit best. We use the following scaling functions:

$$I_{\text{RSB}} = a_1/L^{\theta'} + c, \tag{4}$$

$$I_{\text{DS}} = a_2/L^{b}, \tag{5}$$

for RSB fits and droplet fits, respectively.

The exponent θ' within the RSB theory, controls the algebraic decay of the correlation function within the $q = 0$ sector. We use the known exponents $\theta' = 0.38(2)$ in three dimensions [19,53] and $\theta' = 1.0(1)$ in four dimensions [54] to reduce the degree of freedom. For the droplet picture, one may like to use the stiffness exponent θ which is $\theta \approx 0.2$ in three dimensions [23] and $\theta \approx 0.7$ in four dimensions [55,56]. However, these fits are going to be poor as one can easily see especially for PBCs that such strong decays do not present for the system sizes accessible. Therefore, we relax this exponent as a fitting parameter b. In this way, one can compare b with θ to see if the $1/\ell^{\theta}$ decay is observed. Note that this also makes both fits have two fitting parameters. The results are listed in Table II.

One interesting result is in the c column. We see that the asymptotic I of PBCs and FBCs with the RSB fits are compatible within statistical errors, in agreement with our conjecture. On the other hand, I would become 0 for the droplet picture by construction. The goodness of fits Q for RSB and droplet are similar. However, some of the exponents b have very large statistical errors, suggesting the absence of the $1/\ell^{\theta}$ decay. Furthermore, the exponents b are far from θ. Therefore, it is reasonable to conclude the data fit the RSB picture better than the droplet picture.

IV. CONCLUSIONS AND FUTURE CHALLENGES

In this work, we studied whether the finite $P(0)$ observed in numerical simulations of the EA model in three and four dimensions is dominated by domain walls or droplet excitations. To this effort, we compared the spin overlap distribution functions of periodic and free boundary conditions, as the two effects make dramatically different predictions for $P(0)$ when we change the boundary conditions from PBCs to FBCs. Our results suggest that droplet excitations, not domain walls, are the main contribution to small overlaps. Our data at different temperatures and dimensions also suggest that the overlap distributions of PBCs and FBCs are likely to have the same thermodynamic limit. A rigorous proof of this would be interesting, yet challenging as FBCs are not gauge related to PBCs.

If we believe in this conjecture, our results show that the initial decrease of $P(0)$ of FBCs is a result of finite-size effects, not the onset of the droplet picture. Therefore, our data for the statistic I in FBCs are still a support of the RSB picture, as in PBCs. Furthermore, our results indicate that it is important

TABLE II. Fitting parameters of the RSB and droplet fits of the statistic I using Eqs. 4 and 5. D is the dimensionality, T is the temperature, BC is the boundary condition, a_1,a_2,b,c are fitting parameters, and Q_1, Q_2 are the goodness of fits.

D	T	BC	a_1	c	Q_1	a_2	b	Q_2
3	0.42	FBC	0.0235(33)	0.0508(16)	0.9837	0.0709(16)	0.0684(111)	0.9759
3	0.42	PBC	−0.0023(98)	0.0430(46)	0.6468	0.0405(55)	−0.0267(660)	0.2688
3	0.20	FBC	0.0185(259)	0.0158(129)	0.0794	0.0323(123)	0.1364(2008)	0.0614
3	0.20	PBC	0.0098(71)	0.0244(35)	0.8520	0.0162(35)	−0.1092(1107)	0.6591
4	0.72	FBC	0.1540(240)	0.0509(49)	0.0311	0.1542(133)	0.3856(522)	0.0386
4	0.72	PBC	0.0123(141)	0.0560(29)	0.6381	0.0635(52)	0.0489(478)	0.6777
4	0.36	FBC	0.0475(115)	0.0246(26)	0.5065	0.0558(58)	0.2975(671)	0.5548
4	0.36	PBC	−0.0029(176)	0.0279(39)	0.3927	0.0261(69)	−0.0150(1632)	0.3087

to compare FBCs with PBCs for future studies with FBCs to avoid misleading conclusions due to the strong finite-size effects of FBCs.

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