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Finite-Size Scaling of the Domain Wall Entropy Distributions for the 2D $\pm J$ Ising Spin Glass

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The statistics of domain walls for ground states of the 2D Ising spin glass with $+1$ and -1 bonds are studied for $L \times L$ square lattices with $L \leq 48$, and $p = 0.5$, where p is the fraction of negative bonds, using periodic and/or antiperiodic boundary conditions. When L is even, almost all domain walls have energy $E_{dw} = 0$ or 4. When L is odd, most domain walls have $E_{dw} = 2$. The probability distribution of the entropy, S_{dw}, is found to depend strongly on E_{dw}. When $E_{dw} = 0$, the probability distribution of $|S_{dw}|$ is approximately exponential. The variance of this distribution is proportional to L, in agreement with the results of Saul and Kardar. For $E_{dw} = k > 0$ the distribution of S_{dw} is not symmetric about zero. In these cases the variance still appears to be linear in L, but the average of S_{dw} grows faster than $\sqrt{L}$. This suggests a one-parameter scaling form for the L-dependence of the distributions of S_{dw} for $k > 0$.

KEY WORDS: Ising spin glass, domain wall entropy, finite-size scaling

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1. INTRODUCTION

There continues to be a controversy about the nature of the Ising spin glass. The Sherrington-Kirkpatrick model,[1] with its infinite-range interactions between the spins, is described by the Parisi replica-symmetry breaking mean-field theory.[2,3] To understand models with short-range interactions on finite-dimensional lattices, however, it is necessary to include the effects of interfaces, which do not exist in a well-defined way in an infinite-range model. The droplet model of Fisher and Huse,[4–6] which starts from the domain-wall renormalization group ideas of McMillan[7–9] and Bray and Moore,[10–12] and studies the properties of interfaces, provides a very different viewpoint on the spin-glass phase.

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In two dimensions (2D), the spin-glass phase is not stable at finite temperature. Because of this, it is necessary to treat cases with continuous distributions of energies (CDE) and cases with quantized distributions of energies (QDE) separately.[11,13]

In three or more space dimensions, where a spin-glass phase is believed to occur at finite temperature T, the general framework of thermodynamics requires that the CDE and the QDE should be treated on the same footing. The way this comes about is that in these cases the typical domain wall energy increases as a positive power of the size of the lattice. Thus the quantization energy becomes a negligible fraction of the domain wall energy for large lattices. All bond distributions behave in a qualitatively similar way, except that the QDE have finite ground state entropies.[6,11]

Amoruso, Hartmann, Hastings and Moore[14] have recently proposed that in 2D there is a relation

$$d_S = 1 + \frac{3}{4(3+\theta_E)}, \tag{1}$$

where d_S is the fractal dimension of domain walls, and θ_E is the exponent which characterizes the scaling of the domain wall energy with size. For the CDE case, the existing numerical estimates of d_S and θ_E satisfy Eq. (1). However, it is unclear if Eq. (1) should continue to be correct when the scaling exponent for spin correlations, η, is not zero. For the QDE, the current estimates[15,16] find $\eta \approx 0.14$.

In three dimensions it is known from the droplet theory,[5,6,12] that for the QDE, which have a positive entropy at $T = 0$, in the spin-glass phase

$$d_S = 2\theta_S. \tag{2}$$

θ_S is the exponent for the scaling of domain wall entropy with size. Thus, for the QDE, Eq. (1) provides a relation between the scaling of the energy and the entropy of domain walls. It is not known how to calculate d_S directly for the QDE case, so we need to use Eq. (2) to check Eq. (1) in that case. One might hope that this relation would also hold in 2D, even though the spin-glass order only occurs at $T = 0$.

For the QDE, it is known that $\theta_E = 0$.[13,17] Then using Eq. (1) gives $d_S = 5/4$, or using Eq. (2), $\theta_S = 5/8$. The calculation of θ_S by Saul and Kardar,[18,19] found $\theta_S = 0.49 \pm 0.02$. Since d_S cannot be less than 1, this result was interpreted as a strong indication that $\theta_S = 1/2$.

In this work we will find that Eq. (1) may not work for the QDE case in 2D. It appears, however, that Eq. (2) is still correct in 2D, except when the domain wall energy, E_{dw}, is zero. The actual behavior of the QDE probability distributions under finite-size scaling turns out to be more subtle than what has been assumed until recently.[20,21] As pointed out by Wang, Harrington and Preskill,[22] domain walls of zero energy which cross the entire sample play a special role when the energy is quantized.

We will analyze data for the E_{dw} and for the domain wall entropy, S_{dw}, for the ground states (GS) of 2D Ising spin glasses obtained using a slightly modified version of the computer program of Galluccio, Loebl and Vondrák,[23] which is based on the Pfaffian method. The Pfaffians are calculated using a fast exact integer arithmetic procedure, coded in C++. Thus, there is no roundoff error in the calculation until the double precision logarithm is taken to obtain S_{dw}. This extended precision is essential, in order to obtain meaningful results for entropy differences at large L. An earlier version of the domain wall entropy calculation,[21] using data provided by S. N. Coppersmith,[24] was limited to small $L \times L$ lattices with even L and came to somewhat different conclusions.

We will demonstrate that for $L \times L$ square lattices the Edwards-Anderson[25] (EA) model with a $\pm J$ bond distribution has a strong correlation between E_{dw} and S_{dw} for the GS domain walls. Because of this correlation, we will need to treat domain walls of different energies as distinct classes. We will find that the scaling parameter identified by Saul and Kardar[18,19] is the one associated with domain walls having $E_{dw} = 0$. It is not, however, the one which controls the dominant behavior for large L.

The Hamiltonian of the EA model for Ising spins is

$$H = -\sum_{\langle ij \rangle} J_{ij} \sigma_i \sigma_j, \tag{3}$$

where each spin σ_i is a dynamical variable which has two allowed states, $+1$ and -1. The $\langle ij \rangle$ indicates a sum over nearest neighbors on a simple square lattice of size $L \times L$. We choose each bond J_{ij} to be an independent identically distributed quenched random variable, with the probability distribution

$$P(J_{ij}) = p\delta(J_{ij} + 1) \; + \; (1 - p)\delta(J_{ij} - 1), \tag{4}$$

so that we actually set $J = 1$, as usual. Thus p is the concentration of antiferromagnetic bonds, and $(1 - p)$ is the concentration of ferromagnetic bonds.

2. GROUND STATE DOMAIN WALLS

We define the GS entropy to be the natural logarithm of the number of ground states. For each sample the GS energy and GS entropy were calculated for the four combinations of periodic (P) and antiperiodic (A) toroidal boundary conditions along each of the two axes of the square lattice. We will refer to these as PP, PA, AP and AA. In the spin-glass region of the phase diagram, the variation of the sample properties for changes of the boundary conditions is small compared to the variation between different samples of the same size,[19] except when p

is close to the ferromagnetic phase boundary and the ferromagnetic correlation length becomes comparable to L.

We define domain walls for the spin glass as it was done in the seminal work of McMillan.[8] We look at differences between two samples with the same set of bonds, and the same boundary conditions in one direction, but different boundary conditions in the other direction. Thus, for each set of bonds we obtain domain wall data from the four pairs (PP,PA), (PP,AP), (AA,PA) and (AA,AP). The reader should remember that the term "domain wall," as used in this work, refers only to this procedure. Saul and Kardar[18,19] follow the same procedure used in this work, but use the term "defect" instead of "domain wall."

The domain-wall renormalization group of McMillan[7] is based on the idea that we are studying an effective coupling constant which is changing with L. For the CDE case we can use the energy as the coupling constant. For the quantized energy case, what we need to do is a slight generalization of this idea. We should think of the coupling constant as the free energy at some infinitesimal temperature. When we do this, the entropy contributes to the coupling constant. As we will see, the distribution of E_{dw} rapidly becomes essentially independent of L as L becomes large, except that there are separate distributions for even L and odd L. Under these conditions, it becomes possible to treat each value of E_{dw} as a separate class, representing a different coupling constant.

The domain wall entropy, S_{dw}, is defined, by analogy to E_{dw}, to be the difference in the GS entropy when the boundary condition is changed along one direction from P to A (or vice versa), with the boundary condition in the other direction remaining fixed. $[S_{dw}]$, where the brackets [ ] indicate an average over random samples of the J_{ij}, is expected to increase as a positive power of L for any E_{dw}. Therefore, these coupling constants must eventually, at large enough L, be controlled by $[S_{dw}]$ for any $T > 0$. Of course, the value of L which is needed for this to happen depends in T. The droplet model assumes that all these coupling constants, except for the $E_{dw} = 0$ case which has a special symmetry, are equal.

As long as $E_{dw} > 0$, the two boundary conditions which we are comparing are not on an equal footing. As Wang, Harrington and Preskill[22] express the situation, the $E_{dw} > 0$ domain wall does not destroy the topological long-range order. However, in the $E_{dw} = 0$ case the two boundary conditions are on an equal footing, and the topological order is destroyed. Therefore the $E_{dw} = 0$ class of domain walls can be expected to behave in a special way, which differs from the prediction of the droplet model.

It is natural to wonder if topological long-range order can be related to replica-symmetry breaking, and if the $E_{dw} = 0$ domain walls can be described by the replica-symmetry breaking theory. We will not attempt to do this here.

It is important to realize that the meaning of a domain wall is very different when the GS entropy is positive, as in the model we study here, as compared to the standard case of a doubly degenerate ground state. In the standard case one can identify a line of bonds which forms a boundary between regions of spins belonging to the two different ground states. It is not possible, in general, to do that when there are many ground states. Despite this, we continue to use the term "domain wall."

When L is even, the energy difference, E_{dw}, for any pair must be a multiple of 4. When L is odd, E_{dw} is $4n + 2$, where n is an integer.[11] The sign of E_{dw} for a pair is essentially arbitrary for $p = 1/2$. Thus we can, without loss of generality, choose all of the domain-wall energies to be non-negative.

3. NUMERICAL RESULTS

Our calculated statistics for E_{dw} at $p = 0.5$, as a function of L, for even L and odd L are given in Table I and Table II, respectively. For each L, 500 distinct random configurations of bonds were studied. We obtain four McMillan pairs for each random sample, so we have 2000 sets of E_{dw} and S_{dw} at each L. For even $L > 10$ it turns out, crudely speaking, that about 77% of the time we find $E_{dw} = 0$, and 23% of the time $E_{dw} = 4$. For odd $L > 20$, $E_{dw} = 2$ about 98.5% of the time. No domain walls with energies greater than 8 were observed at any L for these values of p. This, however, does not have much fundamental significance. The probability distribution for E_{dw} is also a weak function of p,[21] and a strong function of the aspect ratio of the lattice.[28] Our results are consistent with the results of Amoruso *et al.*[13]

It is interesting to note that Wang, Harrington and Preskill[22] use an analytical argument to predict that f_0, the fraction of $E_{dw} = 0$ walls, is approximately 0.75, independent of p, in the spin-glass regime. However, the value of f_0 depends strongly on the aspect ratio of the lattice,[28,29] and it is not clear why this analytical

Table I. Domain wall energy statistics for $p = 0.5$ with even L.

L	n_0	n_4	n_8	f_0	f_4
8	1467	530	3	0.7335	0.265
12	1542	458	0	0.771	0.229
16	1515	484	1	0.7575	0.242
24	1578	422	0	0.789	0.211
32	1530	470	0	0.765	0.235
48	1546	450	4	0.773	0.225

Note. The number of random bond configurations studied for each L was 500, and there are four McMillan pairs for each of these. n_i is the number of domain walls of each type having $E_{dw} = k$. f_k is the fraction of domain walls having $E_{dw} = k$.

Table II. Domain wall energy statistics for $p = 0.5$ with odd L.

L	n_2	n_6	f_2
7	1944	56	0.972
11	1960	40	0.980
15	1957	43	0.9785
21	1973	27	0.9865
29	1967	33	0.9835
41	1973	27	0.9865

Note. Column labels as in Table I.

argument should apply only when the aspect ratio is equal to one. It is also completely unclear to this author where the argument uses the fact that $E_{dw} = 0$ domain walls can only occur when L is even.

Estimating the statistical uncertainties in the data precisely is not trivial, due to the fact that the values of E_{dw} obtained from the same set of bonds with the four different pairs of boundary conditions are not statistically independent.[26] An upper bound on the statistical uncertainties is obtained by counting the number of samples, rather than the number of McMillan pairs of boundary conditions.

The probability distribution of S_{dw} for the cases where $E_{dw} = 0$ should be symmetric about 0, and our statistics are consistent with this. If we look at the L-dependence of $[|S_{dw}|]$, shown in Fig. 1(a), we find a scaling exponent

$$\theta_S(0) = 0.500 \pm 0.020 \tag{5}$$

for $E_{dw} = 0$. The result of Saul and Kardar,[18,19] obtained by looking at the distribution of S_{dw} for all values of E_{dw} combined, was $\theta_S = 0.49 \pm 0.02$. To

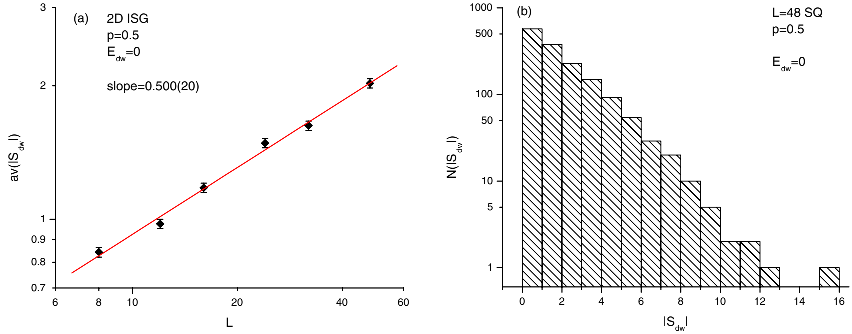

Fig. 1. (color online) (a) Average $|S_{dw}|$ vs. L for the $E_{dw} = 0$ domain walls, log-log plot. The error bars indicate one standard deviation. (b) Histogram of $|S_{dw}|$ for $E_{dw} = 0$ with $L = 48$. The vertical scale is logarithmic.

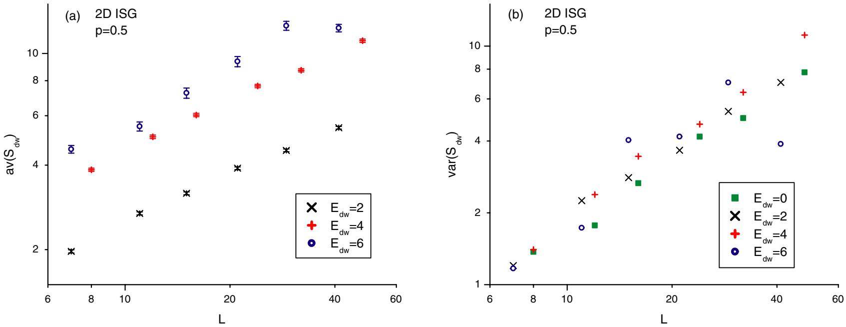

Fig. 2. (color online) (a) Average S_{dw} vs. L for the $E_{dw} > 0$ domain walls, log-log plot. The error bars indicate one standard deviation. (b) Variance of S_{dw} vs. L, log-log plot.

obtain this exponent, Saul and Kardar fit their data at small values of S_{dw}. When L is even, which was the case for all of their data, this part of the data belongs almost entirely to the $E_{dw} = 0$ component.[21]

The calculated means and skewness of these essentially symmetric distributions for S_{dw} is, naturally, consistent with zero, but their kurtosis is not. The reason for this is shown in Fig. 1(b), which is a histogram for $|S_{dw}|$ of $E_{dw} = 0$ when $L = 48$. We see that the distribution is approximately exponential, and therefore far from Gaussian. The computed kurtosis of this $L = 48$ distribution is 2.0, somewhat less than the value of 3 which would be found for an exact two-sided exponential distribution. The basic shape of these distributions is similar for the smaller values of L, with the width of each distribution given by the square root of its variance.

When E_{dw} is not zero, the relative signs of E_{dw} and S_{dw} are not arbitrary. Having chosen E_{dw} to be nonnegative, we then find that, when E_{dw} is positive, it turns out that S_{dw} is usually positive. In Fig. 2(a) we show the behavior of $[S_{dw}]$ for the cases where $E_{dw} = k$, with $k = 2$, 4 and 6, as a function of L. We see that for $k > 0$, the average value of $S_{dw}(L)$ grows approximately as $L^{0.58}$. More precisely, least-squares fits to the form

$$[S_{dw}(L)] = AL^{\theta_S} \tag{6}$$

gives the results for $\theta_S(k)$ shown in Table III. The result for $k = 6$ is rather uncertain, due to the small number of examples of this type. These results are consistent with the prediction of droplet theory,[6] that θ_S should be independent of k (aside from the $k = 0$ case, which is clearly exceptional). However, there also appears to be a tendency for $\theta_S(k)$ to increase as k increases. Therefore, the possibility that $\theta_S \to 5/8$ as $k \to \infty$, which would be consistent with Eq. (1), cannot be excluded by these data.

Because of the large GS degeneracy in the $\pm J$ Ising spin glass, one does not know how to compute d_S directly for this model. However, if we use the droplet model prediction, that there is a single value for θ_S, the result is not consistent with Eq. (1). The author's opinion is that Eq. (1) must be generalized when $\eta > 0$.

As shown by Saul and Kardar,[18,19] the variance of S_{dw} when $E_{dw} = 0$ increases with L in approximately a linear fashion. Calculating the variance of these distributions, and using linear least squares fits on the log-log plot shown in Fig. 2(b), we find that assuming the increase of the variance with L is a power law gives the results shown in Table III. These numbers are reasonably consistent with the hypothesis that the scaling exponent for the variance of the S_{dw} distributions is equal to 1, independent of E_{dw}. It is also interesting to observe that the magnitude of the variance, and not merely the slope of the fit, seems to be independent of E_{dw}. Except in the special $E_{dw} = 0$ case, $2\theta_S$ is greater than 1. Therefore, the exponent d_S should be controlled by θ_S, as predicted by Eq. (2).

4. SCALING OF THE DISTRIBUTIONS

In Fig. 3 we show histograms for the S_{dw} distributions for $E_{dw} = 2$ at $L = 41$ and $E_{dw} = 4$ at $L = 48$. In contrast to the $E_{dw} = 0$ case, the skewness and kurtosis of the S_{dw} distributions for $E_{dw} > 0$ are both small. It is possible that these distributions become Gaussian in the large L limit. However, the author is not aware of any reason why this must happen.

The basic shapes of the histograms in Fig. 3(a) and Fig. 3(b) appear to be the same. Since $2\theta_S > 1$, it seems that the histogram for the $E_{dw} = 4$ case can be mapped onto the histogram for the $E_{dw} = 2$ case at a larger L. A way of expressing this is that for large L the S_{dw} histograms for $E_{dw} = k > 0$ should obey one-parameter scaling in the dimensionless variables

$$g_k(L) = \frac{[S_{dw}]^2}{[(S_{dw})^2] - [S_{dw}]^2}. \tag{7}$$

Table III. Scaling exponents for the first and second cumulants of the S_{dw} distributions.

E_{dw}	θ_S	ϕ_S
0	0.500 ± 0.020	0.992 ± 0.047
2	0.565 ± 0.019	0.972 ± 0.051
4	0.584 ± 0.015	1.107 ± 0.047
6	0.617 ± 0.062	0.85 ± 0.28

Note. θ_S is the scaling exponent for $[S_{dw}]$, and ϕ_S is the scaling exponent for the variance of (S_{dw}).

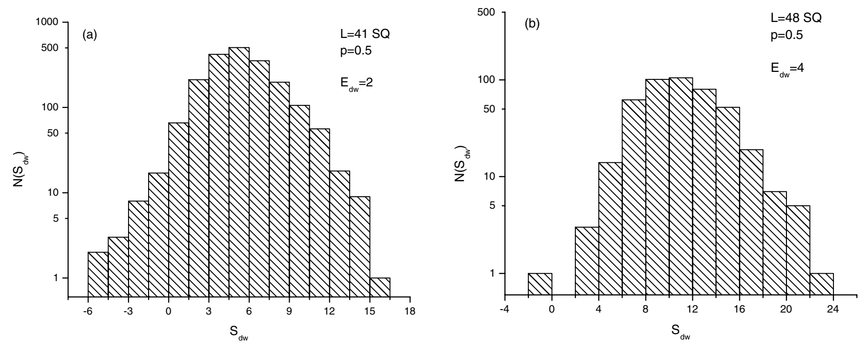

Fig. 3. Histograms of S_{dw} for (a) $E_{dw} = 2$ with $L = 41$ and (b) $E_{dw} = 4$ with $L = 48$. The vertical scales are logarithmic.

If θ_S is independent of k, then, assuming $\phi_S = 1$,

$$g_k(L) = (L/L_k)^{2\theta_S - 1}, \tag{8}$$

where we define L_k by the condition $g_k(L_k) = 1$.

What we have learned is that in this model there appear to be two distinct classes of domain walls, the $E_{dw} = 0$ domain walls and the $E_{dw} > 0$ domain walls. As we have seen, the $E_{dw} > 0$ domain walls behave in a way which appears to be essentially consistent with the predictions of the droplet model, but the $E_{dw} = 0$ domain walls do not. This difference in behavior is due to the symmetry of the $E_{dw} = 0$ case, which forces the average S_{dw} to be zero.

For an $E_{dw} > 0$ domain wall, a large contribution to S_{dw} comes from the shift in the average GS entropy with the shift in the GS energy.[20] What remains to be understood is why $[S_{dw}]$ should scale with L in the way predicted by the droplet model. The conventional derivation of the droplet model[4] uses the assumption that the GS is unique, up to a reversal of the entire state, in an essential way. What follows immediately from this is that $\eta = 0$. An extension of the droplet model to the more general case was given by Fisher and Huse.[6] However, the author hopes that by now he has convinced the reader that a better understanding of the $\eta > 0$ case is needed.

5. SUMMARY

We have studied the statistics of domain walls for ground states of the 2D Ising spin glass with $+1$ and -1 bonds for $L \times L$ square lattices with $L \leq 48$, and $p = 0.5$, where p is the fraction of negative bonds, using periodic and/or antiperiodic boundary conditions, for both even and odd L. Under these conditions, most domain walls have an energy $E_{dw} < 8$. The probability distribution of the entropy, S_{dw}, is found to depend strongly on E_{dw}, but it appears possible to parameterize this dependence in a simple way. The results for S_{dw} do not appear to agree quantitatively with the prediction of Amoruso, Hartmann, Hastings and Moore,[14] Eq. (1). Our results for $[|S_{dw}|]$ when $E_{dw} = 0$ agree with those of Saul and Kardar,[18,19] but in addition we find that the distributions are close to being exponential in that case, even in the limit of large L. Due to the special role of the $E_{dw} = 0$ domain walls, we can understand the difference between the scaling exponent found by Saul and Kardar and the prediction of the droplet model.

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