

Influence of the ground-state topology on domain-wall energy in the Edwards-Anderson $\pm J$ spin glass model

F. Romá and S. Risau-Gusman

Centro Atómico Bariloche and CONICET, R8402AGP San Carlos de Bariloche, Río Negro, Argentina

A. J. Ramirez-Pastor and F. Nieto

Departamento de Física, Universidad Nacional de San Luis and CONICET, Chacabuco 917, D5700BWS San Luis, Argentina

E. E. Vogel

Departamento de Física, Universidad de La Frontera, Casilla 54-D, Temuco, Chile

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We study the phase stability of the Edwards-Anderson spin glass model by analyzing the domain-wall energy. For a bimodal $\pm J$ distribution of bonds, a topological analysis of the ground state allows us to separate the system into two regions: the backbone and its environment. We find that the distributions of domain-wall energies are very different in these two regions for the three-dimensional (3D) case. Although the backbone turns out to have a very high phase stability, the combined effect of these excitations and correlations produces the low global stability displayed by the system as a whole. On the other hand, in two dimensions (2D) we find that the surface of the excitations avoids the backbone. Our results confirm that a narrow connection exists between the phase stability of the system and the internal structure of the ground state. In addition, for both 3D and 2D we are able to obtain the fractal dimension of the domain wall by direct means.

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The spin glass state has been studied extensively during the last thirty years, but the role played by low-energy excitations is still a matter of debate. These excitations are crucial to understand the nature of the ordering of the spin glass phase. Most studies have focused on the predictions of two theories: the replica-symmetry breaking (RSB) picture¹ and the droplet picture.² RSB, rigorously true for the Sherrington-Kirkpatrick model of spin glasses, predicts that there are excitations which involve flipping a finite fraction of the spins and, in the thermodynamic limit, cost only a finite amount of energy. The fractal dimension of the surface of these excitations, d_s , is expected to be equal to the space dimension d . On the other hand, in the droplet picture the lowest-energy excitations of length L have $d_s < d$ and typically cost an energy of order L^θ (θ is known as the stiffness exponent). Thus, contrary to RSB, the droplet picture predicts that excitations involving a finite fraction of spins cost an infinite amount of energy in the thermodynamic limit.

The exponent θ plays a central role in this debate. It is usually calculated by using the concept of defect energy $\Delta E = E^a - E^p$, which is the difference between the ground-state (GS) energies for antiperiodic (E^a) and periodic (E^p) boundary conditions, in one of the directions of a d -dimensional system of linear size L . In ferromagnetic systems, $\Delta E \sim L^\theta$, with $\theta = d_s = d - 1$, because the induced defect is a $(d-1)$ -dimensional domain wall with *all* its bonds frustrated. For spin glasses, the average over the distribution of bonds (denoted by $[\dots]$) must be taken and the scaling ansatz becomes

$$[\Delta E] \sim L^\theta. \quad (1)$$

Assuming that, because of frustration, the defect energy is the sum of many correlated terms of different signs, Fisher and Huse² have shown that for spin glasses $\theta \leq (d-1)/2$.

It is well known that the Edwards-Anderson (EA) $\pm J$ model³ has a degenerate GS. In addition, it has been shown⁴⁻⁶ that, for each realization of the disorder in two dimensions (2D), there are bonds that are either always satisfied or always frustrated in all the GSs. These bonds define the *rigid lattice* (RL) or backbone of the system. Spins connected by it are called *solidary* spins (the rest are denoted *nonsolidary*). Numerical studies in three dimensions (3D) of a similar structure, the *diluted lattice*⁷ (defined by the satisfied bonds of the RL), seem to confirm the existence of the RL in the thermodynamic limit.

Recently, an interesting connection has been found between the RL and both thermodynamic and dynamic properties.⁸⁻¹⁰ For example, in Ref. 10 the slow and fast degrees of freedom associated to the out-of-equilibrium dynamics of the 2D EA $\pm J$ model were shown to be closely related to the solidary and nonsolidary spins, respectively. In this context, one expects that the contributions of the backbone and its environment on the domain-wall energy will be rather different. The present Rapid Communication represents a step in that direction.

In this work we show that in 3D a significant portion of the domain wall is contained in the backbone. Moreover, in this region we find that the defect energy is positive and has a strong size dependence, similar to what happens in a ferromagnetic system. The rest of the system has a negative defect energy and could therefore be considered as an excited phase. The sum of these two defect energies results in the cancellation effect responsible for the weak size dependence observed for the domain-wall energy.^{11,12} On the other hand, we find that in 2D the portion of the domain wall inside the backbone is vanishing. We have also obtained the fractal dimensions of domain wall for both 2D and 3D.

We start by considering the Hamiltonian of the EA model for spin glasses³ on square and cubic lattices,

TABLE I. Parameters of the simulation for each lattice size L in 3D. N_T is the number of temperatures used in the parallel tempering, chosen inside the interval T_{min} to T_{max} (temperatures in units of J/k_B), MCS is the number of Monte Carlo steps needed to reach the GS, and N_S is the number of samples used. N_{GS} is the mean number of GSs used to approximate the average $\langle \langle \dots \rangle_{GS}$ for the antiperiodic system.

L	N_T	T_{min}	T_{max}	MCS	N_S	N_{GS}
3	20	0.1	1.6	2×10^2	1×10^4	3×10^4
4	20	0.1	1.6	2×10^2	1×10^4	5×10^4
5	30	0.1	1.6	2×10^3	6×10^3	2×10^5
6	30	0.1	1.6	2×10^5	3×10^3	4×10^5
7	40	0.1	1.6	2×10^5	1×10^3	1×10^6
8	40	0.1	1.6	2×10^6	3×10^2	2×10^6

$$H = \sum_{(i,j)} J_{ij} \sigma_i \sigma_j, \quad (2)$$

where $\sigma_i = \pm 1$ is the spin variable and (i,j) indicates a sum over nearest neighbors. The coupling constants are independent random variables chosen from $a \pm J$ bimodal distribution.

For 3D lattices and periodic boundary conditions, we determine the RL by using an improvement of the algorithm introduced in Ref. 13, where parallel tempering¹⁴ has been implemented for reaching the GS. The present scheme, called the rigid lattice searching algorithm (RLSA), allows us to obtain true GSs up to $L=12$, where L is the lattice size. However, the maximum size used in this work is $L=8$, because, to obtain the RL, the GS must be reached $3N$ ($N=L^d$) times. An important point is that the set of parameters used in the parallel tempering (see Table I) has not been chosen to equilibrate the system, but to reach quickly a GS configuration. To check this, for each lattice size we have compared the average GS energy per spin, e_0 , calculated from our algorithm, with the value reported in the literature.^{15,16} For example, for $L=8$ we obtain $e_0 = -1.780(1)$, in good agreement with the value $e_0 = -1.7802(5)$ reported in Ref. 16.

For 2D lattices, we have used a different algorithm. It is well known¹⁵ that the problem of finding the GS for a 2D lattice with at least one free boundary condition can be mapped to a minimum weighted perfect matching problem, for which very efficient algorithms exist. To implement the RLSA we have used one of these routines, which has allowed us to calculate the RL up to $L=100$.

As mentioned above, the RL is formed by bonds (*rigid bonds*) which are either always satisfied or always frustrated in all the GSs. The remaining bonds, called *flexible bonds*, form the *flexible lattice* (FL). This allows us to write the Hamiltonian (2) as $H = H_r + H_f$. The subscript r (f) refers to the Hamiltonian restricted to only rigid (flexible) bonds.

To calculate the defect energy we write the GS energy of a particular sample (p) as

$$E^p = E_r^p + E_f^p. \quad (3)$$

Note that, although the GS is degenerate, E^p , E_r^p , and E_f^p remain constants on all configurations of the GS. Next, a

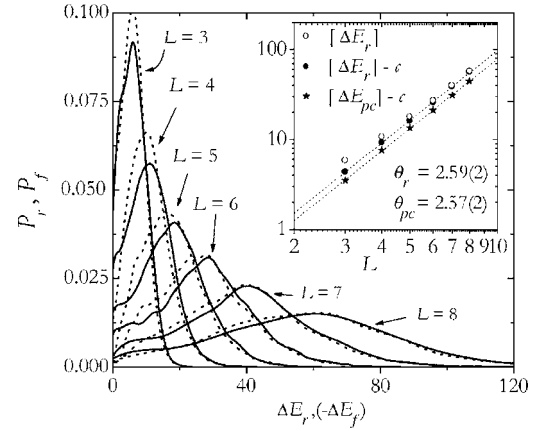


FIG. 1. Distribution P_r (full line) and P_f (dotted line) for 3D. The energy is given in units of J . The inset shows the scaling of $[\Delta E_r]$, $[\Delta E_r] - c$, and $[\Delta E_m] - c$. Error bars are smaller than the symbols.

new sample is generated (a), by introducing antiperiodic boundary conditions in one direction. Its energy can be written as

$$E^a = \langle E_r^a \rangle_{GS} + \langle E_f^a \rangle_{GS}, \quad (4)$$

where the subscripts r and f correspond to the restriction of the Hamiltonian to the bonds that form the RL and FL of the periodic system, and $\langle \dots \rangle_{GS}$ denotes an average over all the GSs of the antiperiodic system.¹⁷ Notice that this average is necessary, because now E_r^a and E_f^a are not constants in all the GSs. Using Eqs. (3) and (4), we write the defect energy as

$$\Delta E = \Delta E_r + \Delta E_f, \quad (5)$$

where $\Delta E_r = \langle E_r^a \rangle_{GS} - E_r^p$ and $\Delta E_f = \langle E_f^a \rangle_{GS} - E_f^p$.

In 3D, we have measured $[\Delta E]$ for each lattice size (due to symmetry arguments, $[\Delta E] = 0$) and we have obtained a finite-size dependence with a small stiffness exponent $\theta \approx 0.2$, in agreement with the result of Refs. 11 and 12. This is seen as an evidence of the existence of a finite critical temperature. We have also measured the distribution of $|\Delta E|$. For the sizes considered, this function extends up to $|\Delta E| = 12J$ (the values of the defect energy are multiples of $4J$). In contrast, for the 3D ferromagnetic Ising model, the defect energy takes the value $128J$ for $L=8$. The small values obtained for the EA model indicate the presence of large sets of frustrated or satisfied bonds that compensate each other.

The main point of this paper is that these sets can be very clearly related to the topology of the system. This can be seen on Fig. 1, which shows the distributions of the contributions of the RL, $P_r(\Delta E_r)$, and the FL, $P_f(\Delta E_f)$, to the domain-wall energy. Two features stand out. On the one hand, ΔE_r is almost always positive. Only a small fraction of samples have $\Delta E_r < 0$, and this fraction decreases with L . Our measurements indicate that on the portion of the domain wall that crosses the RL, the fraction of excitations (rigid bonds always satisfied that appear frustrated in the GS of the antiperiodic system) seems to tend to 0.72. On the other hand, P_r is a broad distribution and extends up to high values

of ΔE_r . In addition, our simulations show that the distribution of ΔE_r seems to be very broad also for fixed values of $|\Delta E|$. For example, for $L=8$, we have found samples with $\Delta E_r = -\Delta E_f = 123.59J$ or $\Delta E_r = -\Delta E_f = 11.63J$, both corresponding to $\Delta E = 0$.

The inset in Fig. 1 shows the scaling of $[\Delta E_r]$ with L . It tends toward a power law behavior of the form

$$[\Delta E_r] \sim L^{\theta_r}. \quad (6)$$

To determine θ_r , we have fitted the data with the function $[\Delta E_r] = c + bL^{\theta_r}$ (which is the simplest correction to scaling). We obtain a good fit for $c=3/2$ and $\theta_r=2.59(2)$. The inset in Fig. 1 shows the scaling of $[\Delta E_r] - c$ with L . Notice that the exponent θ_r is an order of magnitude bigger than the usual stiffness exponent θ (≈ 0.2 for 3D).

The behavior of $P_f(\Delta E_f)$ is very similar to the one observed in P_r , but now ΔE_f is always negative (see Fig. 1). The vanishing of the average domain-wall energy implies that $-\Delta E_f$ follows a power law with the same exponent as $[\Delta E_r]$.

The previous results indicate that the proposal of separating the system in two regions is not trivial: the sections of the domain-wall energy with positive (negative) sign, prevail on RL (FL). However, the system has a small but positive stiffness θ , because on average the defect energy $[\Delta E_r]$ overcomes the defect energy $[\Delta E_f]$.

Our numerical results also allow us to infer that the exponent θ_r is equal to the fractal dimension of the domain wall, d_s . To justify this conjecture, let us consider the topological characteristics of the RL. Our simulations up to $L=8$ indicate that the RL consists mainly of a compact *percolation cluster* (PC).¹⁸ The fraction of the RL that corresponds to this cluster converges to 0.78. The fact that the distributions P_r are vanishing for negative ΔE_r shows that compensation effects are not important in the RL. Assuming that the same happens in the PC and that it behaves as a natural box containing (on average) always the same fraction of domain wall as the whole RL, it is natural to conjecture that the area of the domain wall inside the RL follows a power law L^{d_s} . Therefore, $d_s \approx \theta_r = 2.59(2)$, which agrees with the values reported in the literature for the EA model with Gaussian distributed couplings.¹⁹

To refine this, measurements were carried out separating the system into two new regions: the PC and its environment (now, FL plus small clusters of RL). Then, the defect energy can be written as $\Delta E = \Delta E_{pc} + \Delta E_e$, where the subscripts pc and e refer to the defect energy of PC and its environment, respectively. If we assume again a power law, $[\Delta E_{pc}] \sim L^{\theta_{pc}}$, we obtain $\theta_{pc} = 2.57(2)$, which gives $d_s = \theta_{pc} = 2.57(2)$, consistent with the value quoted above. The inset in Fig. 1 shows the scaling of $([\Delta E_{pc}] - c)$ with L for $c=3/2$.

The picture in 2D is very different. The main problem is that, even though the RL spans a significant portion of the square lattice, it does not percolate.^{6,18} It consists instead of a large number of relatively small islands. The analysis of the difference between periodic and antiperiodic systems reveals that the number of bonds in the RL that belong to the domain wall grows as $\sim L^{0.6}$. But the size of the domain wall is

necessarily larger than L , which implies that the fraction of it that crosses the RL is vanishing with L . Geometrically, what is happening is that the domain wall crosses the sample avoiding the RL islands (notice that this is further evidence that the RL does not percolate). Consequently, in the following we shall use a different strategy for studying the influence of the backbone on the domain-wall energy in the 2D case.

Thus, for each sample, the domain wall depends on the pair of GSs (one GS for the periodic and another for the antiperiodic system) that are being compared. However, with the hope of capturing its relevant properties, for each sample we have picked a single random pair of GSs. But even for a pair of fixed GSs the determination of the domain wall is not trivial. It can be shown¹⁸ that there are some sets of bonds of the periodic system that appear flipped (in the sense that their satisfied bonds become frustrated and vice versa) in the antiperiodic system but do not contribute to the energy change. Notice that this implies that they can also appear flipped in other GSs of the periodic system. Therefore, one must weed out these sets of bonds to get the correct domain wall. The plaquette picture²⁰ provides the best framework for this.

The 2D lattice can be seen as a set of squares, called plaquettes, bounded by four bonds. If an odd number of these bonds are frustrated, the plaquette is called frustrated. It has been shown that plaquettes are frustrated if and only if there is an odd number of ferromagnetic bonds in the boundary.^{20,21} Every spin configuration can be mapped to a perfect matching, which is a set of paths, made of frustrated bonds, that join pairs of frustrated plaquettes. The energy of the system is proportional to the total length (also called weight) of these paths. Thus, finding a GS is equivalent to finding a minimum weighted perfect matching.

To define the domain wall we use, as an example, the system shown in Fig. 2 (generalization is straightforward). To account for the free boundaries two plaquettes must be added, at the top and the bottom (outside the lattice in Fig. 2).¹⁵ The top (bottom) plaquette is called frustrated if there is an odd number of frustrated bonds in the top (bottom) boundary. The antiperiodic boundary condition changes only the frustration of these two plaquettes, which in turn leads to a new matching as GS. From the comparison of the two GSs a set of contours can be defined, where each contour is

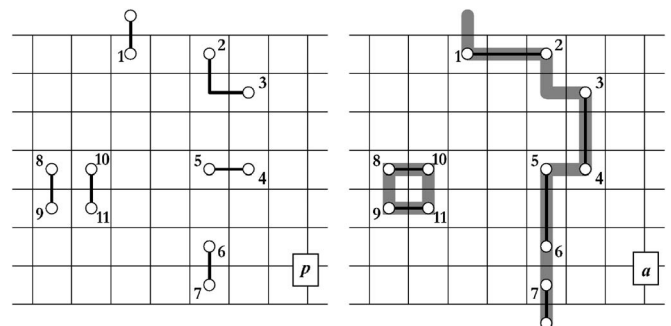


FIG. 2. Matchings corresponding to the ground states of a 2D sample with periodic (left) and antiperiodic (right) boundary conditions on the horizontal direction. Points represent frustrated plaquettes. The gray line crossing the sample is the resulting domain wall.

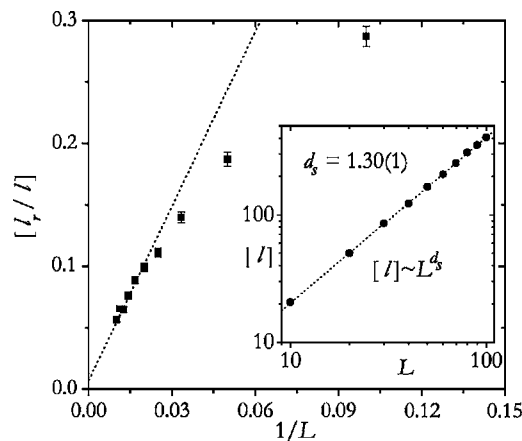


FIG. 3. Scaling of ratio $[l_r/l]$ with $1/L$ for 2D. The inset shows the scaling of $[l]$ with L . Error bars are smaller than the symbols. Averages have been taken over 1000 samples of each lattice size up to $L=100$.

formed by alternating paths from each matching (see Fig. 2). All these contours will be closed (as the one joining plaquettes 8 to 11 in Fig. 2), except for one that runs from the top plaquette to the bottom one. This last contour is the domain wall (it can be proved that the loops do not contribute to the energy change).

The results of simulations performed for several sample sizes are shown in Fig. 3, where both the average length of the wall, $[l]$, and the average fraction of RL bonds in the domain wall, $[l_r/l]$, are shown. As anticipated, this fraction vanishes for large L although a very small, but nonvanishing value, cannot be ruled out. The average length of the domain wall follows a scaling ($[l] \sim L^{d_s}$) that allows us to find its fractal dimension, with $d_s=1.30(1)$. Remarkably, this value coincides with the fractal dimension reported²² for the 2D EA model with a Gaussian distribution of bonds.

In summary, we have studied the relevance of characterizing the domain wall of the EA $\pm J$ spin glass by using topological information of the GS. The defect energy on the RL in 3D shows a behavior typical of a highly stable phase

(similar to the 3D ferromagnetic Ising model, but with $d_s > 2$). On the other hand, the FL shows a very different behavior, like a system in an excited state. The total defect energy ΔE is the result of these competitive and correlated effects (the whole system shows a low stability with a small stiffness exponent).

The 2D case is very different. We have shown that the defect energy avoids the RL, lying almost completely on FL (which percolates in 2D). If we assume that the RL is the only structure able to support a stable phase, then this behavior is compatible with an unstable phase and a zero critical temperature. This agrees with most recent studies (see, e.g., Ref. 23).

In addition, for both dimensionalities we obtain the fractal dimension of the domain wall by direct means. These values are in good agreement with the ones reported in the literature for the EA model with Gaussian distributed couplings.

We want to stress that our work is yet another indication that separating the contributions of the backbone and its environment provides relevant and nontrivial information about the nature of the critical behavior of the $\pm J$ EA model. We believe that this separation should also be important in the study of other physical quantities. Moreover, this analysis can be applied to the other systems (e.g., K-satisfiability problem,²⁴ Viana-Bray spin glass,²⁵ etc.) that are known to have a backbone.

We are working to extend the concept of backbone to systems with nondegenerated GSs, as happens with continuous distributions of bonds. Results are still too preliminary to be reported here.

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¹⁷Because of the rapid growth of the number of the GSs, the average has been approximated using a large number of randomly sampled GSs, N_{GS} (see Table I).

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