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Ferromagnetic random-bond Ising model: Metastable states and complexity of the energy surface

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Metastable states of the ferromagnetic random-bond Ising model are produced by simulated quenches from infinite to zero temperature. Two-dimensional systems (square lattice) show many domains: the many-valley picture of the energy surface of spin glasses applies to these unfrustrated systems as well. The number of the domains, which serves as a rough measure of the complexity of the energy surface in two dimensions (but not in three), is only 30% greater for a broad bond distribution (uniform from 0 to 1) than for a narrow one (uniform from 0.499 to 0.501). We conclude that the uniform-bond model also has a complex energy surface; for a square lattice the surface has many terraces (or steps) rather than many valleys, but for the honeycomb lattice it has a many-valley structure. The large domains in our two-dimensional systems have holes on many length scales and are highly ramified, with total perimeter proportional to the number of sites; their dimensions from the capacity, information, and radius-of-gyration definitions are 1.82 ± 0.06, 1.84 ± 0.04, and 1.83 ± 0.07, respectively. In three dimensions (simple cubic lattice), the initial concentrations of both up and down spins exceed the percolation threshold and the metastable states are dominated by two large spanning domains; only a few, small, embedded domains are found.

I. INTRODUCTION

Although important advances in the theory of the spin glass (in both the short-range[1] and infinite-range[2] versions of the Edwards-Anderson model[3]) have recently been made, many questions remain open; in particular, the free-energy surface of the short-range model is incompletely understood. The work reported in the present article (which deals only with the short-range Edwards-Anderson model) was undertaken in part to determine whether the complexity of this surface is unique to the spin glass; we conclude that it is not.

Most of the theoretical literature (reviews are given in Refs. 4 and 5; see also Ref. 6) on the energy surface of the spin glass concerns the infinite-range model where the barriers have infinite energy in the thermodynamic limit. The states in this model are ultrametric: for any three pure states, at least two of the three overlaps are equal, and, as a consequence, the space of pure states has a hierarchical structure.[2]

In the short-range spin glass (with nearest-neighbor interactions), the metastable states are domain states.[7,8] Consequently, (i) energy barriers are finite in the thermodynamic limit, (ii) the overlaps violate the ultrametricity condition of the infinite-range model, and (iii) the metastable states have a hierarchical or tree structure,[8] at least in naive mean-field theory. These results obviously carry over to unfrustrated nearest-neighbor models.

The many-valley picture of the energy surface figures prominently in spin-glass articles and talks, and one can easily gain the impression that the many-valley picture is unique to the spin glass. This article shows that such is not the case; although both randomness and frustration are essential to the spin glass, *neither* is required for an energy surface with many valleys.

We show that the frustration is unnecessary by showing that a random but unfrustrated model has an energy surface with many valleys; the frustration, however much it increases the density of states in the important low-energy region, however difficult it makes the determination of the ground state, is not required for the many-valley structure.

To show that the randomness is unnecessary is even easier; the many-valley picture applies to some uniform-bond models (such as Ising spins on a honeycomb lattice) as well.

Since a many-valley surface is then not unique to the spin glass, what property is qualitatively different? Certainly not the ultrametricity. If ultrametricity means equality of the overlaps, then the infinite-range spin glass is ultrametric, but the short-range spin glass and the ferromagnetic random-bond model are not; if ultrametricity means that the states have a tree structure, then all three of these models are ultrametric. The obvious answer to the above question is the degeneracy of the ground state and the high density of states at low energy, but is this all?

If there is no other qualitative feature distinct to the spin glass, is the spin glass at least quantitatively different with respect to the number (as distinct from the density) of metastable states in short-range models? We have no direct numerical evidence, but extrapolation of our results on ferromagnetic random-bond Ising models suggests the contrary: the number of metastable states appears not to be significantly larger in the spin glass than for nearly uniform bonds. In support we offer the following argument. By definition, whether turning over a specified clump of spins yields a local energy minimum is determined by local energy considerations in short-range models; the number of metastable states is therefore relatively insensitive to the bond distribution. Support is provided also by ex-

act calculations[9] on one-dimensional models; the number of metastable states is independent of the bond distribution (as long as the distribution is continuous).

Naturally enough, others have come to conclusions similar to ours. Some aspects of our results were anticipated by Bak;[7] in fact, our work was motivated in part by his. Independently, Cieplak and Gawron[10] have reached some of the same conclusions; in their words, "the ground state of a disordered ferromagnet is but one of many local energy minima" and the differences between a disordered ferromagnet and a spin glass are "more of quantity than of quality."

We turn now to a description of our methods and results.

We have studied the metastable states of a random but unfrustrated model, Ising spins interacting via random, ferromagnetic bonds; the model can be viewed as an Edwards-Anderson model of a randomly diluted ferromagnet (for which, however, more realistic models have already been studied[11]). This model has a twofold-degenerate ground state in zero magnetic field. We simulate quenches from infinite to zero temperature by assigning random (± 1) starting values to the spins and then updating the spins (in random order) using single-spin-flip dynamics (nonconserved order parameter) until the system freezes. We then analyze the resulting domain structure.

Our major result (that the many-valley picture describes the energy surface of an unfrustrated model) is discussed above. The bulk of the article deals with a less important topic, the morphology of the domains; a brief summary of results follows.

The two-dimensional systems (square lattice) show a rich domain structure, with many embedded domains of many sizes. The number of domains is only 30% larger for a broad bond distribution (uniformly distributed from 0 to 1) than for a narrow one (uniform from 0.499 to 0.501). The smaller domains are necessarily compact, the larger diffuse, with a continuous transition between the two. The large domains are ramified, with total perimeter proportional to the number of sites.

The three-dimensional systems (simple-cubic lattice) show very different domain structures, with two large spanning domains (each consisting of roughly half the sites) and a few, very small, embedded domains.

The difference in structure between the two- and three-dimensional systems arises because the initial concentrations of both up and down spins are below the site-percolation threshold in two dimensions and above it in three; these thresholds are $p_c \simeq 0.593$ for square lattices and 0.312 for simple cubic; see, for example, Refs. 12 and 13.

II. PROCEDURES

The systems consisted of Ising spins on square and simple-cubic lattices with periodic boundary conditions and nearest-neighbor interactions; the external magnetic field was zero.

The bonds were generated from a uniform distribution; to reduce correlations, we generated a list of random numbers and then assigned these numbers randomly to the bonds. Broad bond distributions (0 to 1) were used in the simulation of ten two-dimensional systems (512^2 sites), a few smaller two-dimensional systems (128^2 sites), and five three-dimensional systems (64^3 sites); narrow distributions (0.499 to 0.501) were used for two square lattices of 512^2 sites.

Initial values of the spins were assigned randomly (± 1 with equal probability).

The updating method can be viewed either as a zero-temperature Monte Carlo calculation (all favorable changes accepted, all unfavorable changes rejected) or as a mean-field calculation (the spin is set equal to the sign of the total field); the two are identical at zero temperature. A site was chosen at random and the field from its nearest neighbors calculated; the spin was flipped if necessary to align it with the internal field and otherwise left alone. Another site was chosen at random and the procedure repeated. The system eventually reached a local minimum in the energy surface, with each spin aligned with the field from its neighbors; at this stage no further flips are possible and the simulation was terminated. Since we were concerned only with the static properties of the spin configurations, and not with the relaxation processes, in the later systems we accelerated the convergence by avoiding the updating of spins known to be correctly oriented. A site in a list of sites to be checked was chosen at random, the spin updated, and the site removed from the list, its nearest neighbors being added to the list if the spin was incorrectly oriented; no check was made whether the spins at the nearest-neighbor sites were correctly oriented or whether these latter sites duplicated sites already in the list. The list initially contained all sites with incorrectly oriented spins as determined by a global check made after several passes through the lattice.

Different bond configurations, different initial values for the spins, and different updating sequences were used for each system.

III. RESULTS: SQUARE LATTICE, BROAD DISTRIBUTION

Table I gives our results for the broad distributions; listed are the mean and standard deviation (representing system to system fluctuations) for the internal energy (per site and per bond), the average broken bond (bonds J_{ij} with $s_i s_j < 0$ are "broken"), the fraction of broken bonds, the fraction of majority spins (like those of Ref. 10, our systems are unmagnetized), the average chord length (measured along the axes of the lattice), the ratio of the perimeter to the number of members in the domain (for large domains), and the number of domains found in a given simulation. Multiplying the fraction of broken bonds by the number of sites gives the total perimeter of the domains.

It is clear from the last entry in Table I (the number of domains) that the energy surface of the two-dimensional systems is highly complex, with many local minima, even in this model with a unique (twofold-degenerate) ground state; as we show later (but which is already obvious), the domains found in a single simulation are only a tiny frac-

TABLE I. Properties of metastable states of two- and three-dimensional Ising models (square and simple-cubic lattices of 512^2 and 64^3 sites, respectively) with random, ferromagnetic bonds uniformly distributed from 0 to 1.

	Square	Simple cubic
Internal energy per site	-0.7471 ± 0.0010	-1.0631 ± 0.0024
Internal energy per bond	-0.3736 ± 0.0005	-0.3544 ± 0.0008
Average broken bond	0.3451 ± 0.0007	0.3877 ± 0.0007
Fraction broken bonds	0.1829 ± 0.0005	0.1878 ± 0.0007
Fraction majority spins	$0.503\ \pm0.003$	$0.507\ \pm0.005$
Average chord length	$5.468\ \pm0.015$	$5.325\ \pm0.021$
Perimeter per number of members	$0.681\ \pm0.008$	$1.127\ \pm0.021$
Number of domains	1490 ± 24	7 ± 2

tion of those possible for a given realization of the bonds. The energy surface is highly complex in three dimensions also, although this is not clear from the table. Obviously frustration is not necessary for a many-valley structure.

The two-dimensional systems contained either one or two infinite clusters with the following forms (in the ten 512^2 systems with broad distributions):

(i) One domain spanning site to site in both directions (eight cases).

(ii) Two domains spanning site to site in one direction (one case).

(iii) One domain spanning site to site in one direction, with no other domain spanning in either direction (one case); this is possible, as is obvious from percolation clusters—an explicit example is a 3^2 system with up spins at sites (1,2), (2,3), (3,2), and (3,3) and down spins at the remainder. Another configuration, two domains with the topology of the stripes of a barber pole joined end to end, was found in a 128^2 system. Somewhat surprisingly (our site concentrations were well below the site percolation threshold), a fifth possibility, no infinite cluster, was not found in any system (presumably because of the strong short-range correlations in our systems); by definition, this latter case is the only configuration in percolation systems below threshold.

Embedded in these large domains were many domains, with sizes ranging from two members to almost half the number of sites, including large domains which spanned side to side but not site to site.

Figure 1 shows domains in a 128^2 system, sites with up and down spins being shown with white and black squares. A white domain spans site to site in both directions; embedded in it is a large black domain which stretches from the lower left to the upper right. Domains exist within other domains, to four levels. Individual domains are only tenuously connected; many can be cut into two parts by flipping a spin or two. Even the spanning paths have narrow necks–recall that the starting concentration of both up and down spins was below the percolation threshold.

The domains do not have simple geometric shapes. The large ones have many arms which wind about, inflate, narrow, reinflate, split into other arms, etc.; penetrating into the domains are large fjords. The domain surfaces (both internal and external) are rough; the interiors of the domains contain many holes, with a broad distribution of length scales. Only the smallest domains are compact and the average chord length is consequently not a measure of the average linear extent of the domains.

The domains superficially resemble percolation clusters, but have considerably more short-range order at the same site concentration; the probability that two nearest neighbors have the same sign (and thus belong to the same domain) is ~0.82. Figure 2 shows how the correlation functions depend on distance; the anisotropy is small (no more than 4×10^{-3} in the probabilities). We have not investigated whether a correlated site percolation model (with preferential occupation of sites which are nearest neighbors of sites already occupied) would yield similar clusters; there is certainly a minor difference—domains of a single site cannot occur in our systems.

That the domains are ramified is shown by Fig. 3, a log-log plot of the total perimeter of each domain versus the number of sites in the domain; both spanning and embedded domains are included. The origin of the linear relation between perimeter and number of members (for

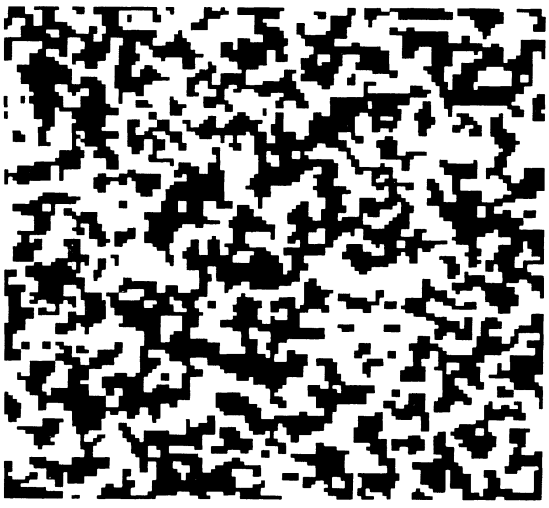

FIG. 1. Domains in a 128×128 Ising system, with periodic boundary conditions, after a simulated quench from infinite to zero temperature, followed by Monte Carlo updating; sites with up (down) spins are shown with white (black) squares.

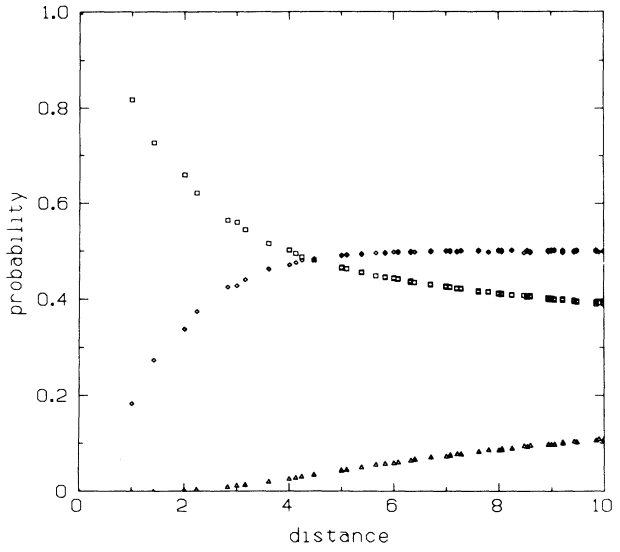

FIG. 2. Spin correlations in a 512^2 system; plotted as functions of distance between the spins are the probabilities that the spins belong to the same domain (squares), have the same sign but belong to different domains (triangles), and have different signs (diamonds).

large domains) is clear from Fig. 1, which shows few homogeneous regions of significant extent; a large region surrounded by spins of one orientation is likely (because of the random starting configuration) to contain a domain of the other. Despite the linear relation, it seems misleading to call the domains stringy, and we have chosen diffuse instead.

Figure 4 shows, for the five largest embedded domains, log-log plots of the number of sites within a circle of radius R (centered at the center of mass) versus R. The plots are too irregular to allow precise determination of an exponent; our systems have strong short-range order, and therefore have strong local inhomogeneities, and the numerical determination of the exponent is more difficult than, for example, for percolation clusters. An exponent of 2 is consistent with the data; that is, the domains appear to be homogeneous on an intermediate length scale. Note the extreme extent of the domains relative to the linear dimension (512 units) of the lattice; a circle of radius 256 units spans the system, but the second largest domain has a site between 527 and 528 units from the center of mass.

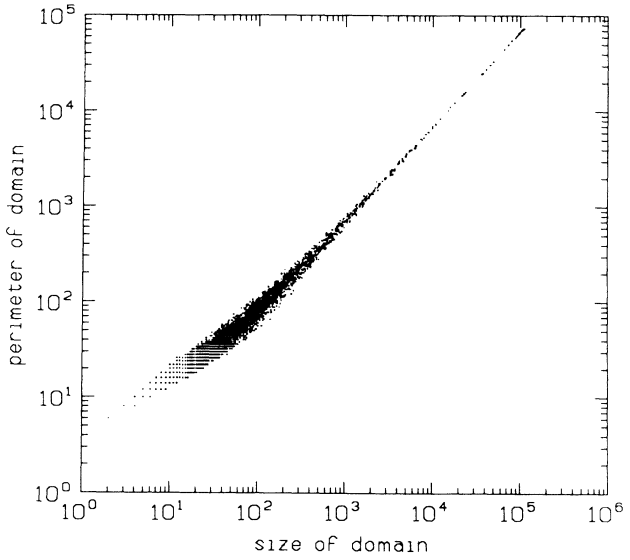

FIG. 3. Log-log plot of the perimeter of each domain vs the number of sites belonging to the domain; the perimeter is proportional to the number of sites for large domains. The knee in the data arises because the smaller domains cannot have holes.

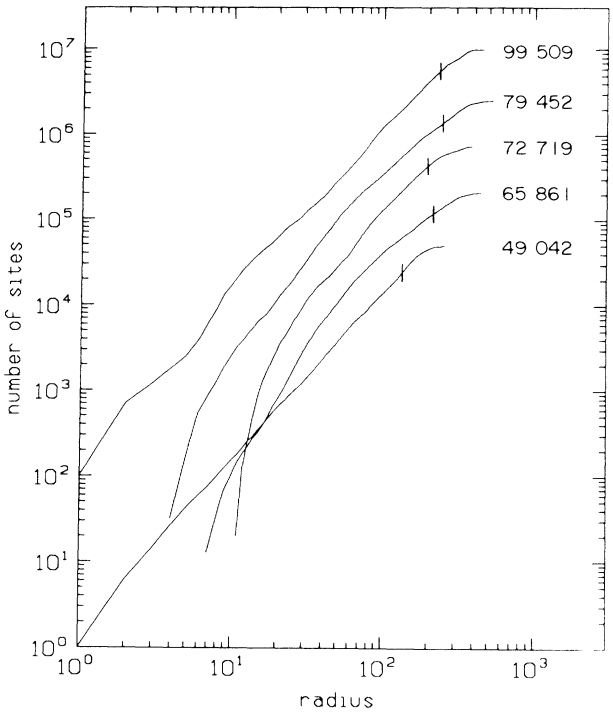

FIG. 4. Log-log plots of the number of sites belonging to a domain and included within a circle of radius R as a function of R for the five largest embedded domains; successive plots are shifted upward by half a decade. The vertical bars mark the radii of gyration; the numbers to the right are the numbers of sites.

Figure 5 plots the radius of gyration of each embedded domain versus the number of sites belonging to the domain. The slope of the best line through the points is 0.54 ± 0.02; that is, the size (number of members) of the domains varies as the radius of gyration to the power 1.83 ± 0.07, definitely less than the Euclidean dimension. This value is consistent with values for the exponent (d_p in Ref. 14) for percolation clusters (both bond and site) at threshold in two dimensions, but the errors are large; our definition of the dimension is the same as in Ref. 14, but we determined the dimension directly whereas Ref. 14 used scaling relations. Our value for the exponent is consistent also with values determined directly[15] (from simulations of site and bond percolation on square lattices at threshold). Note, however, that our site concentration is

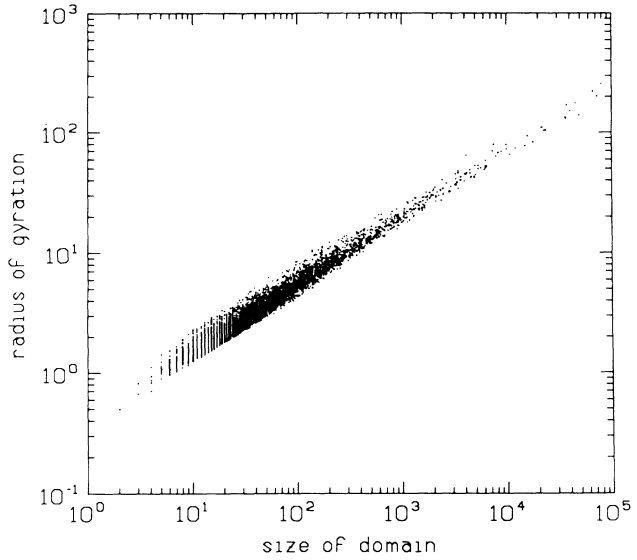

FIG. 5. Log-log plot of the radius of gyration of embedded domains vs the number of members.

considerably below threshold.

Figure 6 shows some examples of the determination of the capacity and information dimensions d_{cap} and d_{inf}. Defining $N(L)$ as the number of squares of side L which contain at least one site belonging to the domain, $P_i(L)$ as the fraction of occupied sites in the ith square, and $S(L)$ as

$$S(L) = -\sum_i P_i(L)\ln[P_i(L)] , \tag{1}$$

we defined d_{cap} and d_{inf} to be the slopes of plots of $\ln[N(L)]$ and $S(L)$ versus $\ln(1/L)$; in the calculation of these quantities, it is necessary to use an extended lattice to treat properly domains which wrap around the boundaries. For obvious reasons the regions of small and large L must be discarded, leaving for the calculation of the dimensions only a small intermediate region ($L = 7$–80 was used), a region so small as to strain, perhaps beyond a reasonable limit, the interpretation of these quantities as fractal dimensions; the plots had noticeable curvature, even over this small interval. Averaging over 15 domains (both spanning and embedded) with more than 4×10^4 members, we find $d_{\text{cap}} = 1.82\pm0.06$ and $d_{\text{inf}} = 1.84\pm0.04$, consistent both with the dimension from the radius of gyration and with the inequality $d_{\text{inf}} \le d_{\text{cap}}$. The information dimension (which arose in another context[16]) and other dimensions are discussed in Refs. 17–19.

Figure 7 shows the distribution of bonds (as a check on the random-number generator) and the distribution of broken bonds; obviously small bonds are more easily broken than large ones, but many large bonds are broken in these quenched systems (which are far from equilibrium).

Figure 8 shows the distribution of internal fields; considerable relaxation will occur at even very small temperatures due to the large weight at small fields; again, the systems are far from equilibrium. Shown for comparison (and as another check on the random-number generator) is the distribution of internal fields in the ferromagnetic state; it approximates a Gaussian, as expected for the sum of four random numbers.

Our systems are likely too small (Ref. 20 studies percolation clusters in lattices of 2.56×10^{10} sites), and certainly too few, to apply a scaling analysis and so we do not present our results on the distribution of domain sizes. There is, in fact, no obvious definition of threshold for our systems, and so it is not all obvious whether a scaling relation should hold.

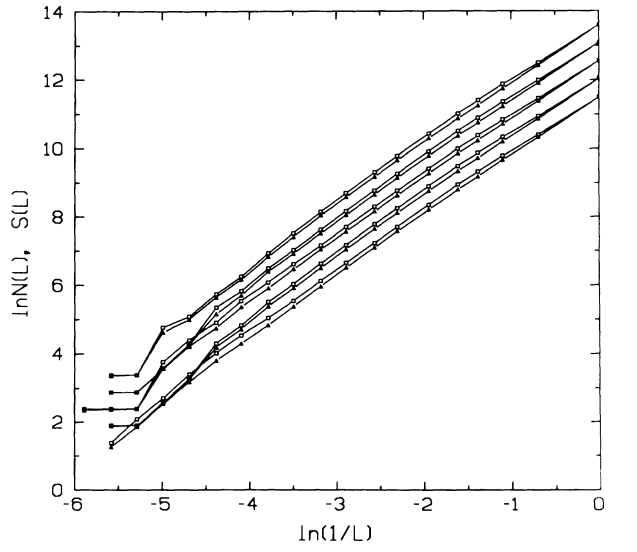

FIG. 6. Sample plots used to determine dimensions from the capacity and information definitions. $\ln[N(L)]$ (squares) and $S(L)$ (triangles) are plotted against $\ln(1/L)$ for the five largest domains, the largest at the top; data are shifted successively upward by 0.5.

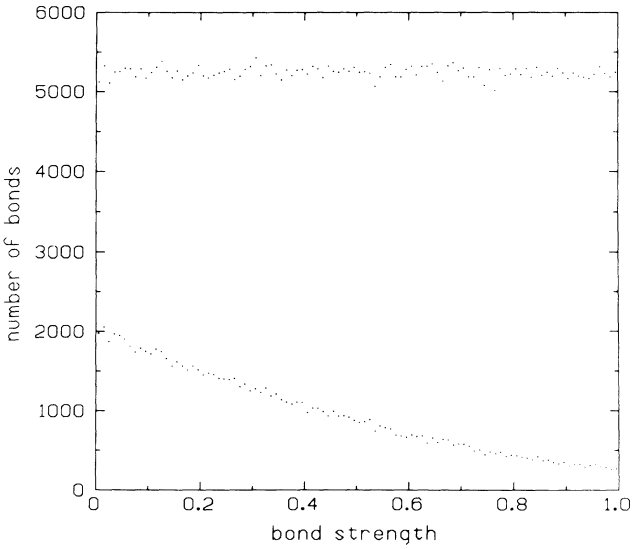

FIG. 7. Distribution of bonds (upper points) and broken bonds (lower points); the bin width is 0.01.

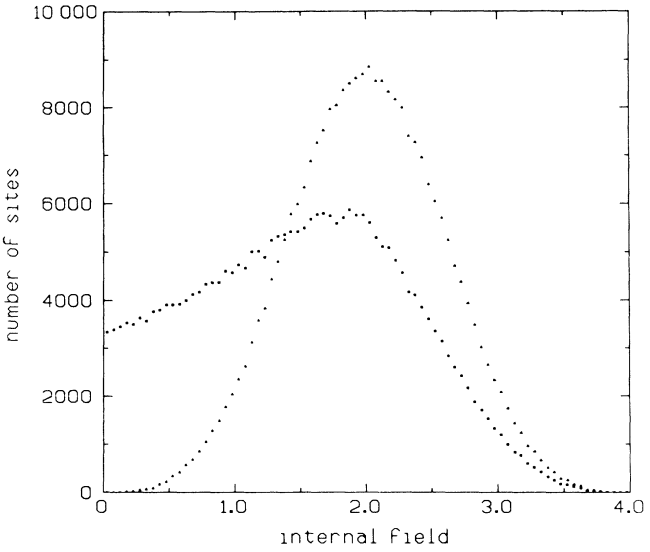

FIG. 8. Distribution of internal fields (squares) and distribution of internal fields in the ferromagnetic state (triangles); the bin width is 0.05.

We investigated the effects of different initial conditions and updating sequences on the final configuration. Three simulations were performed with the same bond configuration, two (numbers 1 and 2) with the same initial spin configuration but different updating sequences, and a third (number 3) with a different initial configuration and a third updating sequence. Defining the overlap of two configurations α and β by

$$q_{\alpha\beta}=\sum_i s_i^{(\alpha)}s_i^{(\beta)}/N \ , \tag{2}$$

where N is the number of sites, we found $q_{12}=0.406$, $q_{23}=-0.002$, and $q_{13}=0.001$; that is, 70% of the spins had the same orientation in systems 1 and 2, but only 50% of the spins in system 3 were parallel to those in the other two systems—a random choice for the spins would also yield 50% parallel. The final spin configuration depends strongly on the updating sequence and even more strongly on the initial spin configuration, demonstrating further the complexity of the energy surface: For a given bond configuration, many domains are found with a single initial spin configuration and updating sequence, and many others are found with different initial configurations and updating sequences.

The numerical results presented in Table I are particular to our choice for the bond distribution; the amount of randomness (in the bonds) is important. For example, in square lattices with ferromagnetic bonds, when the largest and smallest bonds satisfy $J_{\max}<3J_{\min}$ stubs of unit thickness (many can be seen in Fig. 1) cannot occur, although bridges of unit thickness are still possible, and the smallest domain has dimensions 2×2, rather than 2×1 for the broad (0 to 1) distribution discussed above. A decrease in randomness will therefore decrease both the number of domains and the roughness of the surfaces; decreasing the randomness to zero (by going to the uniform-bond model) will, however, not get rid of the domains, as discussed in the next paragraph.

The domain states are not a consequence of the randomness, for they occur also in the uniform-bond Ising model. In discussing the stability of the domains, however, one must distinguish between lattices according to whether the coordination number z is even or odd. In the honeycomb lattice (z odd), there are no ambiguous spins; domains are stable with respect to a nonzero magnetic field. In the square and simple-cubic lattices (z even), spins at the corners of domains are ambiguous; domains are unstable with respect to an infinitesimal magnetic field, apart from some unusual cases (in an up field, a rectangular spanning domain of down spins is metastable, and an up domain in a down matrix is stable). The instability can be seen by starting with a rectangular domain of down spins in a matrix of up spins, in zero magnetic field, so that the four spins at the corners are ambiguous. On the application of any positive (up) field each corner spin will align with the field (the perimeter and the interaction energy are unchanged) to produce two more corner spins, also ambiguous, until the entire down domain is consumed. Domains in the uniform-bond model differ also in that they can be translated without change in energy or loss of self-consistency.

IV. RESULTS: SQUARE LATTICE, NARROW DISTRIBUTION

We investigated the effect of decreased randomness by simulating two 512^2 systems with bonds uniformly distributed in the interval $[0.499, 0.501)$. The results (most of which follow qualitatively from the above) were (average values) as follows: internal energy (per site) $=-0.686$, fraction of broken bonds $=0.157$, average chord length $=6.37$, a linear relation between the perimeter and size of large domains with the ratio of perimeter to number $=0.583\pm0.008$, and number of domains $=1130$. About half the decrease in the number of domains upon going from the broad distribution to the narrow can be accounted for by deleting domains with two and three members from the number (1490) for the former, but the justification for the deletion, that these small domains cannot occur with the narrow distribution, fails under scrutiny. The fractions of sites with two, one, and zero neighbors oppositely oriented were 0.147, 0.332, and 0.520, respectively. The capacity and information dimensions were $d_{\rm cap}=1.84\pm0.06$ and $d_{\rm inf}=1.86\pm0.04$, consistent with the values found for the broad distribution.

We have not simulated quenches of uniform-bond models, but the results of the preceding paragraph should apply, apart from difficulties (which can be resolved, but only arbitrarily) caused by ambiguous spins.

V. RESULTS: SIMPLE-CUBIC LATTICE

Only the broad bond distribution (0 to 1) was used for the three-dimensional systems. As Table I shows, these systems are quantitatively similar to the two-dimensional

ones in many respects (the fraction of broken bonds, the average chord length, etc., and also the distributions of chord lengths), but the numbers in Table I (apart from those on the last line) conceal a radical difference in structure. The number of domains is smaller by a factor of roughly 200 in $d=3$ (even though the number of sites is the same) and the domains have entirely different character; in three dimensions, there are two large spanning domains (taking up fractions 0.487 to 0.513 of the sites) plus a few (two to seven), small (three to twelve members) embedded domains. As discussed in the Introduction, in two dimensions neither the up nor the down spins percolate in the starting (random) configuration, whereas in three dimensions there are already in the starting configuration large spanning domains of both species. The absence of large embedded domains in three dimensions is clearly due to the unlikelihood of creating a large three-dimensional hole, starting from random values.

Although only a few embedded domains are found in three dimensions, the energy surface is nevertheless complex; obviously the walls separating the spanning domains can be relocated in many ways.

The dependence of the character of the domains on dimension has consequences for numerical studies of relaxation at nonzero temperatures following simulated quenches from high temperatures; the article by Fisher,[21] and references therein, deal with predictions for the behavior. The spanning domains have enhanced (topological) stability; after a quench to low temperature, there will be an initial stage during which most spins align with their local fields, followed by slow relaxation dominated by the decay (and growth) of embedded domains in two dimensions, and by wall wandering in three. Boundary conditions will be very important in three dimensions.

Note added in proof. The recent work of Bak, Tang, and Wiesenfeld[22] on the self-organized criticality of systems far from equilibrium seems to explain the sealing behavior which we find above. Our results (including the distribution of domain sizes in two dimensions) are consistent with the lack of a natural length larger than the plus-minus correlation length of roughly two units seen in Fig. 2. Qualitative support for this interpretation (due to Bak[23]) is provided by Fig. 8 which shows a nearly uniform distribution of internal fields in the low-field region.

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