

Anderson clusters and inhomogeneous ordering in the short-range Ising spin glass

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In naive mean-field theory, the initial ordering in the short-range Ising spin glass is in the form of internally inhomogeneous clusters which form in regions with favorable bond configurations. These "Anderson clusters" are identified with the clusters inferred from experiments. The metastable states are domain states and have a tree structure, despite violation of the ultrametricity condition obtained in the infinite-range version of the model.

I. INTRODUCTION AND INTERPRETATION

After a decade of sustained, intensive effort (Ref. 1 reviews hundreds of papers, most of them dealing, however, with the infinite-range version), strong numerical evidence has been obtained²⁻⁶ for a finite-temperature phase transition in the three-dimensional, short-range version of the Edwards-Anderson model⁷ of a spin glass. The two-dimensional short-range model has a transition only at zero temperature.^{5,6} The Monte Carlo work²⁻⁴ suggests a new unit of computational effort, the CEY (Cray-equivalent central-processing-unit year); one paper² alone amounts to 5 CEY. This remarkable effort attests to the interest in the model, to the difficulty of its solution, and, perhaps, also to the seductive simplicity of its starting point. Reference 8 provides a fine summary of the experimental and theoretical situation as of two years ago.

In an attempt to clarify the nature of the transition, which the Monte Carlo work suggests is not an ordinary one (the finite-size scaling analyses of Refs. 3 and 4 show atypical behavior), the present article treats the three-dimensional short-range model in mean-field theory; this theory, one of the most useful guides to the behavior of complex systems, has been largely neglected in the study of the short-range model (only a few articles^{9,10} discuss it), in contrast with the infinite-range model.¹¹ This neglect is hard to understand, for mean-field theory is the natural first step in understanding nonergodic systems.

In a previous article,¹⁰ I investigated the metastable states of a few small systems near the mean-field onset of ordering, in zero magnetic field. This study gave several results whose qualitative features are not expected to change on further "resort to the indignity of numerical simulations,"¹² that is, more and larger systems. For example, the metastable states are domain states in the short-range model.^{4,10} (This result is probably limited to nearest-neighbor interactions if domain is interpreted strictly, as a set of flipped spins, each a nearest neighbor of another.) Walstedt⁸ has described evidence for domain states in another model. The present article deals in greater length with the same systems and draws further conclusions regarding the short-range model. Averaging over bond configurations is not possible with so few sys-

tems, but neither is such averaging desirable for present purposes, for several interesting features are apparent only on detailed investigation using individual bond configurations.

In mean-field theory, the initial ordered state in the short-range model consists of a small cluster of spins, as shown some time ago by Anderson,^{13,14} see also Ref. 15. The second-order transition (from the paramagnetic state to an ordered state) predicted by mean-field theory is a false result, for the ordered state is localized and there is therefore no thermodynamic transition (as discussed by Anderson¹⁴). In mean-field theory, further ordering takes place with growth of the original cluster (all magnetizations increase by a constant factor), followed by the formation of other clusters, some driven by the first, others independent of it, as shown in Sec. VI.

The experimental evidence (see Sec. II) suggests that the clusters should be taken seriously. In order that there be a phase transition (in the thermodynamic limit), an infinite number of such clusters must be present, and an infinite number of them must lie sufficiently close together; an analogy with a percolation transition seems empty, however. Perhaps the closest analogy is to the proximity effect in a random mixture of superconducting particles of different sizes and different bulk transition temperatures. Once an ordered state is established, many low-energy states are available to the system due to the weak interaction between clusters; that is, in mean-field theory irreversibility sets in immediately below the onset of ordering. With decreasing temperature the average magnetizations grow at different rates, and nonthermodynamic first-order transitions (domain flips) are energetically favorable, as shown in Ref. 10; the state which minimizes the free energy at high temperature does not do so at all T .

An open question is the size of the energy barriers to these domain flips (and to the motion of domain walls); as discussed in Sec. IV, barrier heights have so far not been obtained in the mean-field theory of the short-range Ising spin glass, although progress has been made in both Monte Carlo calculations on this model and in a vector model as described by Morgenstern⁸ and Walstedt,⁸ respectively. Even in the thermodynamic limit though, many of the barriers are finite (only a finite number of spins need be flipped) and some states are nearby in con-

figuration space (there are small domains), and so at high temperatures it seems certain that the system can explore many of these states and make transitions to them on laboratory time scales. At the same time the system is nonergodic because it cannot make on the latter time scales the large excursions (in free energy or configuration space, or both) necessary to sample all configurations with appreciable Boltzmann weight. The infinite-range model also has both accessible and inaccessible states; see Ref. 14 (p. 176) and Ref. 16.

The complex behavior of spin glasses is due to the multitude of local minima, to the near degeneracy of many of the lowest, and to the broad spread in energy of the barriers between them. A feature apparently new with Ref. 10 is that the lowest-energy state at one temperature is not necessarily (and probably not ever in the thermodynamic limit) the continuation of the lowest-energy states at nearby temperatures, and so the state of lowest free energy at one temperature evolves continuously into what is a domain state at others. The system must make domain-flip transitions (which become progressively more difficult at lower temperatures) to get to the lowest state in even a restricted region of configuration space. This process may be responsible in part for the long equilibration times found in the Monte Carlo work.²⁻⁴

The domain picture developed in Ref. 10 suggests a continuum of these nonthermodynamic first-order (domain-flip) transitions in the thermodynamic limit, with the result that the temperature axis is a critical line (though perhaps not extending down to $T=0$); a similar result is obtained in the infinite-range version of the model (see Ref. 17 and pp. 232 and 242 of Ref. 14). The same behavior should carry over to nonzero magnetic field (for not too large field), so that a critical *area* (where the thermodynamic functions are nonanalytic at each point) is expected in the magnetic-field-temperature plane. The axial next-nearest-neighbor Ising (ANNNI) model shows similar behavior, as pointed out in Ref. 10, but the second-order and first-order transitions are thermodynamic in the ANNNI model; other similarities between the two models were pointed out in Ref. 18. There is related work on the random-field Ising model.¹⁹

The article is organized as follows.

Clusters of spins have long been recognized as important in spin glasses. In Sec. II I cite some experimental articles, and also define the terms "Anderson cluster" and "domain."

In Sec. III I review the Edwards-Anderson model and the mean-field approximation. In Sec. IV I discuss the solution of the mean-field equations.

In Ref. 10 it was shown that the ordered solutions of the mean-field equations for the short-range model have a tree (hierarchical) structure; such structure had been argued previously for the infinite-range version.²⁰ In Sec. V I discuss the tree structure in the short-range model, where its origin is transparent; this structure is found despite violation of the condition $q_1 \geq q_2 = q_3$ obtained²⁰ in the infinite-range version.

In Sec. VI I show how the Anderson clusters form at the mean-field onset of ordering and how they develop with decreasing temperature.

II. CLUSTERS

In the first part of this section I explain what Anderson clusters are not; in the second part I explain what they are, and identify them (as did Anderson¹⁴) with the clusters inferred from experiment. The discussion of other uses of the term cluster differentiates them from the use here.

(1) Experimental results on spin glasses (see, for example, the articles by Mydosh and Wenger in Ref. 8) are sometimes interpreted²¹ in terms of giant clusters of spins, along the lines of theories²² used to explain the magnetic properties of inhomogeneous systems such as rocks. Unfortunately, these interpretations are sometimes taken literally; the recognition that spin glasses behave as if they are composed of clusters is important, although it is not in itself an explanation of spin glasses, but "spin glasses exhibit rock magnetism"²³ seems excessive. Both the origin of the assumed superparamagnetic clusters and the reason for their rigidity are unclear in these interpretations; while chemical clustering no doubt occurs in some systems, such a mechanism fails in several respects, as discussed by Binder²⁴ (who also discusses the weaknesses of the paramagnetic cluster interpretation).

(2) Smith²⁵ defined a cluster as "a group of spins each of which is coupled to at least one other member of the group by an exchange bond whose magnitude is greater than thermal energy, and is thus not coupled to any spin outside the group"; the other spins are called loose spins "which arise by a fortuitous cancellation of internal fields from different neighbor spins, and are responsible for most of the low-temperature and transport properties." Smith identified the spin-glass temperature as the temperature at which the bonds with magnitude greater than $k_B T$ form an infinite cluster; that is, Smith suggested that the spin-glass transition is a bond-percolation transition. Smith's argument omits two important physical effects, Anderson localization and frustration. In the first part of Ref. 24, Binder used the term cluster in much the same sense as Smith.²⁵

(3) Soukoulis and Levin²⁶ proposed and analyzed a model with regions ("clusters") of enhanced exchange interaction with smaller (but not necessarily small) interactions between clusters. Intracluster interactions were accounted for—the spins in the clusters were not assumed rigid. This model might be appropriate for chemical clusters, but is not necessary to explain the clusters deduced from experiment.

(4) Binder²⁴ recognized the existence of another kind of cluster; starting with a random configuration of spins at $T=0$, he "annealed" it with the Monte Carlo algorithm, and then warmed the system to finite temperature. The spins which changed sign on warming formed groups (see Fig. 12 of Ref. 24) which look very much like domains (defined below); the two are certainly closely related, despite the different definitions. The identification is clouded, however, because the two-dimensional systems of Ref. 24 have no finite-temperature phase transition. Similar "clusters" have been found by Palmer⁸ and in a Monte Carlo study²⁷ of the Mattis-Ising spin glass. Binder's clusters are not Anderson clusters; his Fig. 13 compares

the size distributions of percolation clusters and entities similar to what I call domains.

(5) In a study of the two-dimensional model, Kinzel²⁸ used the term to describe groups of spins which had not changed sign after a given number of Monte Carlo steps at fixed temperature. The spins in the Anderson clusters discussed below probably also relax slowly, but are distributed differently (compare Fig. 3 of Ref. 28 with the figures below); neither are Kinzel's clusters to be interpreted as domains (compare Kinzel's Fig. 3 with Fig. 3 of Ref. 10).

Studies similar to those of Binder²⁴ and Kinzel,²⁸ but on three-dimensional systems, would be of interest, particularly if combined with mean-field calculations on the same systems.

(6) In Ref. 29 (and on p. 252 of Ref. 14) a cluster is a group of spins of volume ξ^d . These "clusters" are similar to what I call domains, but not identical; ξ is only the minimum domain dimension, and domains can have volume larger than ξ^d . They are not Anderson clusters cut off to include only sites with absolute magnetizations $|s_i|$ greater than some value; because of the exponential decay of the $|s_i|$, this cutoff gives entities of volume proportional to $[\ln(\text{const}/\xi)]^d$.

(7) Finally, there are what I call Anderson clusters. These are found in mean-field theories^{14,10} of disordered systems and are closely related to Anderson localization;³⁰ the eigenvector corresponding to the largest eigenvalue of the J_{ij} matrix is localized. In agreement with Anderson (Ref. 14, p. 217), it is proposed here that these "Anderson clusters" are the clusters postulated in Ref. 21.

In mean-field theory, the initial cluster forms in the region where in some vague sense the bond configuration is most favorable, where the frustration is least severe. At lower temperatures, other clusters form independently, each at its own ordering temperature, in regions where the frustration is not severe. Still other clusters can be forced to order by nearby clusters. The figures of Sec. VI suggest the following.

Definition. In mean-field theory, an Anderson cluster is a group of spins with absolute magnetizations $|s_i|$ sharply peaked at the center and decaying approximately exponentially with decay constant independent of temperature and roughly equal to $\frac{1}{2}$ per site.

A typical such cluster contains 20 to 30 sites at which the $|s_i|$ are larger than half the maximum $|s_i|$. A single state is sufficient to recognize a cluster, but in mean-field theory clusters are distinguishable only near the (mean-field) onset of ordering.

A cluster cannot be defined so simply outside mean-field theory. One expects there to be regions where the spins are strongly (but inhomogeneously) correlated with each other, and weakly correlated with spins outside each region.

Clusters differ from domains. A domain is a group of spins, connected by nearest-neighbor bonds, whose magnetizations have different signs in two states compared at the same temperature. This definition is imperfect (because of frustration, there is some straggling—see Fig. 3 of Ref. 10) but may be the best possible in such systems. Domains are recognized easily by multiplying the s_i at

each site; using a reference state to identify special spins apparently originated with Binder,²⁴ but the idea also occurred to Bak.⁴ Domains have been seen in one Monte Carlo study,⁴ and likely in another²⁴ [see point (4) above]. In mean-field theory a test can be made that these are domains in the usual sense of the term; a comparison of the magnitudes of the s_i as well as their signs is given in Sec. VI. The requirement that the two states be compared at the same temperature arises because the magnetizations in a given state rearrange with temperature, as shown in Sec. VI; they change nonuniformly with temperature and so the internal field acting on a given spin can go through zero, several times in some cases.

The Anderson clusters form quite naturally, even in the extreme model of exchange constants $\pm J$ between nearest neighbors and zero otherwise. There is no need to put in by hand regions of enhanced exchange constant in order to explain the cluster interpretation of the experimental results. While there are undoubtedly regions in laboratory spin glasses where there are clusters as defined by Smith²⁵ and Soukoulis and Levin,²⁶ the nearest-neighbor, $\pm J$ model shows that such clusters are not necessary to explain the clusters deduced in Ref. 21. These other explanations for the clusters draw attention from the main point, that sufficient disorder is the *only* requirement for the formation of the clusters; even the frustration is unnecessary.

Anderson clusters differ substantially from Smith's clusters, and the analogy with a percolation transition differs correspondingly. The analogy (which appears to contribute little to the understanding of spin glasses) is to a correlated site-percolation problem³¹ (preferential addition of new sites near existing ones), rather than to a standard bond-percolation problem.

Identification of Anderson clusters in Monte Carlo calculations may be difficult; mean-field calculations on the same systems should be helpful in this respect. In mean-field theory Anderson clusters are easily identified in only a narrow temperature region; they overlap strongly at temperatures well below the mean-field onset of ordering. At these latter temperatures it is domains rather than clusters which are important.¹⁰ In the following, cluster is to be interpreted as Anderson cluster.

III. EDWARDS-ANDERSON MODEL AND MEAN-FIELD THEORY

The suggestion that the Ruderman-Kittel-Kasuya-Yosida (RKKY) interaction³² is important in spin glasses seems due to Marshall;³³ the statistical mechanics of such systems was also studied by Klein and Brout.³⁴ The Edwards-Anderson model⁷ consists of spins occupying every site of a lattice; the exchange constants have random sign to take into account the oscillatory nature of the RKKY interaction. Considerable differences^{35,9} are found between Ising and vector systems; in the latter case, uniaxial and Dzyaloshinsky-Moriya³⁶ terms are usually included to give the anisotropy (automatic in Ising systems) believed necessary for irreversibility.^{35,9}

An interesting alternative to the Edwards-Anderson model has been provided by Walker and Walstedt,³⁵ who

treated both Ising and vector spins with RKKY interactions on a diluted face-centered-cubic lattice; they found several extrema of the energy in a system of vector spins without finding irreversibility. Monte Carlo³⁷ studies of the model have also been made.

The present article is limited to the Edwards-Anderson model with Ising spins on a simple-cubic lattice with periodic boundary conditions and nearest-neighbor interactions randomly ± 1 with equal probability, as in the recent Monte Carlo work.²⁻⁴ Gaussian bonds are more realistic and (unlike the ± 1 choice) do not yield ambiguous spins at low temperature. The model is treated in the naive mean-field approximation which, though inadequate for the infinite-range version,¹⁷ is generally accepted for the short-range version.

The defects of the mean-field approximation are well known and are listed in Ref. 10 but bear repeating here. It gives false transitions in finite systems, false transitions in systems of dimensionality lower than critical, usually poor numbers for the critical exponents, frequently a poor value for the transition temperature, and occasionally the wrong order of the transition; its virtues are its simplicity and the insight which it provides.

In naive mean-field theory, extrema of the free energy are obtained when the thermally averaged magnetization s_i at the i th site satisfies ($\beta = 1/T$)

$$s_i = \tanh \left[\beta \sum_j J_{ij} s_j + \beta H \right]; \quad (1)$$

the magnetic field H is taken to be zero in the following, but the results are expected to be qualitatively correct for $H \neq 0$ as long as $|H|$ is not too large. Unfortunately, Eq. (1) can be solved only numerically for general values of the temperature.

Equation (1) falsely predicts a second-order transition from the paramagnetic state (all $s_i = 0$) to an ordered state at the temperature T' where the determinant of the linearized equations vanishes.¹⁴ Whether a localized solution is obtained also in treatments which go beyond this naive mean-field theory is uncertain (see Ref. 14, p. 241); there are serious numerical difficulties with such improved theories.³⁸

Given a solution of the mean-field equations, one can calculate its free energy from

$$F = \frac{1}{2} \sum_{i,j} J_{ij} s_i s_j - \beta^{-1} \sum_i \ln \left\{ 2 \cosh \left[\frac{1}{2} \beta \left(\sum_j J_{ij} s_j + H \right) \right] \right\}. \quad (2)$$

The paramagnetic state is stable for $T > T'$ and unstable for $T < T'$; its free energy (for $H = 0$) is $F_0 = -NT \ln 2$.

IV. SOLUTIONS OF THE MEAN-FIELD EQUATIONS

I have solved Eq. (1) for three bond configurations, two of 10^3 spins and one of 20^3 spins, in which the mean-field onset of ordering occurs at temperatures $T' = 4.52$, 4.53, and 4.55; the large discrepancy with the thermodynamic transition temperature $T_c = 1.2 \pm 0.1$ found in Refs. 2-4 shows that thermal fluctuations are strong (as is already

well known), but part of the difference arises because T' is not a transition temperature. Only the temperature region near T' was investigated.

Solutions to Eq. (1) were found by inserting an initial set of s_i into the right-hand sides to generate a new set and repeating to convergence; to accelerate convergence, new values were used as soon as they were available. This scheme is adequate for the above naive mean-field theory, but problems arise in more sophisticated theories.³⁸ Under both the accelerated and unaccelerated iteration schemes, the physically unstable solutions (maxima and saddle points of the free energy) are, unfortunately, numerically unstable as well;³⁸ means other than simple iteration of Eq. (1) are necessary to estimate the energy barriers between the metastable solutions of Eq. (1).

The convergence criterion was

$$\max_i \left\{ \left| s_i - \tanh \left[\beta \sum_j J_{ij} s_j \right] \right| \right\} \leq \epsilon s_{\text{rms}}, \quad (3)$$

$$s_{\text{rms}} = \left[\frac{1}{N} \sum_i s_i^2 \right]^{1/2}; \quad (4)$$

a convergence parameter ϵ of 10^{-6} was usually sufficient, but much smaller values were required near T' . Typically, several hundred passes through the equations were required for the 10^3 systems and several thousand for the 20^3 system. These numbers increased as T' was approached; here convergence was accelerated greatly by scaling the magnetizations by a factor determined variationally.

Solution branches were generated by starting with spins randomly ± 1 , or randomly ± 0.3 , or all 1, or all 0 but one, etc., and iterating to convergence; other branches were found as the result of decay of known states. Once a solution was found it could be tracked to other temperatures by using the current s_i as starting values for the next temperature. Various updating strategies were used: sequential, completely random, and restricted random (each site updated once and only once in each pass through the equations, in random order).

As in Ref. 9, solutions decayed only on warming (with the two exceptions noted below). The decay of a state is interpreted as due to the vanishing of its local minimum in the free-energy surface.

A second rule was followed (in all but one case); decays occurred to states of lower free energy. This is expected on physical grounds, and therefore reinforces the domain picture, for there is no obvious mathematical reason why all decays should be downward.

A single state, curious for a third reason (it exists for only the narrow temperature interval $\Delta T < 0.03$), violated both these rules.

Only one case was found in which a relative minimum evolved into a relative maximum with decreasing temperature (a pitchfork bifurcation, as at the mean-field onset of ordering).

In Ref. 10 I found a rapid decrease in the number of solutions of the mean-field equations with increasing temperature; this decrease was attributed¹⁰ to the increase of the correlation length ξ with temperature. The minimum linear dimension of a domain is $\sim \xi$ and hence all

domains eventually become unstable as the temperature increases, the smallest going first. That there exists a temperature T_m above which only one ordered solution of the mean-field equations is found was attributed¹⁰ to the increase of ξ with T and to the finite volume (L^3) of the systems; no domain state can exist for $\xi \geq L$.

The success of the interpretations of the preceding paragraph supports the existence of an underlying “shattered” or “staggered” order parameter suggested on other grounds in Refs. 39 and 4; see, however, Ref. 16.

V. TREE STRUCTURE AND ULTRAMETRICITY

The solutions of the mean-field equations for the short-range model have a tree structure, as noted previously;¹⁰ see Figs. 1 and 2 of Ref. 10. The tree structure arises because the metastable states are domain states;^{4,10} it merely reflects the fact that many states decay to the same state. A metastable state can contain many domains, either separated from each other or adjacent, with domains within domains, large domains composed of smaller ones, etc. When a domain becomes unstable, it can either vanish or (probably less frequently) add a domain or two at its periphery to form a larger domain.

Ultrametricity²⁰: Suppose that one has three states α , β , and γ with overlap parameters⁴⁰ $q_{\alpha\beta}$, $q_{\beta\gamma}$, and $q_{\gamma\alpha}$ obtained from

$$q_{\alpha\beta} = \mathcal{N} \sum_i s_i^{(\alpha)} s_i^{(\beta)}, \tag{5}$$

etc., where \mathcal{N} is a normalization constant. If the overlaps are ordered so that $q_1 \geq q_2 \geq q_3$, the ultrametricity condition is²⁰

$$q_1 \geq q_2 = q_3; \tag{6}$$

this last result, derived in the infinite-range model²⁰ after averaging over bond configurations, implies that the space of states is ultrametric (that it has a hierarchical or tree structure²⁰). Numerical tests of Eq. (6) have been made for both the short-range⁴¹ and infinite-range⁴² models, with inconclusive results. The physical origin of the tree structure in the infinite-range model is obscure at present, in contrast to the short-range model where it is transparent.

Because the metastable states are domain states^{4,10} in the short-range model, it is easily seen that Eq. (6) is violated. At zero temperature (where the overlap parameter is most simply interpreted—note, however, that the $\pm J$ model is ill behaved at $T=0$) and if \mathcal{N} is taken to equal 1, the overlap between two states is N minus twice the number of spins inverted from one state to the other. The distribution of overlaps reflects the distribution of domain sizes and the extent to which large domains possess natural fracture lines which can split them into smaller domains; a study⁴³ of the two-dimensional, short-range, Gaussian-bond model at $T=0$ shows such lines and other interesting features. Despite the violation of Eq. (6) in the short-range model, the states have a tree structure.¹⁰ To repeat, in Ref. 10 (and here) no bond averaging is done; the tree structure applies to individual sets of bond

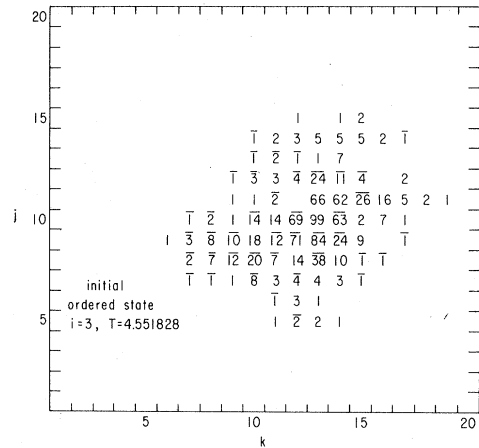


FIG. 1. Magnetizations s_{ijk} in the plane $i=3$ (which contains the site with the largest absolute magnetization) for the initial ordered state at a temperature slightly below ($T' - T \approx 10^{-7} T'$) the mean-field onset of ordering. The integer n at a given site is the integer part of the absolute magnetization as a percentage of the largest absolute magnetization [see Eq. (7)], except that $n=99$ is to be read as $n=100$; bars denote negative values. For example, $n_i=66$ and $\bar{7}$ mean $0.66 < s_i \leq 0.67$ and $-0.08 \leq s_i < -0.07$, respectively.

configurations in the short-range model.

Early work of Krey⁴⁴ (see his Fig. 3) should be cited in a discussion of the tree structure, and an article of Palmer³ as well. Krey's picture, “a continuous sequence of bifurcations”⁴⁴ (a local minimum of the free energy changes with decreasing temperature into a local maximum with two subsidiary local minima), is not correct in detail,¹⁰ but it does anticipate several later developments.

VI. ANDERSON CLUSTERS

The comments are brief here; the results have been discussed both above and in Ref. 10.

Figures 1 to 6 show selected planes of the 20^3 system ($T' \sim 4.55$) at various temperatures. The number n_i at site i is

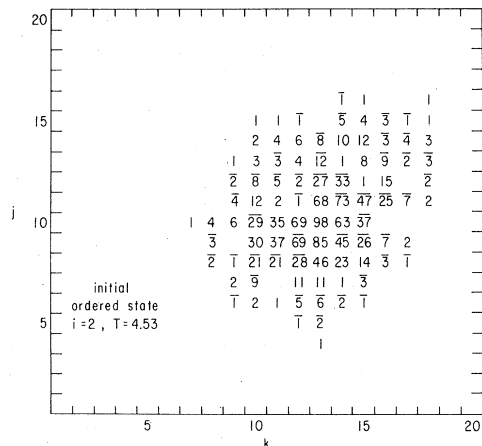


FIG. 2. s_{ijk} : $i=2$, initial ordered state, $T=4.53$.

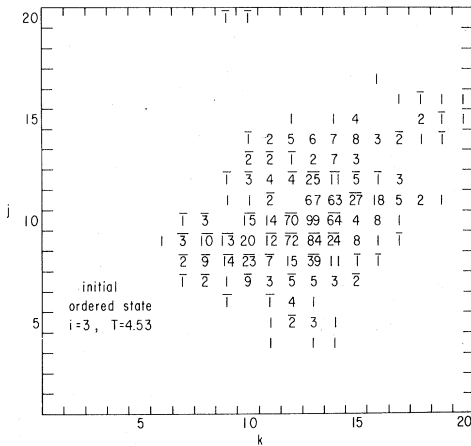


FIG. 3. s_{ijk} : $i=3$, initial ordered state, $T=4.53$.

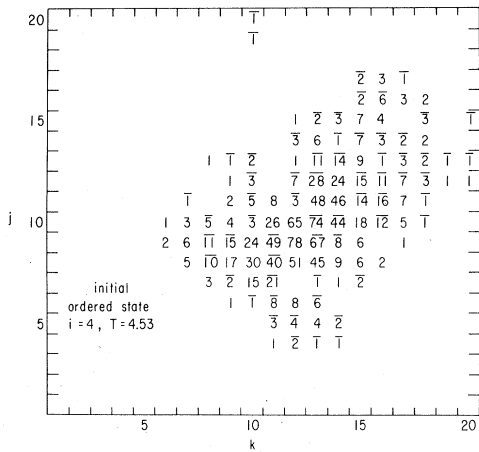


FIG. 4. s_{ijk} : $i=4$, initial ordered state, $T=4.53$.

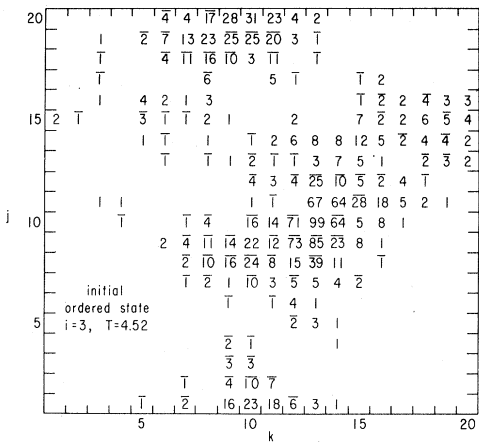


FIG. 5. s_{ijk} : $i=3$, initial ordered state, $T=4.52$.

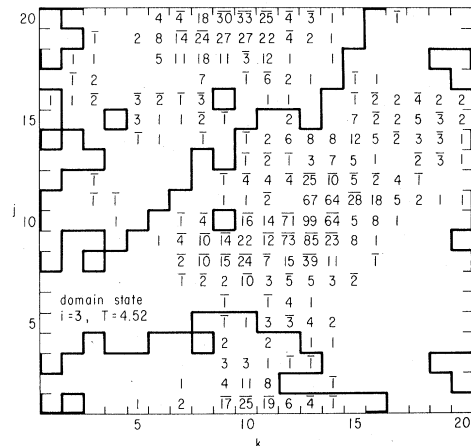


FIG. 6. s_{ijk} : $i=3$, domain state, $T=4.52$. The heavy lines separate sites whose magnetizations have the same sign in the initial ordered state and the domain state from those which have different signs in the two states.

$$n_i = |\text{int}[100(1-10^{-7}) |s_i| / S]|, \quad (7)$$

where int is the integer part and $S = \max_i \{|s_i|\}$ is the maximum absolute magnetization in the state at the temperature. $n_i = 100$ is shown as $n_i = 99$ (for lack of space), while bars over the n_i denote negative values.

Figure 1 shows the magnetizations in a plane ($i=3$) containing the site with the maximum $|s_i|$, at a temperature $T \sim T' - 5 \times 10^{-7}$.

Figures 2 to 4 show the same plane ($i=3$) and the two neighboring planes at the lower temperature $T=4.53$. Comparison of Figs. 1 and 3 shows some growth of the original cluster at the edges. Note the two sites at $k=9$ and $10, j=20$ in Fig. 3.

Figure 5 shows the plane $i=3$ at the slightly lower

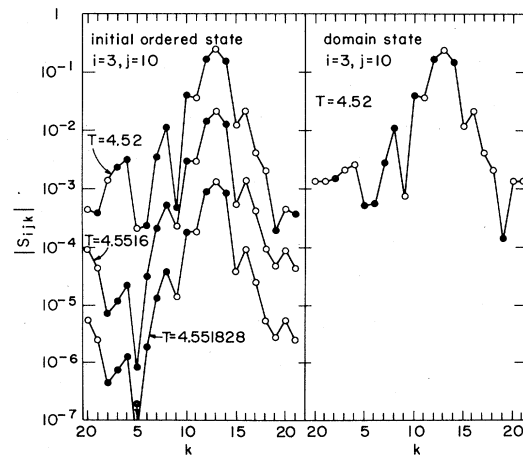


FIG. 7. Absolute values of the magnetizations along the line $i=3, j=10$ for the initial ordered state (left-hand side) and the domain state (right-hand side) at three temperatures; the domain state exists only for $T \leq 4.528$. Sites at which the magnetization is positive (negative) are shown as open (solid) circles. For clarity, lines connect the points.

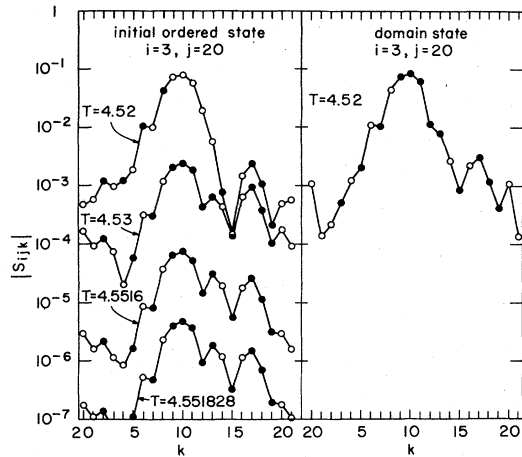


FIG. 8. Absolute values of the magnetizations along the line $i=3, j=20$ for four temperatures. For further explanation, see the caption for Fig. 7.

temperature 4.52. Another strong cluster (with maximum $|s_{ijk}|$ also in the plane $i=3$) has formed and several weak clusters are apparently being forced to order by the two strong ones. Two other strong but connected clusters (maximum $|s_{ijk}|=49$ and 34 on the same scale) are centered in the plane $i=6$.

Figures 1 through 5 apply to the initial ordered state which is the only ordered state for $T \geq 4.528$. At $T=4.52$, however, there is another state (called the domain state here and in the figures). Apparently no other ordered state exists at this temperature; ten random starts at $T=4.52$ gave only the two. Figure 6 shows the

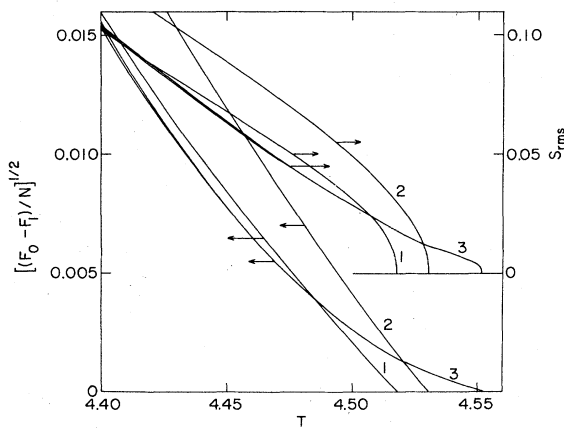


FIG. 9. Free energy per spin (relative to the paramagnetic state) and the root-mean-square magnetization s_{rms} [Eq. (4)] for the three systems (numbered 1, 2, and 3) as functions of temperature T . For system 1 ($N=10^3$), only the initial ordered state exists in the temperature interval shown. For system 2 (also $N=10^3$) a domain state exists for $T \leq 4.43$ but is not shown. For system 3 ($N=20^3$) the free energy and s_{rms} are plotted for both the initial ordered state and the domain state; the latter exists only below $T \approx 4.528$ and is the only domain state at $T=4.52$. At least 12 more domain states exist at $T=4.50$, and many, many more at lower temperatures.

magnetizations in the domain state; comparison of Figs. 5 and 6 shows that the two states are domain states relative to each other.

Figure 7 is a plot of $|s_{ijk}|$, the magnitude of the magnetization, as a function of the index k for $i=3, j=10$ (along a line through the center of the original cluster) for three temperatures. From the highest temperature to $T=4.5516$, the magnetizations increase by virtually the same factor at each site. The larger $|s_i|$ scale from $T=4.5516$ to $T=4.52$ as well, but there are rearrangements at some of the other sites. A plot of the absolute magnetizations in the domain state (which exists only for $T \leq 4.528$) is given on the right-hand side.

Figure 8 is again a plot of the absolute magnetization as a function of the index k , here for $i=3$ and $j=20$ (through the center of the second cluster). Again the spins change by almost the same uniform factor from the highest temperature to $T=4.5516$, and the same is roughly correct from $T=4.5516$ to $T=4.53$. From $T=4.53$ to 4.52 , however, there are major changes in both the magnitudes and signs of the s_{ijk} at many of the sites. The right-hand part of the figure shows the magnetizations in the domain state at $T=4.52$; the signs are, perversely, in most cases identical to those at the same sites in the initial ordered state at $T=4.53$.

At $T=4.50$, four or five more strong clusters have appeared; there are at least 14 states with energies (per spin, relative to the paramagnetic state) ranging from -6.7×10^{-6} to -5.8×10^{-6} , roughly uniformly distributed. The distribution of energies becomes centrally peaked at lower temperatures.

Figure 9 shows the free energies (per site, relative to the paramagnetic state) and the root-mean-square magnetizations [Eq. (4)] of the three systems as functions of T near T' . The clusters cause unusual behavior; the reduced free energy is proportional to $(T' - T)^2$ near T' , but the coefficient behaves roughly as $1/N$. The root-mean-square magnetization is roughly linear in T until it turns over and vanishes as $(T' - T)^{1/2}$; the turnover is sharper and closer to T' for the larger system. The tails in the free energy and s_{rms} are due to the finite size of the initial clusters and will extend to higher temperatures (and decrease in magnitude) with increasing size of the system; in the $\pm J$ model used here, the tails will extend ultimately to $T' = 6$ (the mean-field transition temperature of the model with all nearest-neighbor bonds = 1), since in an infinitely large system there will exist arbitrarily large unfrustrated regions. The approach to the limit is expected to be very slow, however, as indicated also by Fig. 9. In the Gaussian-bond model, the tails will extend ultimately to $T' = \infty$, but much more slowly than in the $\pm J$ model; T' will likely have a reasonable value even in systems of macroscopic size.

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