Frustration and ground-state degeneracy in spin glasses

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The problem of an Ising model with random nearest-neighbor interactions is reformulated to make manifest Toulouse's recent suggestion that a broken "lattice gauge symmetry" is responsible for the unusual properties of spin glasses. Exact upper and lower bounds on the ground-state energy for models in which the interactions are of constant magnitude but fluctuating sign are obtained, and used to place restrictions on possible geometries of the unsatisfied interactions which must be present in the ground state. Proposed analogies between the ferromagnet–spin-glass phase boundary at zero temperature and a percolation threshold for the "strings" of unsatisfied bonds are reviewed in the light of this analysis. Monte Carlo simulations show that the upper bound resulting from a "one-dimensional approximation" to the spin-glass ground-state energy is reasonably close to the actual result. The transition between spin glass and ferromagnet at 0 K appears to be weakly first order in these models. The entropy of the ground state is obtained from the temperature dependence of the internal energy, and compared with the density of free spins at very low temperatures. For a two-dimensional spin glass in which half the bonds are antiferromagnetic, $S(0) \approx 0.099\ k_B$; for the analogous three-dimensional spin glass the result is $S(0) \approx 0.062\ k_B$. Monte Carlo kinetic simulations are reported which demonstrate the existence and stability of a field-cooled moment in the spin-glass ground state.

I. INTRODUCTION

Recent theories of disordered magnets give convincing evidence[1-3] that in the presence of random competing ferromagnetic and antiferromagnetic interactions, a continuous phase transition into a "spin-glass" state can occur. The details of the low-temperature phase that results, however, remain largely unknown. It is certainly unlikely that a random-ordered state will be unique, so these models should exhibit metastability at low temperatures. Since the experimental literature on spin glasses[4] is dominated by discussion of metastable relaxation phenomena, any simple insights into the nature of the low-temperature phase in models of spin glasses should help in establishing contact between theory and experiments.

In this paper we direct attention to the question of the degeneracy of the spin-glass ground state, a quantity for which theoretical estimates differ widely. Edwards,[5] considering a model with random nearest-neighbor interactions governed by a continuous probability distribution, has estimated that there may be $O(2^N)$ ground states for a model with N spins. Computer studies[6] of a similar model suggest, however, that there are $O(N^\alpha)$ metastable states, where $3 \gtrsim \alpha \gtrsim 1$. We give below estimates of the ground-state degeneracy (and thus the entropy at 0 K) for a class of models in which all interactions have the same magnitude but random signs. We find rather fewer states than Edwards estimates, but more than would be present if the interactions were continuously distributed in magnitude as well as sign. The model does have a nonzero entropy in the zero-temperature thermodynamic limit.

The central feature of spin-glass models is that not all interactions can simultaneously be satisfied. Anderson (private communications) has suggested the phrase "frustration" to describe this effect. Adopting Toulouse's recent precise definition of the frustration effect,[7] we shall in Sec. II present an explicit transformation of the partition function of a random Ising model which makes the frustration manifest. For models with interactions of random sign but constant magnitude, the disorder enters only through the frustration effect, and any two such models with the same extent of frustration are easily seen to have the same thermodynamic properties, even though the models may differ in other respects. For example, a model such as was described recently by Mattis,[8] constructed to have a unique random ground state and no frustration, is equivalent to a pure Ising ferromagnet, and is not a model of a spin glass in zero field.

In discussions of the possibility of an amorphous antiferromagnetic state (in which all interactions are negative but the spins are so arranged that there is no natural decomposition into two interpenetrating Néel sublattices), the same concept is given the name "misfit." The first term seems clearly preferable, since the misfit which leaves some spins in unfavorable magnetic environments when one attempts to construct a ground state for

an amorphous antiferromagnet is just a special case of the frustration effect. Similarly we hope that focussing on the extent to which magnetic interactions are inevitably frustrated in a particular system may help to unify treatment of the wide variety of materials[4] in which spin-glass behavior is observed. This contrasts with the recent proliferation of terminology and definitions in the experimental literature,[4] since the intent of those has been to differentiate different classes of materials.

II. THE MODEL

Consider a random Ising model described by the Hamiltonian

$$\mathcal{H} = -\sum_{\langle ij \rangle} J_{ij}\mu_i\mu_j , \tag{1}$$

where $\langle ij \rangle$ denotes the site indices of two adjacent spins, the μ_i may be ± 1, and the interactions J_{ij} are random and may be either >0 (ferromagnetic) or <0 (antiferromagnetic). We shall discuss only two-dimensional (2D) square, three-dimensional (3D) simple cubic, and higher hypercubic lattices. On such lattices, the shortest nontrivial closed paths visit four sites, and will be denoted $[ijkl]$. Define

$$\Phi_{[ijkl]} \equiv \mathrm{sgn}(J_{ij}J_{jk}J_{kl}J_{li}) \tag{2}$$

to be the sign of the product of the interactions around such an elementary circuit. Toulouse[7] has observed that Φ is a local measure of frustration since whenever $\Phi = -1$ there is no arrangement of the spins around the square in which all four adjacent pairs are aligned according to their respective interactions.

To demonstrate the role of this frustration density Φ in the statistical mechanics of a spin glass, we rewrite the partition function

$$Z = \mathrm{Tr}_{\{\mu\}} \prod_{\langle ij \rangle} \exp(\beta J_{ij}\mu_i\mu_j), \tag{3}$$

where $\beta = (k_B T)^{-1}$, in terms of pseudospins σ_{ij}:

$$\sigma_{ij} \equiv \mu_i\mu_j \,\mathrm{sgn}(J_{ij}) . \tag{4}$$

The bond $\langle ij \rangle$ is satisfied whenever $\sigma_{ij} = +1$. There are d times as many σ's as μ's in a d-dimensional model, but (2) provides a constraint which can be used to eliminate the redundant degrees of freedom. Thus

$$Z = \mathrm{Tr}_{\{\sigma\}} \prod_{\langle ij \rangle} \exp(\beta |J_{ij}| \sigma_{ij}) \times \prod_{[ijkl]} \tfrac{1}{2}(1 + \Phi_{ijkl}\sigma_{ij}\sigma_{jk}\sigma_{kl}\sigma_{li}), \tag{5}$$

where the second product in (5) vanishes unless (2) is satisfied, in which case it is unity. Since

$$\prod_{[ijkl]} \tfrac{1}{2}(1 + \Phi_{ijkl}\sigma_{ij}\sigma_{jk}\sigma_{kl}\sigma_{li}) = \lim_{\beta' \to \infty} \prod_{[ijkl]} \exp\beta' (\Phi_{ijkl}\sigma_{ij}\sigma_{jk}\sigma_{kl}\sigma_{li} - 1), \tag{6}$$

we can write Z as

$$Z = \lim_{\beta' \to \infty} \mathrm{Tr}_{\{\sigma\}} \prod_{\langle ij \rangle} \exp(\beta |J_{ij}| \sigma_{ij}) \times \prod_{[ijkl]} \exp\beta' (\Phi_{ijkl}\sigma_{ij}\sigma_{jk}\sigma_{kl}\sigma_{li} - 1) \tag{7a}$$

$$= \lim_{\beta' \to \infty} \mathrm{Tr}_{\{\sigma\}} z_1(\beta) z_4(\beta') . \tag{7b}$$

Information about the strength of the $\langle ij \rangle$ bond is now contained in z_1, while the possibility of frustrated interactions is contained in z_4. It should be apparent from (7) that no further details of the arrangement of the antiferromagnetic interactions are required to specify the thermodynamics of the system. Therefore, instead of characterizing a model by x, the fraction of negative interactions, it will prove convenient to use x_f, the fraction of frustrated squares. If there is no correlation between the signs of adjacent bonds, one obtains

$$x_f = 4x(1-x)[x^2 + (1-x)^2], \tag{8}$$

by summing the probabilities that one or three bonds are antiferromagnetic, and $0 \le x_f \le \frac{1}{2}$. Note that $x_f \approx \frac{1}{2}$ for a considerable range of x, from roughly 0.2 to 0.8, as shown in Fig. 1. There are

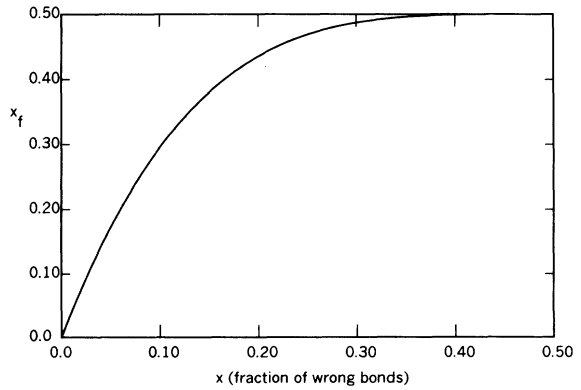

FIG. 1. Fraction of frustrated squares x_f given by (8) as a function of the fraction of the antiferromagnetic interactions present in a random Ising model. The values for $x > 0.5$ are obtained by reflection about $x = 0.5$.

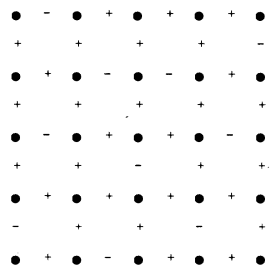

FIG. 2. Section of a random magnetic system. The dots represent spins on a 2D square lattice, and "±" signs indicate the sign of the interaction between adjacent spins. For this arrangement of bonds, all squares are frustrated.

nonetheless random magnetic systems with x_f as large as 1. Figure 2 shows a section of such a model.

The density matrix $z_4(\beta')$ describes a lattice gauge field model of the sort introduced by Wilson[9] and by Balian *et al.*[9] and studied recently by Migdal[10] and by Kadanoff.[11] The special property of such models is their invariance under local transformations reminiscent of a redefinition of the gauge in electrodynamics. In the spin systems we consider there are two local transformations of interest. First, using the bare Hamiltonian (1), one can change the sign of any μ_i and the sign of all interactions J_{ij} which involve the site i. This has no effect on the free energy, as (5) makes clear, since the σ_{ij}'s are unaffected. Toulouse[7] has described this transformation as the true "gauge transformation" for a magnetic Hamiltonian. In addition, our density matrix z_4 has a local symmetry which is a broken symmetry in the full Hamiltonian. The local transformation in which $\sigma_{ij} \to -\sigma_{ij}$ for each of the four σ's about a common site leaves z_4 unchanged. This symmetry is broken by the "external field" $\beta|J_{ij}|$, which appears in z_1.

Other lattice models known to exhibit phase transitions can be transformed into a form analogous to (7b). For example, the 2D ferroelectric eight- and six-vertex models[12] can be represented in this form by identifying the pseudospins σ with the directions of the displacements of the protons along the bonds of "planar-ice" lattices whose vertices lie at the centers of the elementary squares $[ijkl]$. (Divide the vertices into two interpenetrating sublattices, denoted A and B. Let $\sigma = +1$ denote a displacement towards the nearest A site, and away from the nearest B site.) The projection operator (6) for $\Phi = +1$ restricts us to the eight vertices in which 0, 2, or 4 protons are attracted to any vertex. Breaking the local symmetry of $z_4(\Phi = 1, \beta' = \infty)$ with the various two-spin interactions which can fit into a square yields all the common six-vertex models.[12] Thus, the totally symmetric combination, $\sigma_{ij}\sigma_{jk} + \sigma_{jk}\sigma_{kl} + \sigma_{kl}\sigma_{li} + \sigma_{li}\sigma_{ij} + \sigma_{ij}\sigma_{kl} + \sigma_{jk}\sigma_{li}$, distinguishes the "ice-model" configurations with two protons attracted to each vertex from those with zero or four. The other invariant combination, $\sigma_{ij}\sigma_{jk} + \sigma_{jk}\sigma_{kl} + \sigma_{kl}\sigma_{li} + \sigma_{li}\sigma_{ij} - 2(\sigma_{ij}\sigma_{kl} + \sigma_{jk}\sigma_{li})$, splits the four "polar" from the two "nonpolar" ice-model configurations, and thus will generate the F model.[12]

In this context, "frustration" associated with some of the Φ's having the value -1 forces the admixture of odd eight-vertex configurations into the ground state. In the ice problem, this would imply that some vertices will have one or three protons attracted to them, instead of the usual two. This type of disorder would in fact occur in ferroelectrics doped with ions of differing valence. Therefore such alloys should show "frustration" effects akin to those of spin glasses.

III. THE GROUND STATE: EXACT RESULTS

The hidden local symmetry in a spin glass can also be described by noting that z_4 in (7b) requires that one bond in each frustrated square be unsatisfied, but does not determine which one. If the interactions fluctuate in magnitude the bond with smallest $|J_{ij}|$ will be unsatisfied at sufficiently low temperature. Even if all interactions have the same magnitude, however, the requirement from $z_1(\beta)$ that the smallest possible number of bonds remain unsatisfied in the ground state still provides a stringent constraint. To study the latter case we now restrict J_{ij} to be ± 1.

Toulouse[7] has given a geometric interpretation of the possible ground-state configurations of the resulting restricted models. The interpretation is slightly different in two and three dimensions. Unsatisfied bonds in 2D can be visualized by drawing "strings" made up of lines joining centers of adjacent squares and crossing the broken bonds. Strings must begin and end in frustrated squares; thus there are half as many strings as frustrated squares.[13] If we denote the length of the string leaving the square $[ijkl]$ by $L_{[ijkl]}$ (which may be zero), the ground-state energy E_0 is given in two dimensions by

$$E_0 = -2 + N^{-1} \sum_{[ijkl]} L_{[ijkl]} = -2 + x_f L , \tag{9}$$

where L is the average length of the strings present in the ground state. In the special case $x_f = 1$ (Fig. 2) strings of unit length joining adjacent squares are sufficient to pair all frustrated squares, but in general L will exceed 1. Thus, in two dimensions,

$$E_0 \geq -2 + x_f . \tag{10}$$

Bounding or determining E_0 for any specific 2D model therefore yields information about the structure of possible random ground states.

The degeneracy of the ground state is simply the number of minimum length pairings of all the frustrated squares.[7] For the special case of Fig. 2 the number of pairings is known[14] to be $\approx 1.791^{N/2} \approx \exp(0.291N)$, corresponding to a ground-state entropy of $S(0) \approx 0.291 k_B$.

Any heuristic for the assignment of spins to an approximate ground state for a particular model yields an upper bound to E_0 which complements (10). For example, comparison with the energies of ferromagnetic and antiferromagnetic arrangements gives $E_0 \leq -2|1-2x|$. A quasi-1D construction of a random ground state gives a stronger bound at intermediate values of x: Choose the signs of the spins in the row which forms one edge of the sample so that all the interactions between them are satisfied. Next, choose signs for the spins in the adjoining row to minimize the energy due to interactions within that row plus the interactions with the spins in the previous row. A construction which accomplishes this is given in Appendix A. Assign the remaining spins, a row at a time, in the same manner. The energy per spin in this assignment is asymptotically equal to that of an Ising chain with random ± 1 interactions, each spin also feeling a random external field of ± 1. By the gauge symmetry discussed in Sec. II, this problem is equivalent to a uniform chain with all $J=+1$ in a random external field of ± 1. The calculation of the ground-state energy of the latter is straightforward if the signs of the bonds are uncorrelated (see Appendix A). The result is $-\frac{4}{3}$.

We therefore obtain, in two dimensions for models with a fraction x of uncorrelated negative bonds,

$$E_0 \leq \min[-2|1-2x|, -\tfrac{4}{3}]\,. \tag{11}$$

For the case $x = x_f = \frac{1}{2}$, E_0 is restricted by (10) and (11) to lie in the fairly narrow interval $[-\frac{4}{3}, -\frac{3}{2}]$, and $L(\frac{1}{2}) \leq \frac{4}{3}$. Bounds on L for other values of x are also fairly restrictive:

$$L(x) \leq \begin{cases} (1-x)^{-3}, & 0 \leq x \leq \frac{1}{6}, \\ 2/3x_f \leq 1.67, & \frac{1}{6} \leq x \leq \frac{5}{6}, \\ x^{-3}, & \frac{5}{6} \leq x \leq 1\,. \end{cases} \tag{12}$$

It is clear from (12) that the defect strings need never be very long in two dimensions.

Toulouse[7] has suggested that the boundary between the spin glass and ferromagnet at $T=0$ might be signaled by some change in the nature of the configurations of minimum length strings. A natural analogy is to the changes seen in cluster statistics near the percolation threshold,[15,16] where the mean cluster size passes through a cusp, with a finite maximum, and the mean-square cluster size diverges. Equation (12) restricts the maximum average string length, but does not rule out a cusp. However, (9) can be used to rule out any divergence in the mean-square string length. Calculate

$$\langle N(E-E_0)^2 \rangle = N^{-1} \sum_{[ijkl]}{}' (L^2_{[ijkl]} - L^2)\,, \tag{13}$$

where the prime restricts the summation to frustrated squares. The left-hand side of (13) is $k_B T^2 C(T)$, and must vanish at low temperatures. This requires fluctuations in $L_{[ijkl]}$ to be irrelevant in the thermodynamic limit as $T \to 0$.

The numerical studies discussed in Sec. IV show that $L(x)$ does have a slight maximum in the concentration range where the ferromagnet–spin-glass transition is seen. They also provide estimates of the ground-state degeneracy away from $x_f = 1$.

The construction of minimum-energy configurations of unsatisfied bonds is more complicated in 3D than in 2D. Two examples are shown in Fig. 3. If one draws a line of unit length normal to the center of each frustrated square, the lines, like lines of magnetic field, will close on themselves or run off to infinity.[7] (Since the edges of any elementary cube in the lattice form a planar graph, there will always be an even number of frustrated faces,[13] so that as many lines enter as leave each cube.) Each closed line subtends surfaces of elementary squares; the bonds cut by such a surface are taken to be unsatisfied; and the ground-state configurations can be described as those covering surface(s) of minimum area. As shown in Fig. 3(b), even for simple closed curves there may be several minimal covering surfaces. For the cases of physical interest when $x_f \approx \frac{1}{2}$ there will be on average three lines entering or leaving each cube defined by six adjacent plaquettes. The resulting "frustration network"[7] of lines will be quite complex, so one expects a large number of distinct ground-state configurations.

In 3D the surface to perimeter ratio λ of a minimal covering plays the same role in the total energy as did L, the string length, in 2D. For the isolated antiferromagnetic bond that gives rise to Fig. 3(a), $\lambda = \frac{1}{4}$, and one unsatisfied bond is associated with four frustrated squares. At higher densities, situations like Fig. 3(b), with $\lambda = \frac{1}{2}$, become common. Thus $\lambda \geq \frac{1}{4}$ and should grow with increasing density. Since there are three squares per site, in 3D,

$$E_0 = -3 + 6\lambda x_f\,, \tag{14}$$

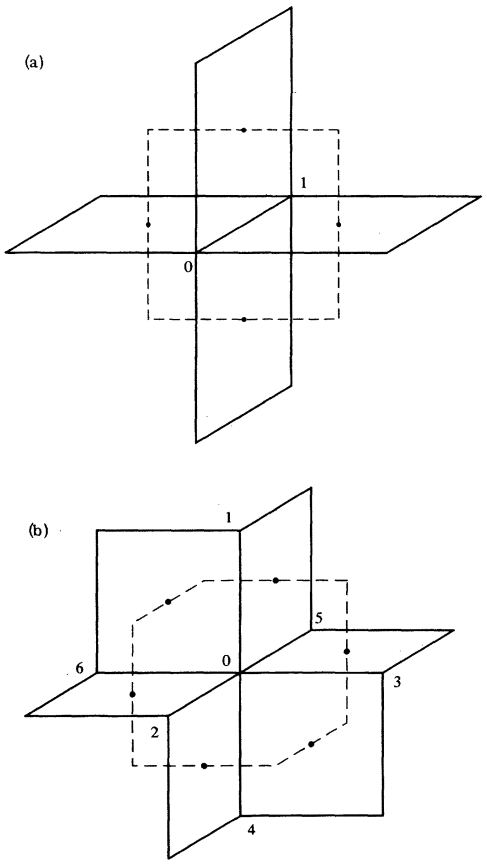

FIG. 3. (a) Simplest case of a 3D frustration network (dashed line). The bond between spins at 0 and 1 is unsatisfied in the ground state. (b) 3D frustration network with $\lambda = \frac{1}{2}$, and two possible covering surfaces. One surface cuts the bonds 01, 02, and 03, the other cuts 04, 05, and 06.

and the lower bound is

$$E_0 \geq -3 + \tfrac{3}{2}x_f . \tag{15}$$

Upper bounds to E_0 are derived as before. The energies of ferromagnetic and antiferromagnetic arrangements of spins are, respectively, $\pm 3(2x-1)$. If we set the spins into an approximate ground state one row at a time, taking into account only spins previously assigned, the energy per spin of the resulting configuration will be asymptotically equal to that of a row of spins with uniform +1 interactions, and a random external field which takes the values 0, ±2. This is worked out in Appendix A for the uncorrelated case $x = \frac{1}{2}$ (which should be concentration with the highest ground-state energy). The resulting upper bound is $E_0 \leq -1.5$, so, in 3D,

$$E_0 \leq \min\left[-3\left|1-2x\right|, -\tfrac{3}{2}\right] . \tag{16}$$

For $x = \frac{1}{2}$, $x_f = \frac{1}{2}$ this constrains E_0 to lie between -2.25 and -1.5 and λ between $\frac{1}{4}$ and $\frac{1}{2}$, the two extremes shown in Fig. 3. Although $\lambda = 1$ is geometrically possible and corresponds to an infinite open frustration network, it does not appear to have significant weight when the interactions in the model are uncorrelated.

IV. MONTE CARLO RESULTS

Monte Carlo calculations were carried out on fairly large samples of 2D and 3D Ising models, prepared with random ±1 interactions, uncorrelated in position, with a fraction x of the interactions antiferromagnetic. Calculations of the specific heat, susceptibility and internal energy at finite temperature, studies of the possible ground states [and hence of $L(x)$ and $\lambda(x)$], and some results on relaxation kinetics are reported in this section.

Ising models in which the interactions are continuously distributed have been studied by several groups. In particular, Binder *et al.*[17] have considered 2D and 3D models with nearest-neighbor interactions. At sufficiently low temperatures, there are important differences between ±1 models and models in which the J_{ij} are continuously distributed. One can think of the ground state of a ±1 model as having a fourfold degeneracy per frustrated square, constrained by the requirement that the defect surfaces be of minimal area or length. The degeneracy within each frustrated square is removed when the interactions fluctuate in magnitude.

When x_f is sufficiently large, there may no longer be a phase transition in the ±1 model. An example where this is known to occur is the Ising antiferromagnet on a planar triangular lattice,[18] a model in which $\Phi = -1$ for all elementary circuits (triangular faces). By analyzing high temperature series for the ±1 model (taking $x = x_f = \frac{1}{2}$), Fisch and Harris[19] have recently suggested that the paramagnet–spin-glass transition changes at four spatial dimensions from a second-order transition to one with infinite exponents. The singularity in the susceptibility which they calculate moves off the real temperature axis below four dimensions. Thus 2D and 3D ±1 models may be below the lower critical dimensionality.

This inference from Fisch and Harris's work conflicts with lattice renormalization-group calculations which indicate that a second-order transition from spin glass to paramagnet will occur in 3D and perhaps in 2D as well.[20-22] Under lattice rescaling, the discrete ±1 distribution of interactions quickly smears into a continuous distribution centered about $J = 0$ (see especially Fig. 3 of Ref. 22), so close to any phase tran-

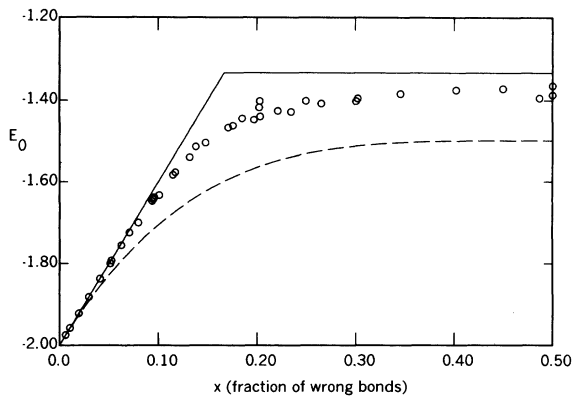

FIG. 4. Ground-state energy for 2D samples of 80 $\times$80 spins, plotted vs x. The upper bound given by (11) is indicated by a solid line, the lower bound (10) by a dashed line.

sition, there should be no distinction between models with discretely and with continuously distributed interactions. Finally, Binder's simulations[17] seem to show a phase transition in the magnetic susceptibility at a temperature which is consistent with (lower than) mean-field-theory estimates.[1]

Results that bear on ground states of the 2D ± 1 model are presented in Fig. 4 [$E_0(x)$] and Fig. 5 [$L(x)$ from the same data]. Ground states were reached by performing Monte Carlo simulations at successively lower temperatures, until the internal energy reached a limiting value. Each data point represents the lowest value of E_0 obtained for a particular sample. For $x \lesssim 0.15$, the lowest energies were obtained by starting with all spins ferromagnetically aligned and cooling rather quickly to low temperatures. Above $x \gtrsim 0.2$, better ground states were obtained by first warming the sample to randomize spin directions, then cooling in very slow steps. We expect, therefore,

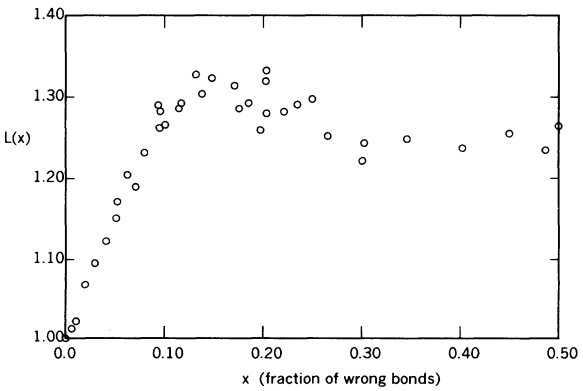

FIG. 5. Average ground-state string length $L(x)$ observed in 80$\times$80 spin 2D samples with various values of x.

that the transition from ferromagnet (perturbed by local fluctuations) to spin glass occurs somewhere in the range 0.15–0.2 for this model.

Figure 4 shows that the 1D construction gives a fairly accurate estimate of E_0 for $x_f \approx 0.5$. Values of E_0 obtained at $x = 0.5$ cluster about -1.39 (we did not investigate the dependence of E_0 on sample size), so the error is of order 5%. It is not possible to tell from the data as plotted in Fig. 4 whether the transition between ferromagnetic and spin-glass phases is first order at $T = 0$, signaled by a change in the slope of $E_0(x)$, or second order, with $\partial E_0(x)/\partial x$ continuous. (For the infinite-range Ising model of Ref. 2, the transition was found to be second order, but that model represents the high-dimensionality mean-field limit, and should not be compared in detail with 2D or 3D spin glasses.)

Figure 5 also shows distinct regions of low- and high-concentration behavior. At very low concentrations the most common magnetic defect is an isolated wrong bond. The probability of a wrong bond bordered by two squares with no other wrong bonds is $x(1-x)^6 \sim x - 6x^2$. This gives rise to a string with $L_{[ijkl]} = 1$. The probability of finding (by sampling bonds at random) a configuration with two wrong bonds in a square is $\sim 3x^2$. For small x this produces two frustrated squares separated by a normal square, with $L_{[ijkl]} = 2$. There are arrangements of three wrong bonds which enter to order x^3 and force, at small x, strings of length 3. These isolated configurations correspond to Toulouse's picture[7] of the frustrated squares separating from their partners as x increases. To leading order in x, the predicted dependence of $L(x)$ for small x is $\sim (x - 6x^2 + 6x^2)/(x - 6x^2 + 3x^2) \sim 1 + 3x$, in agreement with the data in Fig. 5.

At high densities ($x \gtrsim 0.15$ or $x_f \gtrsim 0.4$), clusters of wrong bonds and their surrounding squares are no longer isolated, and a defect structure with relatively short strings is always possible. Examination of computer generated ground states in this concentration range turned up no strings of more than four steps. The transition seems most like the condensation of a liquid from vapor and thus would normally be first order. Consequently we suspect that $L(x)$ should have a cusp somewhere near $x \approx 0.16$, and that the ferromagnet–spin-glass transition is first order for this "pure-frustration" Ising model.

The Monte Carlo calculations provide several pieces of information about the degeneracy of the spin-glass ground state. For 2D samples with $x \approx 0.5$, it was found that at $T = 0$ about 0.08 of the spins experience a completely canceled exchange field, and thus are still free to flip. This fraction

decreased monotonically when x tended to 0 or to 1. Although any one of these spins is free to flip, it is not true that any combination of the spins in zero-exchange field can flip, since some of them are neighbors. Thus this observation does not directly determine the ground-state entropy. We also kept track of the fraction of spins which had flipped one or more times at $T=0$ during a Monte Carlo chain of 20–50 time steps (attempted moves) per spin, after the system had been cooled into a ground state. This quantity appears to saturate after about 20 time steps per spin, at a value roughly twice the fraction of spins found in zero field at any one time. (It did not, as one might have expected, tend to unity.) For $x \approx 0.5$ in 2D, roughly 0.18 of the spins were in this category. From this measurement we obtain an upper bound on the ground-state degeneracy (for $x=\frac{1}{2}$) of $2^{0.18N}$, or $S(0)<0.125k_B$.

If the internal energy is known for all temperatures, $S(T)$ can be extracted by

$$\frac{S(T)}{k_B} = \ln 2 - \int_T^\infty \left(\frac{dU}{dT}\right)\frac{dT}{T}. \tag{17}$$

At sufficiently high temperatures, $U(T)$ is given by

$$U(T) \sim -d \tanh(1/k_B T) \tag{18}$$

for a cubic lattice in d dimensions. Figure 6 shows that (18) is a good approximation for $T \gtrsim 4$ in the case $x \approx 0.5$. We therefore calculated $S(T)$ by "computer calorimetry"[23] using (17) with $U(T)$ given by (18) when $T > 10.0$, and determined from the Monte Carlo simulations when $T \leq 10.0$. Results for four different concentrations are plotted in Fig. 7. The data for $x=0.5$ were obtained by averaging results from three samples; the other points represent one sample each. $S(0)$ is nearly constant (and $=0.099k_B$ for $x=0.5$) from $x=0.5$ to 0.2, i.e., in the spin-glass phase. It decreases steadily to zero in the ferromagnetic phase. $S(0)$ for the case $x=\frac{1}{2}$ implies a ground-state degeneracy of order $2^{0.14N}$. Thus the number of independent degrees of freedom in the "frustrated" ground state exceeds the number of spins free to flip at any one time!

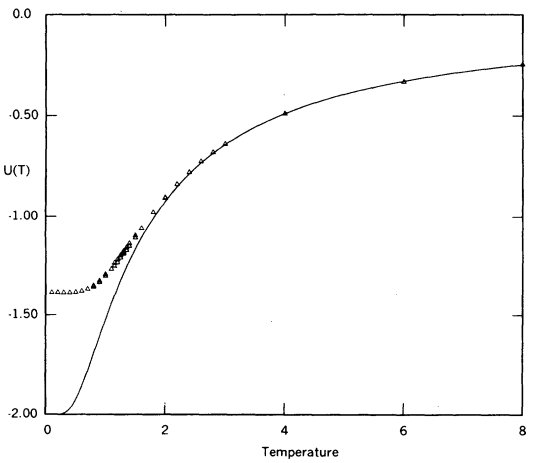

FIG. 6. Internal energy vs T for three 80×80 samples with $x=0.5$. The solid line is the high temperature approximation to $U(T)$, given by (18).

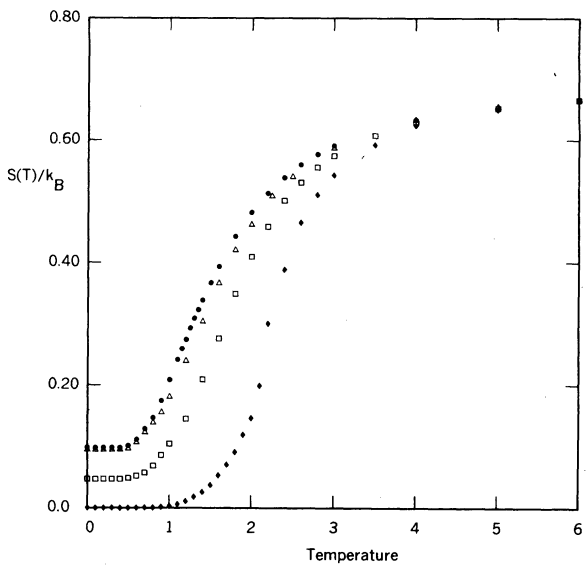

FIG. 7. Entropy as a function of temperature for 2D Monte Carlo samples with the following concentrations of wrong bonds: $x=0.5$ (dots); $x=0.2$ (triangles); $x=0.1$ (squares); and, as a check, $x=0.0$ (diamonds).

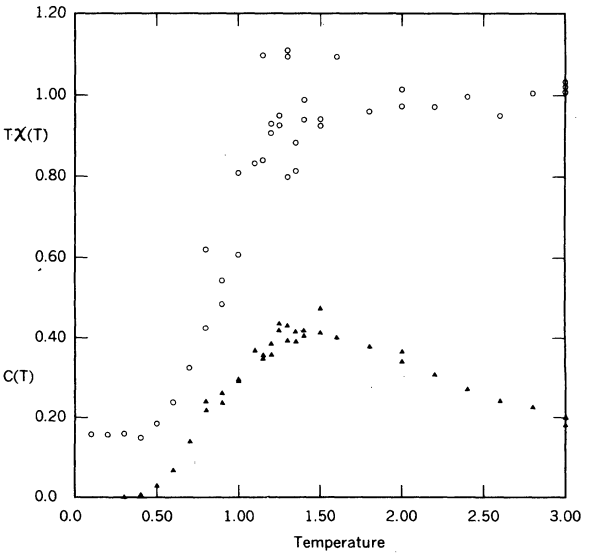

FIG. 8. Spin-spin correlations (circles) and specific heat (solid triangles) for the 2D random-bond spin glass with $x=0.5$.

The static thermodynamic properties obtained for finite temperatures in the case $x = 0.5$ are summarized in Fig. 8. The circles give spin-spin correlations in the form

$$\left\langle \left(\sum_i \mu_i \right)^2 - \left\langle \sum_i \mu_i \right\rangle^2 \right\rangle \Big/ N \equiv T\chi(T) .$$

For this case, since $\langle J_{ij} \rangle = 0$, $T\chi(T) = 1 - q$, where q is the Edwards-Anderson order parameter.[1,2] The susceptibility is seen in Fig. 8 to follow a Curie law down to a temperature of roughly 1.5, and to drop rapidly below $T \approx 1.25$. Similar behavior is observed in Binder's Monte Carlo simulations[17] of 2D spin glasses with continuously distributed interactions, and his value of $T_{sg}/\langle J^2 \rangle^{1/2}$ is comparable to ours. The decrease is consistent with $q \propto (T_{sg} - T)^{\beta}$, for a value of $\beta \lesssim 1$, but the data are not good enough for any quantitative estimates. Since there are spins free to flip in the ground state, $q(T)$ does not saturate at 1, but at a smaller value, as Fig. 8 indicates.

The specific heat, shown with solid triangles in Fig. 8, has a rounded maximum, as was also seen in Binder's calculations. This maximum occurs at nearly the same temperature as the break in $T\chi(T)$, however, while in the models with continuously distributed interactions the maximum in C occurs at a higher temperature. Presumably the formation of small clusters of strongly coupled spins at temperatures $\gtrsim T_{sg}$ is enhanced by the continuous distribution of J_{ij}'s.

Ground-state energies found for 3D samples of the ± 1 model are plotted against x in Fig. 9. For $x \lesssim 0.20$ the lowest-energy states are obtained by cooling from an initially ferromagnetic arrangement of spins, and $E_0(x)$ is not much less than the energy of the unrelaxed ferromagnetic state. Above $x \approx 0.25$, lower energies were obtained by first randomizing the spins. Thus the ferromagnet–spin-glass transition occurs between 0.2 and 0.25 in 3D for this model. The 1D construction is a weaker bound here than in 2D. We find $E_0(x = 0.5) \approx -1.75$, which is about 17% lower than the quasi-1D estimate.

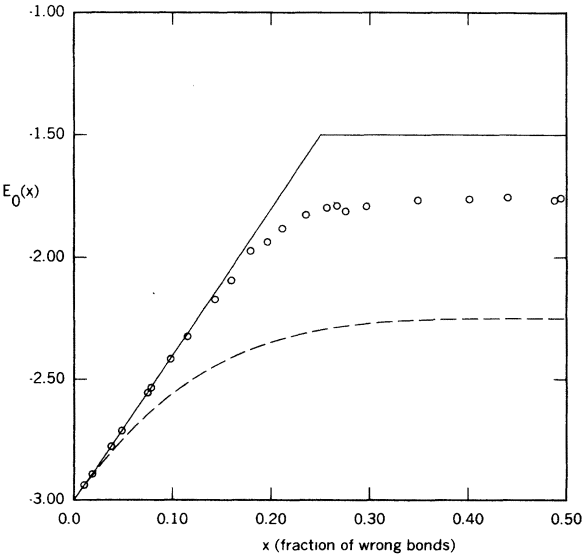

FIG. 9. Ground-state energy for small (16×16×16) samples of 3D random-bond model, plotted vs x. The upper bound given by (16) is indicated with a solid line, the lower bound (15) by a dashed line.

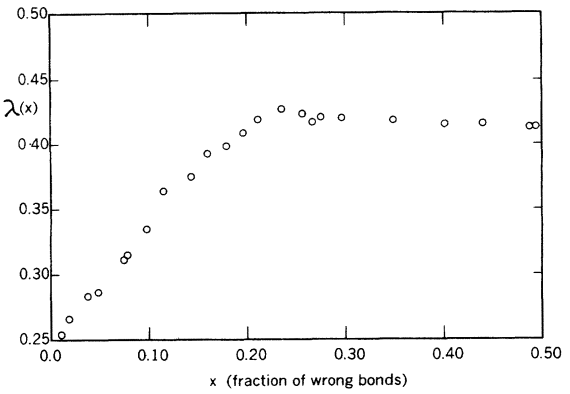

FIG. 10. Ratio of defect surface area to perimeter for 3D random-bond model, as a function of x, using the data of Fig. 9.

We plot values of $\lambda(x)$, the ratio of defect surface area to the perimeter or frustration network length, in Fig. 10. As in 2D (Fig. 5), the maximum in $\lambda(x)$ coincides with the concentration range in which the ferromagnet–spin-glass transition occurs. The data seem to show two lines, for the low- and high-concentration regimes, intersecting with discontinuous slope at $x \approx 0.24$. This again suggests a first-order transition.

The 3D ground state is not as highly degenerate as the 2D. For $x = \frac{1}{2}$ we find (5–6)% of the spins at a time are free to flip at $T = 0$; (10–12)% of the spins had flipped one or more times after 20 time steps in equilibrium at low temperatures. The entropy was estimated from $U(T)$ for a single 3D sample of $20 \times 20 \times 20$ spins with $x = 0.5$, using (17) and (18). The result is $S(0) = 0.062 k_B$, which implies a ground state degeneracy of order $2^{0.09N}$.

Recent real-space renormalization-group calculations[20,21] have also predicted that the spin-glass phase narrows with increasing dimensionality. Jayaprakash *et al*,[21] using an approximate version of the Migdal recursion relation,[10,11] find the zero-temperature critical concentration to be 0.05 in 2D and 0.17 in 3D, while Southern and Young[20] have also considered more elaborate decimation schemes, and find a transition at $x = 0.21$

in 3D. Southern and Young's 3D result is in reasonable agreement with the data of this paper, while the Migdal scheme evidently overestimates the tendency to form a spin glass. Also, lattice-rescaling calculations inevitably seem to predict[20] a second-order boundary between the ferromagnetic and spin-glass phases. Our conclusion that the transition may be first order is supported by low-temperature series on this model [M. Wortis (private communication)], which show no simple critical behavior as a function of x.

The phenomenon of field cooling is one of the most dramatic experimental signatures of a spin glass,[4] the one responsible for the term "glass" in this context. A spin-glass sample cooled to very low temperatures in zero magnetic field is demagnetized; the same sample, cooled in a small applied field, develops a net moment which remains after the field is turned off. The moment of the field-cooled sample is then stable against small perturbations, e.g., hysteresis loops taken at low temperature are displaced from the origin in a field-cooled sample.

We have studied the Monte Carlo time evolution of relatively large ($20 \times 20 \times 20$ spin) 3D samples of the ± 1 model Ising spin glass to determine whether simplifying this model to include frustration but not fluctuations in the magnitude of exchange has eliminated or altered the field cooling and other relaxation effects. In the limit $x_f = 1$, one would not expect to be able to freeze in a moment at $T = 0$ K, since different ground states are readily transformed into one another by flipping spins in zero-exchange field. For small values of x_f, however, transforming one ground state into another may require some activation energy. An example is given in Fig. 11, which shows a portion of a 2D system. For the system to move from the ground state indicated by the heavy dashed strings to the state of equal energy indicated by the vertical light dashed strings, first spin 1 must flip against its exchange field, then before spin 1 can flip back spins 2 and 3 must flip (in zero field), leaving spin 4 unstable, able to gain energy by flipping and completing the transformation. Processes like this will be frozen out at low temperatures.

Figure 12 and 13 show the existence of a field cooling effect in the ± 1 models with $x_f \lesssim 0.5$. The influence of a weak external field h, with $JS > g\mu_B h > k_B T$ was simulated by modifying the rules for transitions between successive Monte Carlo states. When $h = 0$, any spin found to have zero exchange field flips over each time step. When $h \neq 0$, a spin with zero exchange field is left aligned with h. (For each Monte Carlo time step, the spins were sampled in a different random sequence.) A sample in an external field reaches a local equilibrium (with no free spins) in a few time steps per spin.

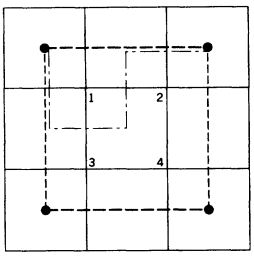

FIG. 11. Configuration in 2D in which an activation barrier separates two degenerate ground-state configurations. The spins lie at the intersections of the solid lines, heavy dots mark the frustrated squares, and the two possible pairs of ground-state strings are indicated by light and heavy dashed lines. Flipping spin 1 stretches the upper string to the position shown by the short-long dashes. Subsequently, flips of spins 2, 3, and 4 bring the system to the other ground state.

For $x \approx x_f \approx 0.5$, starting a 3D sample with all spins ferromagnetically aligned and allowing it to evolve at low temperature in a field quickly leads to a stable state with a net moment of 0.5 to 0.6. The field was then turned off and the sample allowed to evolve to a state of lower energy (and magnetization). The net moment at the end of each subsequent time step is plotted for two such samples in Fig. 12 over 2000 time steps, a relatively long time. From the ground state energy and entropy calculations we know that this model has a large number of ground states with moment

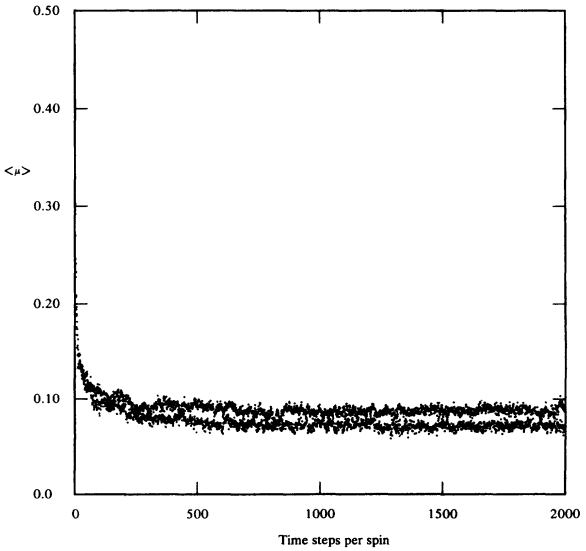

FIG. 12. Decay of the magnetization frozen in by cooling a spin-glass sample in a small external field. Data are from two $20 \times 20 \times 20$ spin samples with $x = 0.5$.

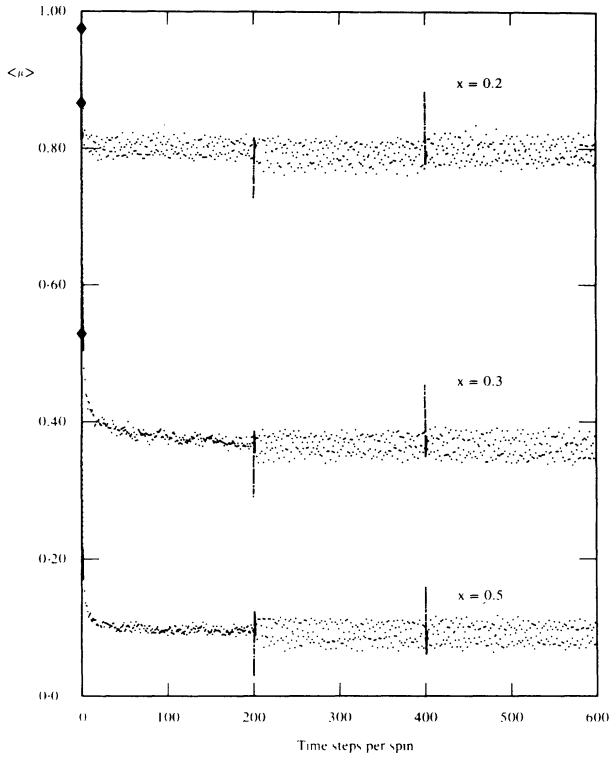

FIG. 13. Relaxation of the magnetization in field-cooled $20\times20\times20$ spin random-bond models at three concentrations, $x=0.2$ (just inside the ferromagnetic phase), $x=0.3$ (just inside the spin glass phase), and $x=0.5$. The spikes are the result of applying a small external field. Diamonds indicate the magnetization in each case when external field is initially turned off.

nearly zero. If the 6% of free spins were independent, one would predict ground state moments in the range $\langle \mu \rangle = 0 \pm 0.003$ for this size sample. Yet both samples relax to a stable set of ground states with $\langle \mu \rangle \approx 0.07$–$0.09$. The field-cooled states in Fig. 12 reached energies which exceeded the lowest observed energies for the same samples by no more than 2%. The rate of relaxation is much greater than Binder observes in models with continuously distributed interactions.[17] We do not find the slow power law or logarithmic decay which he has analyzed and therefore attribute that effect to single spin-flip activation barriers caused by the fact that the finite number of interactions seen by each spin will almost never add to zero when the interactions fluctuate in magnitude.

A further test of the local stability of the field-cooled ground states is given in Fig. 13 for three concentrations. States prepared as in Fig. 12 were allowed to relax in zero field for 200 time steps per spin. Then a field in the opposite directions was applied for long enough to freeze all free spins. Subsequent relaxation quickly returns the system to the same average moment. Application of a second external field, in the direction of the original field, also does not change the average magnetization. Thus, Figs. 12 and 13 confirm that frustration is sufficient to produce activation barriers between ground states for $x_f \lesssim 0.5$.

The relaxation behavior seen in Figs. 12 and 13 is qualitatively different from the kinetics of long-lived domains studied in pure Ising ferromagnets.[24] Large clusters of reversed spins persist in equilibrium at elevated temperatures, but they will decay at sufficiently low temperatures since the domain wall area can always be shrunk to zero by a sequence of spin flips which never encounters an activation barrier. In the ferromagnetic phase of the random ±1 model, the frustrated squares act as pinning centers for domain walls bounding clusters of reversed spin. The effect is most easily pictured in 2D. Figure 14 shows a particularly clear example of pinning. Most of the defect strings connect adjacent frustrated squares, but one large cycle at the center of the sample forms a conventional domain boundary. This is stabilized at a dozen places by pairs or small groups of frustrated squares. The activation energy to shrink the domain wall by first detaching it from any of the pinning centers is at least $2|J|S$, so the domain is stable at $T=0$. A

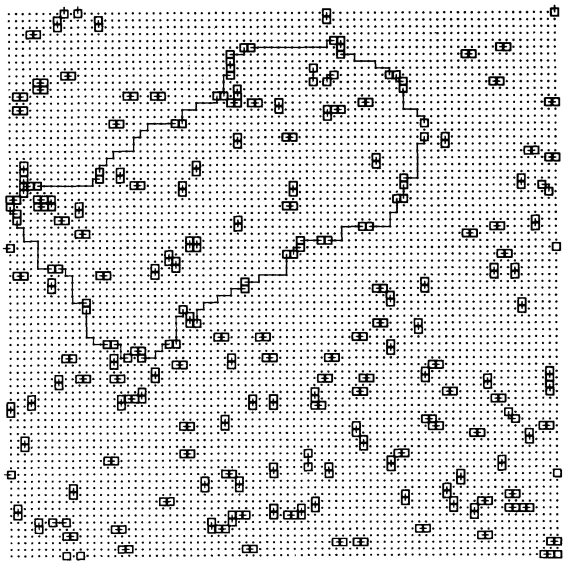

FIG. 14. Stable magnetic defect structure for an 80×80 spin 2D sample with $x=0.015$, $x_f=0.06$. The squares denote frustrated squares, the dots mark the centers of squares in which $\Phi=1$, and the lines represent defect strings. The magnetization is reduced to 0.56 by the large region of reversed spins at the center of the sample.

similar pinning effect has been shown to occur in dilute Ising models.[25]

The pinning phenomena which stabilize the various spin-glass ground states are more complex, but the focus on frustration and the magnetic defect structure suggested in Ref. 7 appears to provide the necessary tools to analyze them. (In a report received after this work was completed, Vannimenus and Toulouse[26] have observed that the energy cost of an extended defect or domain wall like that of Fig. 14 can vanish for sufficiently large x_f. This provides another probe for the transition from ferromagnet to spin glass. The critical concentrations estimated in this way are slightly smaller than those we quote above.) We hope to continue the analysis of low energy states and their consequences for the low-temperature physics of a spin glass in a future paper.

Note added in proof. Random Ising models in which $J = \pm 1$ have also been discussed by Y. Veno and T. Oguchi [J. Phys. Soc. Jpn. 40, 1513 (1976)]. These authors predict the occurrence of a spin glass phase at intermediate concentrations. Monte Carlo studies of these models by I. Ono [J. Phys. Soc. Jpn. 41, 345, 1425 (1976)], using relatively small 2D and 3D samples, predict ground state energies and transition concentrations in good agreement with the results of the present work.

ACKNOWLEDGMENTS

A stimulating correspondence with Gerard Toulouse and Jean Vannimenus is gratefully acknowledged. I am also indebted to K. Binder, M. Wortis, and A. P. Young for preliminary reports of unpublished work and to R. Fisch for bringing the work in Ref. 25 to my attention.

APPENDIX A: GROUND STATE OF A RANDOM 1D ISING CHAIN

Consider the 1D Ising Hamiltonian

$$\mathcal{H} = -\sum_i J_i \mu_i \mu_{i+1} - \sum_i h_i \mu_i , \qquad \text{(A1)}$$

where $J_i = \pm 1$ and h_i represents the interaction with μ's previously assigned orientations in the course of constructing an approximate ground state to a 2D or 3D spin glass. In the 2D construction $h_i = \pm 1$, while in the 3D example h_i describes two spins, and takes tne values $0, \pm 2$. We redefine the μ's in order to transform (A1) into a more convenient form. Start at one end of the chain, say $i = 1$. If $J_i = -1$, replace J_i by $+1$, and $(J_{i+1}, \mu_{i+1}, h_{i+1})$ by $(-J_{i+1}, -\mu_{i+1}, -h_{i+1})$, and continue the process with J_{i+1}. The result is a chain with

$$\mathcal{H}' = -\sum_i \mu_i' \mu_{i+1}' - \sum_i h_i' \mu_i' , \qquad \text{(A2)}$$

in which $(\mu_i', h_i') = (-1)^{n_i}(\mu_i, h_i)$, where n_i is the number of negative J_j for $j \le i$.

Since we need only the ground-state energy we shall now drop the primes and study (A2) instead of (A1). We treat the case of equal numbers of $\pm$ bonds, which leads in (A2) to equal numbers of $h_i = \pm 1$. It is assumed that there are no correlations in the positions of negative bonds. It is probably possible to calculate the ground-state energy of (A2) under more complicated assumptions, but the result should be a lower energy, and we are interested here in obtaining an upper bound to the energy of a 2D or 3D spin-glass ground state.

Consider a cluster of n adjacent spins with the same value of the external field h. For sufficiently large n the spins must align along h, leaving at most two unsatisfied bonds at the two ends of the cluster. We can construct a ground state by identifying all such clusters. First group all those adjacent spins with the same value of h_i into clusters. Assign orientations to the clusters, starting from one end of the sample. For the $h_i = \pm 1$ case, if a cluster has two or more spins, align it with its external field; if it consists of a single spin, align it with the preceding (say, left-hand) cluster.

The calculation of the average energy per spin resulting from this assignment is as follows: The probability that a spin belongs to a cluster of exactly n spins with the same h_i is $n/(2^{n+2})$. Thus $\frac{1}{8}$ of the spins are isolated in 1-spin clusters with $h_i = +1$, $\frac{3}{8}$ in clusters of 2 or more with $h_i = +1$, and likewise for $h_i = -1$. The total energy of a cluster of n (> 2) spins is $-2n + 2$, assuming that the bond extending to the left of the cluster along the chain is unsatisfied, and counting the bond to the right as part of another cluster. Therefore the average energy per spin in clusters with $n > 2$ is

$$\left(\sum_{n=2}^{\infty} \frac{-2n+2}{2^{n+2}}\right) \Big/ \left(\sum_{n=2}^{\infty} \frac{n}{2^{n+2}}\right) = \left[\tfrac{3}{8}(-2) + \tfrac{1}{4}\right] / \tfrac{3}{8} = -\tfrac{4}{3} , \qquad \text{(A3)}$$

The remaining spins occur in groups of one or more consecutive 1-spin clusters found between two clusters with $n > 2$. The probability that a spin is one of m consecutive 1-spin clusters is $m/2^{m+3}$ (counting both signs of h_i). If m is even, interactions with the h_i cancel and the energy is given by just the bonds along the chain: $E_0^{(\text{even})} = -m$. If m is odd, $\sum_i h_i \mu_i = +1$, and the bond to the large cluster on the right is satisfied. Since this was assumed to be unsatisfied in calculating (A3) we add -2 to the energy to correct, and obtain $E_0^{(\text{odd})} = -(m+1)$. The average energy per spin

in the 1-spin clusters is therefore

$$\left(-\sum_{m=1}^{\infty}\frac{m}{2^{m+3}}-\sum_{m=1,3,5}^{\infty}\frac{1}{2^{m+3}}\right)\left(\sum_{m=1}^{\infty}\frac{m}{2^{m+3}}\right)^{-1}=-\tfrac{4}{3}. \qquad \text{(A4)}$$

From (A3) and (A4) we have $E_0=-\frac{4}{3}$ for the 1D chain with both J_i and $h_i=\pm1$ at random.

To find an asymptotic upper bound on the energy of the 3D spin-glass ground state we need the ground-state energy of a 1D chain (A2) with $h_i=0$ with probability $\frac{1}{2}$, and $h_i=\pm2$ each with probability $\frac{1}{4}$. Again group consecutive spins with the same external field into clusters. This time all clusters with $|h_i|=2$ are aligned along the external field, while clusters with $h_i=0$ are aligned with their neighbors to the left. The probability per spin of finding a cluster of n consecutive $h_i=+2$ is $(\frac{3}{4})^2n/4^n$, and the energy of such a cluster is $-3n+2$ if the following cluster has $h=-2$, $-3n$ if it has $h=0$. The probability of the first case is $\frac{1}{3}$, of the latter, $\frac{2}{3}$. Thus the average energy per spin in the clusters with $|h|=2$ is

$$-3+\left(\frac{9}{16}\sum_{n=1}^{\infty}\frac{\frac{2}{3}}{4^n}\right)\left(\frac{9}{16}\sum_{n=1}^{\infty}\frac{n}{4^n}\right)^{-1}=-2.5. \qquad \text{(A5)}$$

A cluster of n spins in zero external field has total energy $-n$ if the clusters to the right and left are aligned in the same direction, and $-n+2$ if they are not. The two cases are equally probable. Averaging them we obtain the average energy per spin for the spins in zero field:

$$-1+\left(\sum_{n=1}^{\infty}\frac{2}{2^{n+3}}\right)\Big/\left(\sum_{n=1}^{\infty}\frac{n}{2^{n+3}}\right)=-0.5. \qquad \text{(A6)}$$

Taking the average of (A5) and (A6) gives the ground-state energy per spin for the chains which occur in the 3D spin-glass ground-state construction $E_0=-1.5$.

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*Permanent address.

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