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Frustration, randomness, and the spin-glass transition

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Numerical simulations are reported on a periodic fully frustrated Ising system in three dimensions and on the same system after the introduction of disorder; with less than 10% random interactions the system is transformed into a spin glass. The striking differences in the physical properties of the system with and without disorder are discussed in terms of phase-space geometry. This approach provides us with a general scenario that can explain why in spin glasses one observes a broad featureless specific-heat maximum at a temperature exceeding the freezing temperature.

Spin glasses have been intensively studied for many years because they represent the conceptually simplest examples of the vast panoply of complex systems, but despite considerable progress (mainly through numerical work) there is still no consensus concerning the correct description of the freezing transition in finite-range spin glasses. This problem is clearly of crucial importance to the understanding of the physics of spin glasses and through them of complex systems in general.

We have studied by numerical simulations the static and dynamic properties of a regular fully frustrated three-dimensional (3D) Ising system, and of the same system after we introduced random interactions. A small degree of randomness transforms the regular system into a spin glass. A discussion of the results in terms of a comparison of the respective phase-space geometries of the fully frustrated and the modified system provides an intuitive image of the spin-glass transition and allows concrete predictions to be made. We suggest that the phase-space approach can provide a general method for understanding nonstandard types of phase transitions.

We first study the periodic fully frustrated 3D Ising system with $\pm J$ near-neighbor interactions on a simple cubic lattice illustrated in the inset of Fig. 1, which we will refer to as the FFI* system. Each plaquette in the lattice is frustrated with three interactions of one sign and one of the other. The FFI* lattice is equivalent by gauge transformation to another fully frustrated system (with three times as many positive interactions as negative), FFI; this latter has been extensively studied.[1–5] Through the gauge transformation the thermodynamic properties of the two lattices will be identical (we have checked that we find the same specific heat and ordering results on FFI* as obtained on the FFI system).[4,5] The FFI has a λ pointlike divergence of the specific heat at an ordering temperature $T_c=1.355$.[4,5] (All temperatures will be quoted in units of J.) The transition has unusual characteristics; theoretically predicted to be first order,[2,3] simulations show it to behave as second order, but with a crossover in effective critical exponents at a temperature of about $1.08T_c$.[4] Weak first-order behavior may set in for very large samples.[5] Just below the ordering temperature there are 16 different ordered states[3,5] and at low temperatures the degeneracy tends to $\sim 2^{N^{2/3}/4}$.[2] We prefere to work with the FFI* system as it contains globally as many positive as negative interactions so one can go continuously and transparently from this regularly frustrated lattice to the $\pm J$ 3D Ising spin glass (ISG) by replacing at random a fraction p of the regular interactions by interactions of random sign (note that the fraction of interactions whose signs have changed is then $p/2$).

We have carried out simulations on lattices of L^3 spins with L up to 32 and periodic boundary conditions, using spin-by-spin heat-bath updating. We followed a step-by-step anneal procedure with a long final anneal at the measuring temperature. We used the criterion of Ref. 6 to establish when thermal equilibrium was attained and checked that further annealing did not affect the measurements. Our results on FFI* show that the dynamics at and close to T_c are unconventional: in contrast to a standard ferromagnet or spin glass where at the ordering temperature the autocorrelation function, $q(t)=\langle S_i(t)S_i(0)\rangle$, behaves as t^{-x} with preasymptotic effects only showing up at short times [$t\sim 1$ MCS (Monte Carlo steps)], the FFI* system shows a wide preas-

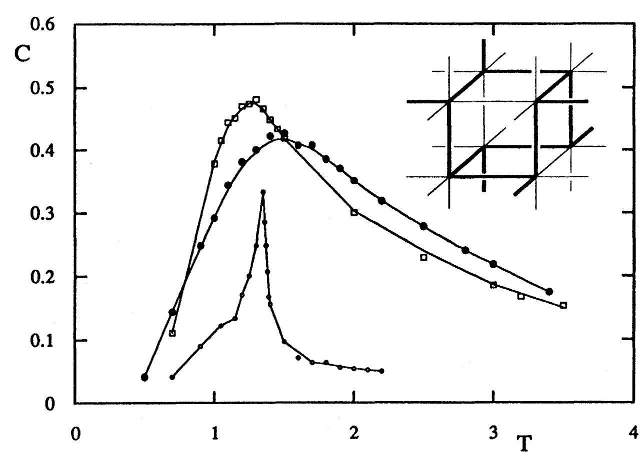

FIG. 1. The specific heats for the FFI* system (see Ref. 4), and for perturbed FFI* systems with random interaction concentrations $p=0.1$ (open symbols) and 0.2 (closed symbols) as functions of temperature. The FFI* data are multiplied by $\frac{1}{4}$. Inset: a one-eighth unit cell of the periodic fully frustrated FFI* lattice. Heavy lines: $+J$, light lines: $-J$. The signs of the interactions alternate along each lattice row.

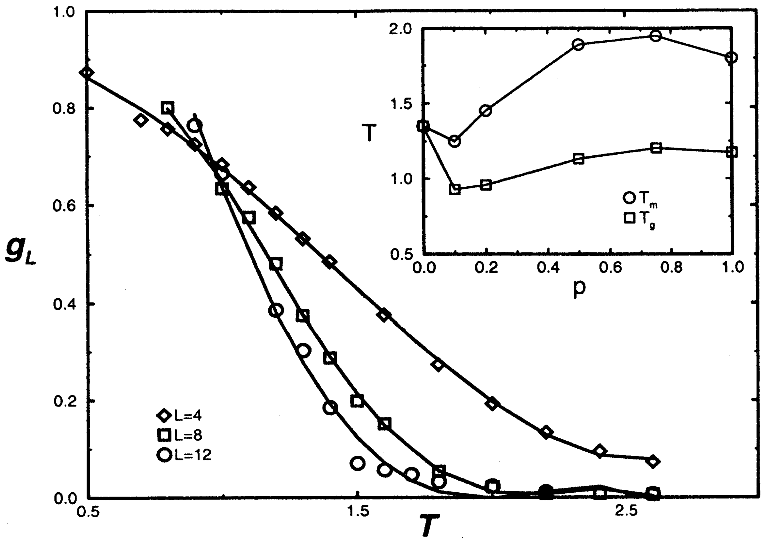

FIG. 2. The scaling function g_L for the perturbed FFI* system with random interaction concentration $p=0.2$ for sample sizes $L=4$, 8, and 12. Inset: specific-heat maximum temperatures (upper curve) and spin-glass ordering temperatures (lower curve) as functions of p.

ymptotic regime (up to $t\sim100$ MCS). We will discuss this behavior elsewhere.

Using the same numerical procedures we then studied the system where a fraction p of the interactions of the periodic FFI* lattice are replaced by interactions of random sign;[7] we have taken data on samples with p equal to 0.1, 0.2, 0.5, and 0.75. Averages were taken over from 100 to 1000 samples depending on sample size. Our results can be compared with data on the standard ISG ($p=1$).[8] For all the p values we have studied, the specific heat of the perturbed lattice is a broad featureless hump with a maximum which is clearly the ghost of the sharp specific-heat singularity at T_c in the unperturbed system (Fig. 1). In order to estimate the spin-glass ordering temperature, we used the scaling technique:[6] we measured the Binder cumulant

$$g_L=[3-\langle q^4\rangle/\langle q^2\rangle^2]/2$$

for samples of size $L=4$, 8, and 12. As an example (Fig. 2), from the intersection point of the $g_L(T)$ curves we estimate that $T_g=0.96\pm0.05$ for $p=0.2$, considerably below the specific-heat maximum. For this p the $g_L(T)$ curves appear to cross and fan out below T_g which is the signature of a bona fide phase transition.[6] The shape of the specific-heat curve as a function of temperature and the ratio of the specific-heat maximum temperature to T_g are for each nonzero p similar to those observed in the standard 3D ISG.[8] The specific-heat maximum and T_g only vary gently with p (Fig. 2 inset). In addition we found that the form of the relaxation of the autocorrelation function $q(t)$ for T approaching T_g is of the Ogielski ISG type,[8]

$$q(t)\approx t^{-x}\exp[-(t/\tau)^{\beta}]$$

with the exponent β tending to close to one third at the ordering temperature.

Thus while the regularly frustrated system is *not* a spin glass, the introduction of even a small degree of randomness has a dramatic effect on the ordering, with the system acquiring the main characteristics of the standard 3D ISG. At small p both the specific-heat maximum temperature and the ordering temperature drop sharply compared with the T_c of the unperturbed system. (We have not yet explored the limit p tending to zero but our lowest p is already small.) At high p the maximum temperature and perhaps the ordering temperature go through a maximum before reaching the ISG values. The key observation, however, is that for all nonzero p that we have studied, the specific-heat maximum is always broad and the spin-glass ordering always occurs at a temperature well below this maximum; we are seeing a major qualitative change in the ordering process when we introduce even weak randomness into the FFI* lattice. This is in striking contrast to the robustness of the Ising *ferromagnet* transition where a sharp specific-heat singularity persists under strong random dilution (60% vacant bonds).[9]

Rather than attempting to interpret the results from a real-space point of view, we will discuss the behavior in terms of the geometry of phase space. Phase-space images have been widely used in discussions of spin glasses, particularly in the regime below the freezing temperature;[10] the phase space is generally represented by a one-dimensional "mountain range" picture, but it is important to keep in mind that the real phase space is very highly dimensional. Consider any Ising system of N interacting spins. There are 2^N configurations each with a well defined energy; the total phase space is a hypercube of dimension N. Knowing the set of interactions, one can in principle (though not in practice except for small N) make a catalog of the number of microconfigurations $n(E)$ at each energy E and plot $\ln[n(E)]$ against E, i.e., the entropy S against the energy U. The thermodynamic relation $dS/dU=1/\mathrm{kT}$ has an obvious graphic solution giving S and U at each temperature. The "available phase space" at temperature T is the thermodynamically attainable set of configurations, those having $E\approx U(T)$. Any phase transition is the reflection of a sudden qualitative change in the form of this available phase space as the temperature is swept, so any transition must have a phase-space interpretation. The phase-space description of certain standard phase transitions can be given fairly easily (and is instructive). Thus the standard second-order transition in the Ising ferromagnet corresponds to a phase space consisting of two clusters of configurations at low temperatures which merge into one single cluster at the ordering temperature [Fig. 3(a)].

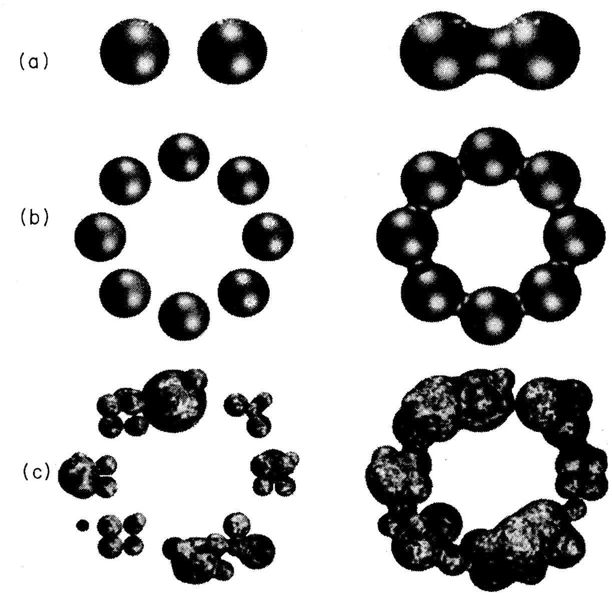

FIG. 3. (a) Schematic phase-space image of an Ising ferromagnet transition, from below T_c (left) to above T_c (right). (b) Schematic phase-space image of the transition in the FFI* system. (c) Schematic phase-space image of the perturbed FFI* spin-glass transition.

Any such merging in phase space will necessarily give rise to a sharp specific-heat peak.[11] It is important that the ordering corresponds to a localization of the system in phase space. Below the ferromagnetic ordering temperature the two clusters are separated by an "infinite free-energy barrier" in the thermodynamic limit, i.e., there are so few states with energy $E=U(T)$ between the clusters that once the system is in thermal equilibrium the relaxation by random walk in the available phase space will "never" (in the thermodynamic limit) take it from the cluster of $+M$ configurations to the $-M$ configuration cluster or vice versa. Above T_c the system is not localized as it can explore all the available phase space, which is topologically connected.

First- and second-order transitions do not represent the only possible "catastrophic" modifications of phase space that one can imagine, and we will argue that the spin-glass transition in particular appears to have characteristics corresponding to a different order of transition with a basically different phase-space geometry. Let us turn first to the periodically frustrated FFI* system. Below T_c there are 16 different ordered states,[3,5] all with similar structures to within a permutation of spin labels. The system will be localized in one of these ordered states, i.e., clusters of configurations. As the temperature is increased the clusters will expand and will come into contact at T_c. We can then represent the transition in phase space schematically as in Fig. 3(b); below T_c there is a "necklace" of clusters while just above T_c each of the clusters has made contact with its immediate neighbors to form a "halo" in phase space. All of phase space is now topologically connected (paramagnetism), with the system no longer localized in an isolated cluster. Because of the periodicity of the real-space lattice, all clusters will have the same size and shape and all contacts of Fig. 3(b) will form at one single temperature, giving a sharp specific-heat peak at exactly the temperature where localization breaks down. Whether in this particular case the transition is second order or very weakly first order (2–5) does not affect the pictures we have given for the phase space just below and just above the ordering temperature. (At some much higher temperatures the hole in the center of the halo will fill in; we identify[12] this upper change of morphology with the "active bond percolation" or "damage spreading" transition.[13])

Now let us consider the same system with a few of the regular interactions replaced by interactions of random sign. When some randomness is introduced into the periodically frustrated system, each configuration will have its energy somewhat modified so the phase space will be perturbed. The numerical data show that there is a nonzero ordering temperature for the system we have studied, so below this temperature isolated clusters exist but will be inequivalent to each other because of the randomness. Then at low temperatures instead of being a necklace of identical beads the phase space will become ragged, with each cluster deforming and splitting up [Fig. 3(c)]. As the temperature is increased the individual clusters expand, and contacts between pairs of neighboring clusters will form over a range of temperature instead of at one single temperature; each local contact in phase space between a pair of clusters will contribute to a broad specific-heat peak which will replace the original singularity. The mode of breakdown of localization will also change fundamentally; as the temperature is raised, the isolated clusters will join together topologically into a single giant cluster well before all links between pairs of neighbor clusters are connected up. In phase space with a high number of clusters, if the links between pairs of clusters are put in at random then a giant cluster can already be formed when only a fraction of the links have been closed. As a consequence, the ordering temperature (which corresponds to the transition from a fragmented phase space with localization to a topologically connected phase space, not to a closing of all the links) can lie well below the maximum of a broad featureless specific-heat hump. At temperatures just above the transition, the labyrinthine nature of the topologically connected phase space (with some links closed but most open) will result in strongly nonexponential relaxation.[14] We can note that neither frustration without topological disorder (the FFI*) nor randomness without frustration (the diluted Ising ferromagnet) produce spin-glass behavior; in the present context both appear as essential ingredients, as is generally accepted.[15] Our picture can be extended naturally to an arborescent low temperature phase-space image for the spin glass below the ordering temperature.[10]

This discussion provides an intuitive geometrical interpretation of the major features which appear from the numerical studies of our regularly frustrated FFI* system perturbed by weak randomness. The main features (a smooth broad specific-heat hump with a freezing transition on its lower temperature flank, the Ogielski form of nonexponential relaxation at temperatures above the ordering transition) are in fact common to these systems, to the standard ISG in dimension 3,[8] to real experimental spin glasses,[15,16] and to other systems in the same family. In view of this we argue that the simple phase-space scenario that we have given can provide a general physical basis for the description of the spin-glass ordering phenomenon in all these frustrated systems with randomness. We expect that, up to an upper real-space dimension, *all* spin glasses with nonzero ordering temperatures should show these same major features, which could be shared by other complex systems.

Assuming this picture is meaningful, a glance at Figs. 3(a) and 3(c) indicates that the spin-glass transition is of a totally different type from the standard Ising ferromagnet second-order transition because the underlying phase-space geometries are fundamentally different. The well established absence in specific-heat data of any singularity at the ordering temperature in 3D spin glasses[8,15] appears in this approach to be an intrinsic property of this type of transition rather than being an "accidental" consequence of the value of the critical exponent α.[15] We expect it to be observed at higher dimensions also. The fact that the Ogielski form of relaxation[8] is observed so ubiquitously close to the ordering temperature in different spin-glass systems[12,16] follows from the general "percolation transition in phase space" character of spin-glass ordering. It is worth noting that de Almeida[17] criticizes on theoretical grounds the use of the generally accepted linear renormalization-group approach[15] for systems with random interactions such as spin glasses. We have shown numerical evidence for the breakdown of universality in ISGs.[18]

In conclusion, we have proposed a simple but predictive phase-space scenario for the spin-glass transition. The phase-space approach that we have sketched out could be relevant not only for spin glasses but in other contexts where complex systems are involved.

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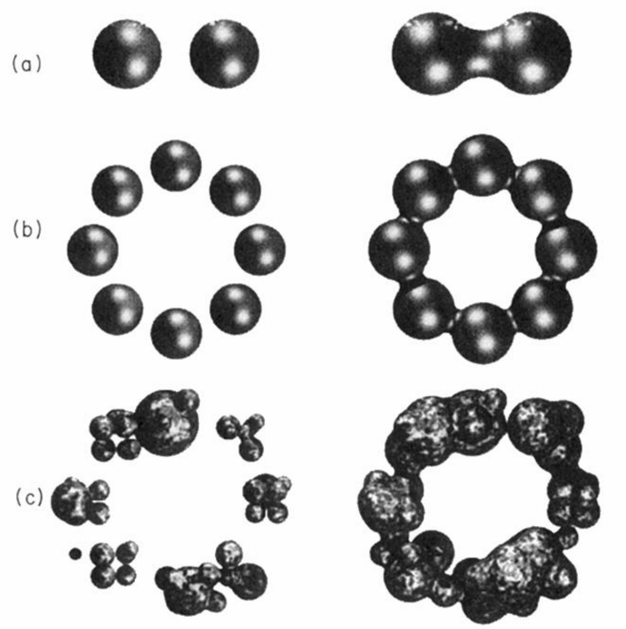

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