Effects of disorder and magnetic field in frustrated magnets

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In this work a site diluted antiferromagnetic Ising model in the FCC lattice is studied by Monte Carlo simulation. At low temperatures, we find that as the external field is increased the transition from the antiferromagnetic phase to the superantiferromagnetic one occurs through an intermediate phase which is not present in the undiluted system. This new phase ordering has three distinct values for the sublattice magnetizations corresponding to one of the phases found in a recent mean field calculation thus suggesting that in strongly frustrated systems many novel spins ordering may arises as found experimentally, for instance, in some pyrochlores.

75.10.Nr, 75.40.Mg, 75.50.Ee

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I. INTRODUCTION

Recently a lot of work has been done on frustrated systems with or without disorder in order to clarify the physical properties of systems exhibiting glassy behavior [4], i.e., systems typically with many metastable states. Among classical fully frustrated systems, one of the earliest to be studied was the nearest-neighbor Ising antiferromagnet on a face-centered cubic (FCC) lattice. The pure FCC Ising antiferromagnet with nearest neighbor interactions and in the presence of a uniform magnetic field $H$, exhibits a variety of stable phases induced by the external field. The field-temperature ($H, T$) phase diagram, which follows from Monte Carlo simulations [2] presents three phases: antiferromagnetic (AF), superantiferromagnetic (SAF), and paramagnetic (PM). This picture is supported by several theoretical approaches and it is well known that the low temperature ordered phases are separated from the paramagnetic phase by two lines of first-order phase transitions. A mean field calculation on the random version of the FCC Ising antiferromagnet in a field shows an even richer scenario [3]. Beside the phases present in the undiluted case, it was found that the addition of disorder may induce another ordered phase where two sublattices have equal magnetizations which is distinct from the others not equal two sublattice magnetizations. Furthermore, the disordered system presents glassy behavior at low temperatures [3,4]. In this letter, we address the issue whether the mean field results are stable against fluctuations in finite dimensions by doing Monte Carlo simulations on the site diluted FCC Ising antiferromagnet and our results seems to vindicate the qualitative mean field results.

II. THE MODEL, SIMULATION AND DISCUSSION

We consider an Ising model with short-range interaction on a regular lattice (FCC) with Hamiltonian given by

$$
\mathcal{H} = \sum_{\langle ij \rangle} J_{ij} \epsilon_i \epsilon_j \sigma_i \sigma_j - H \sum_i \sigma_i, \tag{1}
$$

2
where $J_{ij} = J > 0$ denotes the antiferromagnetic interaction between nearest neighbors spins, $\epsilon_i = 0$ or 1 denotes the site occupation variable (probability $p$ of being occupied), $\sigma_i = \pm 1$ denotes the spin on the sites of the FCC lattice and $H$ is the external field. The simulations were performed on lattices of sizes $4L^3 (L = 20, 40)$ with periodic boundary conditions, and for concentrations of magnetic ions between $p = 0.70$ and $p = 1.00$. We used both the heat-bath and the demon (microcanonical) algorithms. Most of our runs consisted of $4 \times 10^3$ configurations, 5 to 10 MCS apart, and the quoted values for the physical observables came from an average over several independent runs on different disorder realizations. Typically, $\sim 10^4$ MCS were discarded before we start measurements. Several variants of walking through the lattice were considered and, particularly for low temperatures, the results were rather sensitive to this choice. We employed the single demon algorithm to accomplish the microcanonical simulation \cite{5}. It is worth noticing that in a microcanonical simulation the energy is the control parameter, whereas the temperature is measured during the simulation. Most important, within this framework it is possible to probe stable as well as both metastable and unstable states, and a first-order phase transition manifests itself through a S-shaped curve in the temperature-energy plane \cite{2,5}.

We have performed Monte Carlo simulations along of some lines of the $(H, T)$ phase diagram, and for several values of $p$. Here, we will present results for $p = 0.95$ only. Figure 1 shows the field dependence of the sublattice magnetizations for $k_B T/J = 1.3$ and magnetic concentration $p = 0.95$. At this temperature and concentration one has the same behavior as in the pure case, namely, the AF and SAF phases are separated by a paramagnetic phase at intermediate fields. Our microcanonical simulation also indicates that both transitions are of first order as in references \cite{2}.

Lowering $T$, the sublattice magnetizations exhibit a quite different behavior, as shown in figure 2 for $k_B T/J = 1.0$ and the same value of $p$. One can observe the suppression of the paramagnetic phase between the AF and SAF phases; in this region the sublattice magnetizations have a field dependence not observed in the pure system. At lower temperatures this behavior is enhanced as ones sees in figure 3 for $k_B T/J = 0.90$. For some points in
the \((H, T)\) space, where the sublattice magnetizations show a very slow relaxations towards their equilibrium values (within the time scale of our simulations), we needed to make runs as long as \(10^5\) to \(10^6\) MCS.

In figure 4 we plot the sublattice magnetizations as a function of the temperature for \(H/J = 3.6\) and \(p = 0.95\). For this value of \(H\) and high enough \(T\) the ordering is paramagnetic. Lowering \(T\) the system passes through a SAF phase before exhibiting the unexpected behavior as predicted in mean field calculations [3]. Again, we cannot discard that we are observing long-lived metastable states at low temperatures from the simulations alone but at least some (if not all) qualitative features of mean field calculations are present for finite dimensions.

In summary, the FCC Ising antiferromagnet in an external magnetic field seems to change drastically its low temperature behavior when a small amount of disorder is added. It is found that a typical order-by-disorder effect [3] occurs upon dilution. The new sublattice magnetization ordering that follows from our simulation corroborates the suggestion of a mean field calculation carried out for frustrated random magnetic systems with many sub-lattices [3]. The huge relaxation times which we have observed for some values of field and low temperatures indicate that the diluted system might exhibit a glassy phase even for low dilution as suggested by mean field [3] and found experimentally in certain strongly frustrated pyrochlores systems (see the work of Bellier et al in [1] and references therein) which also have a four sublattice structure. A more detailed account of our results should be presented elsewhere.

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Figure Captions

Fig. 1 Sublattice magnetizations (indicated by squares, circles, up and down triangles) as function of the magnetic field for $k_B T/J = 1.3$ and $p = 0.95$. Notice the presence of the paramagnetic (PM) phase between the antiferromagnetic (AFM) and superanti-ferromagnetic (SAF) phases.

Fig. 2 Sublattice magnetizations as function of the magnetic field for $k_B T/J = 1.0$ and $p = 0.95$. The paramagnetic phase occurs only at high fields (not shown). The arrows are a guide to the eye showing the boundaries of the intermediate phase.

Fig. 3 Same as in figure 2, but for $k_B T/J = 0.90$. Notice the increase of the new intermediate phase between the antiferromagnetic (AFM) and superantiferromagnetic (SAF) phases as $T$ decreases.

Fig. 4 Sublattice magnetizations as function of temperature for $H/J = 3.6$ and $p = 0.954$. This graph displays clearly the branching of the sublattice magnetizations in distincts values as $T$ decreases (phases PM SAF INTERMEDIATE).
SUBLATTICE MAGNETIZATIONS

SUBLATTICE MAGNETIZATIONS

H/J

PM

AF

SAF

SUBLATTICE MAGNETIZATIONS

H/J

H/J

0.0

AF

SAF

PM

SUBLATTICE MAGNETIZATIONS

H/J

H/J

0.0

AF

SAF

PM

SUBLATTICE MAGNETIZATIONS

H/J

H/J

0.0

AF

SAF

PM

SUBLATTICE MAGNETIZATIONS

H/J

H/J

0.0

AF

SAF

PM

SUBLATTICE MAGNETIZATIONS

H/J

H/J

0.0

AF

SAF

PM

SUBLATTICE MAGNETIZATIONS

H/J

H/J

0.0

AF

SAF

PM

SUBLATTICE MAGNETIZATIONS

H/J

H/J

0.0

AF

SAF

PM
SUBLATTICE MAGNETIZATIONS

AF  SAF

H/J

-1.0  -0.5  0.0  0.5  1.0

-1.0  -0.5  0.0  0.5  1.0

1.0  2.0  3.0  4.0  5.0  6.0
