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Critical and tricritical behavior of a selectively diluted triangular Ising antiferromagnet in a field

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ABSTRACT

We study a geometrically frustrated triangular Ising antiferromagnet in an external magnetic field which is selectively diluted with nonmagnetic impurities employing an effective-field theory with correlations and Monte Carlo simulations. We focus on the frustration-relieving effects of such a selective dilution on the phase diagram and find that it can lead to rather intricate phase diagrams in the dilution-field parameters space. In particular, in a highly (weakly) diluted system the frustration is greatly (little) relieved and such a system is found to display only the second(first)-order phase transitions at any field. On the other hand, for a wide interval of intermediate dilution values the transition remains second-order at low fields but it changes to first-order at higher fields and the system displays a tricritical behavior. The existence of the first-order transition in the region of intermediate dilution and high fields is verified by Monte Carlo simulations.

1. Introduction

A triangular Ising antiferromagnet is a typical geometrically frustrated spin model which due to a high degree of frustration shows no long-range ordering [1,2]. Nevertheless, a small perturbation, for example in the form of an applied external magnetic field or the injection of quenched non-magnetic impurities, can lift the high degeneracy of the ground state and thus initiate long-range ordering. In particular, it has been shown that for a certain range of the field values the systems displays a transition between the ferrimagnetic phase with two sublattices aligned parallel and one antiparallel to the field at lower temperatures and the paramagnetic phase in which all spins are aligned parallel to the field at higher temperatures [3–5]. On the other hand, the injection of quenched magnetic vacancies in zero field can relieve frustration but only locally, which supposedly leads to a spin-glass order [6–8]. Combining both the presence of the external field and the magnetic impurities can lead to rather interesting phenomena, such as step-wise field-dependence of the magnetization or possibility of multiple reentrants in the phase diagram, as suggested by recent Monte Carlo [9] and effective-field theory [10] studies. Another way of relieving the geometrical frustration is a selective dilution, in which different (in our case three) sublattices are diluted by non-magnetic impurities with different probabilities. Then the geometrical frustration can also be relieved globally, giving rise to long-range magnetic ordering phenomena even in the absence of the field. Kaya and Berker [11] have shown that if only one out of three sublattices of the triangular lattice is randomly diluted then a long-range order can develop in the remaining two sublattices already at relatively low concentrations of the vacancies. Various studies have shown that the presence of either the external magnetic field or the magnetic impurities has generally different effects on the critical behavior of non-frustrated and frustrated spin systems. For example, in the non-frustrated spin systems the critical temperature typically decreases with the field (e.g., Refs. [12–14]) and in some peculiar systems, such as metamagnets [12], the transition in a high-field and low-temperature region can change to a first-order one. On the other

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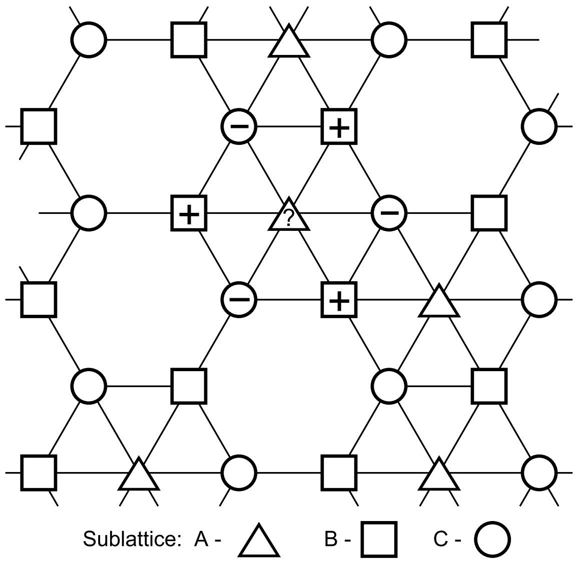

Fig. 1. Triangular lattice partition into three sublattices A, B and C, where the sublattice A is randomly diluted. The signs + and − represent the spin values of +1 and −1, respectively, and the question mark signifies the frustration arising from placing a magnetic A-ion in the center of the antiferromagnetically ordered hexagon of B- and C-ions.

hand, in the frustrated systems the magnetic field can either enhance or suppress the transition temperature, depending on the field range [3–5,10]. Similarly, the introduction of the quenched dilution in the non-frustrated systems typically decreases the transition temperature down to zero at the percolation threshold [15], while the opposite effect also known as "order by disorder" can be achieved by a selective quenched dilution in the frustrated systems [11]. Therefore, by applying the external field to the selectively diluted system we can anticipate different regimes of its effects on the critical properties of the system and thus an interesting phase diagram.

The goal of the present study is to investigate changes in the critical behavior of the system, the frustration of which is systematically controlled by the degree of the selective dilution between the fully frustrated (pure system on triangular lattice) and non-frustrated (pure system on honeycomb lattice) limits.

2. The model and method

The selectively diluted Ising antiferromagnet in a field can be described by the Hamiltonian

$$H = -J \sum_{\langle i,j \rangle} \xi_i \xi_j S_i S_j - h \sum_i \xi_i S_i, \tag{1}$$

where $S_i = \pm 1$, are the Ising spins, h is the external magnetic field, $J < 0$ is the exchange interaction parameter, and $\langle i, j \rangle$ denotes the summation over all nearest neighbor (NN) pairs. ξ_i are quenched, uncorrelated random variables which are equal to 1 with probability p when the site i is occupied by a magnetic atom and 0 with probability $1 - p$ otherwise. Then p represents the mean concentration of magnetic atoms. For the current selectively diluted case with only one (let us say A) sublattice diluted we will consider the sublattice-dependent concentrations $0 \leq p_A \leq 1$, $p_B \equiv p_C = 1$.

In order to study the critical behavior of the system, we apply an effective field theory with correlations (EFT) (for a review see, e.g., Ref. [16]). In contrast to the usual mean-field approach, EFT correctly accounts for the single-site kinematic relations through the Van der Waerden identity. As a result, EFT yields, for example, a non-zero critical concentration for quenched diluted systems, the lack of order in the one-dimensional Ising ferromagnet and the occurrence of order in the two-dimensional case with the critical temperature improved over the usual mean-field theory [16]. However, extra care must be taken when dealing with a frustrated system since a straightforward application of EFT may lead to a complete loss of frustration and consequently meaningless results. Recently, we have applied EFT to an uniformly diluted triangular Ising antiferromagnet [10] and in the present study we will follow the same procedure in order to include the geometrical frustration effects within EFT. Namely, we decompose the triangular lattice into three interpenetrating sublattices A, B and C (see Fig. 1), in such a way that spins on one sublattice can only interact with their NNs on the other two sublattices. Thus all the NN interactions are accounted for and the frustration results from the effort to simultaneously satisfy all the mutual antiferromagnetic intersublattice couplings. Such an approach has correctly reproduced no long-range order behavior down to zero temperature for the pure system in zero field [10].