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Phase diagram of a diluted triangular lattice Ising antiferromagnet in a field

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ABSTRACT

Magnetization processes and phase transitions in a geometrically frustrated triangular lattice Ising antiferromagnet in the presence of an external magnetic field and a random site dilution are studied by the use of an effective-field theory with correlations. We find that the interplay between the applied field and the frustration-relieving dilution results in peculiar phase diagrams in the temperature-field-dilution parameter space.

1. Introduction

The Ising model with nearest-neighbor antiferromagnetic interactions on a triangular lattice is fully frustrated due to local geometric constraints that prevent simultaneous minimization of all the pairwise interactions. It has been solved exactly and found to display no ordering at any finite temperatures [1,2]. Only at $T = 0$ K the model displays a critical phase with algebraically decaying correlations [3]. The ground state is highly degenerated and thus even a small perturbation can cause that the system will choose an ordered state. Such a perturbation can be an external magnetic field, which by several studies has been shown to produce a line of second-order phase transitions for a certain range of the field values [4–6]. At the transition the system passes from the ferrimagnetic phase with two sublattices aligned parallel and one antiparallel to the field at lower temperatures ($\downarrow\uparrow\uparrow$) to the paramagnetic phase in which all spins are aligned parallel to the field at higher temperatures ($\uparrow\uparrow\uparrow$). As a result of the frustration, at low temperatures the magnetization versus field curves display a broad plateau with the value of $m = 1/3$. Similar stepwise plateaus with different magnetization values have also been observed in some other lattices, such as the recursive lattice [7], the zig–zag ladder [8,9] and even on the cluster level [10,11]. However, besides the magnetic field, the degeneracy of the system can also be removed by considering the interactions of more distant neighbors [12–15].

Diluting the system with nonmagnetic impurities in zero field locally relieves frustration and can lead to a spin-glass order [16,17], although this scenario remains controversial for the current 2D system [18]. Spin-glass ordering has also been observed in another highly frustrated Ising antiferromagnet on a fcc lattice for a certain range of the magnetic concentration [19]. In Ref. [20] the effects of doping the triangular Ising antiferromagnet with slow moving holes has been studied. Besides the site-dilution problem, also a bond-dilution problem [21] and a random-bond Ising model [22] on a triangular lattice have been investigated. In contrast to the uniform dilution, if only one sublattice of the triangular lattice is diluted then a long-range order can develop in the remaining two sublattices already at relatively low concentrations of the impurities [23]. Very recently, Yao [24] has studied how dilution can modulate the frustration effect in the system in a field. For example, he found that even a small dilution causes that the broad frustration-induced 1/3 magnetization plateau splits into a stepwise curve. The importance of such studies is amplified by the fact that there are some corresponding real magnetic compounds, such as $Ca_3Co_2O_6$, that have been experimentally found to display some unconventional frustration-induced features [25] and the current model has been successfully employed in their explanation [26,27].

Motivated by the previous interesting findings, the objective of the present work is to systematically study effects of the uniform site dilution on the phase transitions in the triangular lattice Ising antiferromagnet in a field.

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2. Model and effective-field approach

The model Hamiltonian is given by

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

where $S_i = \pm 1$, are the Ising spin variables, h is the external magnetic field, $J < 0$ is the exchange interaction constant, and $\langle i, j\rangle$ is the sum extending over all nearest neighbor (NN) pairs. ξ_i are quenched, uncorrelated random variables chosen to be equal to 1 with probability p, when the site i is occupied by a magnetic atom and 0, with probability $1-p$ otherwise. Then the probability distribution is given by $P(\xi_i) = p\delta(\xi_i - 1) + (1-p)\delta(\xi_i)$ and p represents the mean concentration of magnetic sites.

We employ an effective-field theory (EFT) with correlations (see e.g., [28]), based on a single-site cluster approximation with the attention focused on a cluster comprising just a single spin, labeled i, and the NN spins with which it directly interacts. Following Ref. [29] we get the exact relation

$$\xi_i\langle S_i\rangle = \xi_i\left\langle \tanh\left[\beta\left(J\sum_{j=1}^{z}\xi_j S_j + h\right)\right]\right\rangle, \tag{2}$$

where z is the number of NNs of the site i (i.e., the coordination number), $\beta = 1/k_B T$, and $\langle\ldots\rangle$ denotes a thermal average for a fixed spatial configuration of the occupied sites. Applying the differential operator technique [30] to the identity (2) and using the exact relations

$$\exp(\lambda\xi_j) = \xi_j\exp(\lambda) + 1 - \xi_j, \tag{3}$$

$$\exp(\mu S_j) = \cosh(\mu) + S_j\sinh(\mu), \tag{4}$$

one obtains

$$\xi_i\langle S_i\rangle = \xi_i\left\langle\prod_{j=1}^{z}\left[\xi_j\cosh(\beta JD) + \xi_j S_j\sinh(\beta JD) + 1 - \xi_j\right]\right\rangle \times \tanh(x+\beta h)|_{x=0}, \tag{5}$$

where $D = \partial/\partial x$ is the differential operator. In order to carry out the configurational averaging over the occupational numbers ξ_i, let us assume that NNs of the site i are completely independent of each other by taking an approximation

$$\langle S_j S_k\ldots S_l\rangle \approx \langle S_j\rangle\langle S_k\rangle\ldots\langle S_l\rangle. \tag{6}$$

In spite of this simplification, we note that this approximation is quite superior to the standard mean-field theory, since here, by using Van der Waerden identity (4), the relations like $S_j^2 = 1$ are exactly taken into account.

However, unlike on some other lattices, on a triangular lattice NNs of the central spin i include pairs of spins that are also mutual NNs and, therefore, their decoupling by the approximation (6) could result in rather high inaccuracies. Even more importantly, such a straightforward application of EFT would lead to a complete loss of the frustration and therefore inevitably incorrect results. In order to include all the NN interactions and the effect of the geometrical frustration, we chose to partition the lattice into three interpenetrating sublattices A, B and C in such a way that spins on one sublattice only interact with spins from the other two sublattices (see Fig. 1). Then all the NN interactions are accounted for and the frustration arises from the effort to simultaneously satisfy all the mutual intersublattice interactions, which are antiferromagnetic and isotropic i.e., $J_{AB} = J_{AC} = J_{BC} \equiv J < 0$. As an example, let us consider the situation in a selected triangular plaquette i in Fig. 1. If the spin S_{iA} is in the state $+1$ then the energy is minimized if all its NNs, including S_{iB} and S_{iC}, are in the state -1.

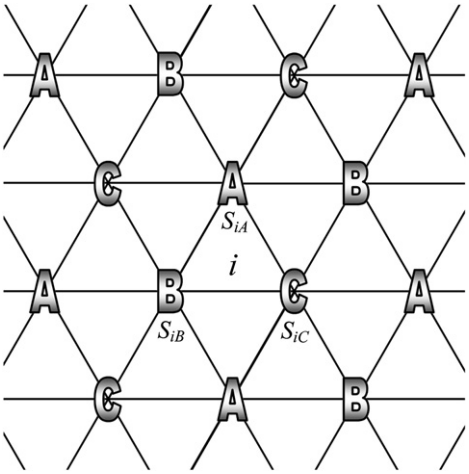

Fig. 1. Triangular lattice partition into three sublattices A, B and C.

However, for the spin S_{iB} in the state -1 it would be energetically favorable if all *its* NNs, including S_{iA} and S_{iC}, were in the state $+1$, which creates frustration for the spin S_{iC}. Given the lattice partition, the expression (5) can be written for individual sublattices in the form

$$\xi_i\langle S_i\rangle = \xi_i\left\langle\prod_{j=1}^{z_1}\left[\xi_j\cosh(\beta JD) + \xi_j S_j\sinh(\beta JD) + 1 - \xi_j\right] \times\prod_{k=1}^{z_2}\left[\xi_k\cosh(\beta JD) + \xi_k S_k\sinh(\beta JD) + 1 - \xi_k\right]\right\rangle \times \tanh(x+\beta h)|_{x=0}, \tag{7}$$

where z_1, z_2 are the numbers of NNs of the spin S_i on a given sublattice that belong to the remaining two sublattices. Then, by performing configurational averaging for all three sublattices, the respective sublattice magnetizations $m_X = \langle\xi_i\langle S_{iX}\rangle\rangle_c$, X = A, B and C, can be calculated from the set of coupled equations

$$\begin{aligned} m_A &= p(a+bm_B)^3(a+bm_C)^3\tanh(x+\beta h)|_{x=0},\\ m_B &= p(a+bm_A)^3(a+bm_C)^3\tanh(x+\beta h)|_{x=0},\\ m_C &= p(a+bm_A)^3(a+bm_B)^3\tanh(x+\beta h)|_{x=0}, \end{aligned} \tag{8}$$

where $a = 1 - p + p\cosh(\beta JD)$, $b = \sinh(\beta JD)$ and $p = \langle\xi_i\rangle_c$ is the same for all three sublattices. The explicit form of Eqs. (8) can be calculated by using the mathematical relation $\exp(\alpha D)f(x) = f(x+\alpha)$. Then we can define the total magnetization per site $m = (m_A + m_B + m_C)/3$ and the order parameter $o = [\max(m_A, m_B, m_C) - \min(m_A, m_B, m_C)]/2$. The latter serves to localize phase boundaries between the ferrimagnetic ($\downarrow\uparrow\uparrow$) and the paramagnetic ($\uparrow\uparrow\uparrow$) phases.

3. Results and discussion

In zero field, Eqs. (8) have only trivial solution at all temperatures, which means that our effective-field approach reproduces the exact result of no long-range order down to $T = 0$ K [1,2]. In Fig. 2 we plot the field dependence of the magnetization at low temperatures for the pure case ($p = 1$) as well as diluted cases ($p < 1$) with different degrees of dilution. For the pure case, the curve displays the typical frustration-induced broad 1/3 plateau, in accordance with some previous theoretical [24,31] and experimental [25] observations. When the system is diluted, we can observe formation of multiple steps at about integer values of the field $h/|J| = 1, 2, 3, 4, 5$, which get more pronounced as the dilution increases. This behavior is in agreement with the Monte