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Tricritical behaviour of the frustrated Ising antiferromagnet on the honeycomb lattice

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ABSTRACT

We use the effective-field theory with correlations based on different cluster sizes to investigate phase diagrams of the frustrated Ising antiferromagnet on the honeycomb lattice with isotropic interactions of the strength $J_1 < 0$ between nearest-neighbour pairs and $J_2 < 0$ between next-nearest neighbour pairs of spins. We present results for the ground-state energy as a function of the frustration parameter $R = J_2/|J_1|$. We find that the cluster-size has a considerable effect on the existence and location of a tricritical point in the phase diagram at which the phase transition changes from the second order to the first one.

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1. Introduction

Since a honeycomb lattice antiferromagnet with only nearest-neighbour exchange interactions (J_1) is considered as a bipartite lattice, the ground state exhibits long-range ordering. The system becomes frustrated like the square lattice, if the next-nearest-neighbour exchange interactions (J_2) are considered. However, spin fluctuations are expected to be larger for the honeycomb lattice than the square lattice because the coordination number $z = 3$ in the honeycomb lattice is smaller than that of $z = 4$ in the square lattice. Hence, it is interesting to study the magnetic ordering on the honeycomb lattice under frustrating interactions.

We note that investigations of the frustrated two-dimensional Ising antiferromagnet (AF) with spin-$\frac{1}{2}$ on a square lattice have a long history (see, e.g. [1–8]). In particular, it has been found that the introduction of competing interactions is accompanied by the appearance of new ground states at the critical point $R \equiv J_2/|J_1| = -0.5$ and due to the ground-state degeneracy there is no long-range order at finite temperatures [4,9–11]. Despite the simplicity of the model, it has been proved difficult to precisely determine the order of the phase transition. Now, it is well established by using different approximate studies [10–12] and the Monte Carlo method [13–18] that in the region of $R < -0.5$, the phase transition changes at a tricritical temperature from the second order to the first order. However, a very recent cluster mean-field calculation [18] with a cluster of the size 4×4 and the effective-field theory with correlations based on the different cluster sizes [19] give change in the order of the phase transition not only for $R < -0.5$ but also in the region of $R > -0.5$.

Interestingly, a similar attention has not been paid so far to the frustrated Ising AF with spin-$\frac{1}{2}$ on the honeycomb lattice. A special feature of this lattice is that it is not a Bravais lattice, i.e., a translation invariance of the full lattice is broken for any type of state [20]. This non-Bravais lattice can be viewed as a composition of two interlacing triangular sublattices and the lattice is constructed by two vectors of the triangular Bravais lattice (see Fig. 1 in [21]). Hence, for a transition from a paramagnetic state to a magnetically ordered phase, the spatial symmetry is not reduced as for the square lattice. We expect that the non-Bravais character of this bipartite lattice results in a behaviour that cannot be observed in the square lattice or other Bravais lattices [22]. Moreover, in view of recent experimental activities [23–28], materials regarded as various types of spin systems on honeycomb lattices are expected to be synthesized.

Motivated by the above considerations, in this paper we investigate the phase diagram and critical properties of the frustrated J_1–J_2 Ising AF on the honeycomb lattice. As far as we know, this model has not been analyzed in the literature. An interest in the honeycomb lattice is also promoted in recent years because of its relevance to graphene [29]. However, when second-neighbour interactions are taken into account or when a magnetic field is

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applied to the honeycomb lattice, the Hamiltonian is no longer exactly solvable and only approximate analytical studies or numerical approaches are possible to attack this more general problem.

In this paper we employ the effective-field theory with correlations (EFT) based on different cluster sizes which has been used for an investigation of frustration in the square case [19]. Therefore, it will be interesting to compare effects of frustration on the phase diagram of these bipartite lattices. This approach is based on the differential operator technique introduced into exact Ising spin identities and has been successfully applied to a variety of spin-$\frac{1}{2}$ and higher spin problems (for a review see, e.g., Refs. [30, 31]) including a geometrically frustrated triangular lattice Ising AF [32–34]. Namely, here we will study the frustrated J_1–J_2 Ising AF on the honeycomb lattice in its parameter space using EFT based on one-, two-, four-, and six-spin clusters. It is important that the present EFT allows us to treat large clusters in a simpler and more efficient computational manner.

2. Theory

We consider the frustrated honeycomb Ising AF with competing nearest-neighbour ($J_1 < 0$) and next-nearest-neighbour ($J_2 < 0$) interactions. The Hamiltonian of the model is given by

$$H = -J_1 \sum_{\langle i,j \rangle} s_i s_j - J_2 \sum_{\langle i,i_2 \rangle} s_i s_{i_2}, \tag{1}$$

with $s_i = \pm 1$, where the first and second sums are taken over all pairs of nearest-neighbours (nn) and next-nearest-neighbours (nnn) of spins, respectively.

Before calculation of the transition line between ordered and paramagnetic phases, it is appropriate to first consider the ground state of this model. For $J_2 = 0$ the ground state of the Hamiltonian (1) is the known AF solution with the energy per site $E_{AF}/N = -3/2|J_1|$. However, adding the nnn AF interactions yields an increase of the ground state energy per site for the AF state:

$$\frac{E_{AF}}{N} = -\frac{3}{2}(|J_1| + 2J_2). \tag{2}$$

In this case each site has its three nn on the other sublattice and six nnn on its own sublattice. For a large negative J_2 the system orders in the collinear striped states (CS) described either by alternate single ferromagnetic columns of antiparallel spins (Fig. 1(a)) or alternate pairs of columns consisting of AF coupled spins (Fig. 1(b)) (see Refs. [35,36]). In such case the ground state is degenerate and its energy per site is given by

$$\frac{E_{CS}}{N} = -\frac{1}{2}(|J_1| - 2J_2). \tag{3}$$

A critical point separating these ordered phases is located at $R_c = -1/4$, where the transition temperature is suppressed to $T = 0$ K. This value may be compared to that of the frustrated J_1–J_2 Ising model on the square lattice $R_c = -1/2$, where the energy of the collinear (or superantiferromagnetic) state depends only on the value of J_2 coupling [14]. Due to the degeneracy of the ground state the system remains disordered at all finite temperatures for $R < -1/4$. Therefore, we focus only on the AF phase which exists for $R > -1/4$.

A starting point of the EFT for our Ising spin system is generalized Callen–Suzuki [37,38] exact identity

$$\langle O_{\{n\}} \rangle = \left\langle \frac{\mathrm{Tr}_{\{n\}}[O_{\{n\}} \exp(-\beta H_{\{n\}})]}{\mathrm{Tr}_{\{n\}}[\exp(-\beta H_{\{n\}})]} \right\rangle, \tag{4}$$

where the partial trace $\mathrm{Tr}_{\{n\}}$ is to be taken over the set $\{n\}$ of spin variables specified by the cluster spin Hamiltonian $H_{\{n\}}$. Here, $O_{\{n\}}$ denotes any arbitrary spin function including the set of all $\{n\}$ spin variables (finite cluster) and $\langle \cdots \rangle$ denotes the usual thermal average.

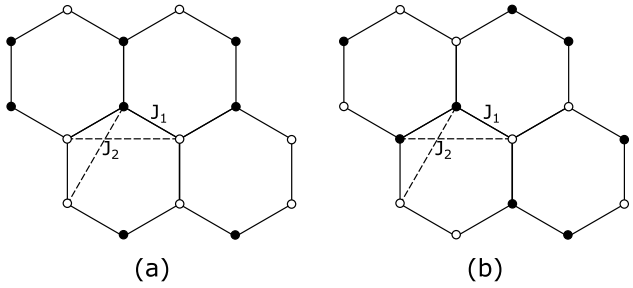

Fig. 1. Ground-state configurations of the J_1–J_2 Ising model on the honeycomb lattice showing two, (a) and (b), degenerate collinear striped states. Two sublattices are marked by black and white circles.

2.1. Single-spin cluster approach

Let us consider first the cluster containing only one spin on site i and A sublattice which interacts with other nn and nnn spins from the neighbourhood. In this approach the multispin Hamiltonian $H_{\{n\}}$ for the AF single-spin cluster ($n = 1$) on the honeycomb lattice is given by

$$H^{AF}_{\{1\}} = -s^A_i h^{AF}_i, \tag{5}$$

with

$$h^{AF}_i = J_1 \sum_{i_1=1}^{3} s^B_{i_1} + J_2 \sum_{i_2=1}^{6} s^A_{i_2}, \tag{6}$$

where s^A_i and s^B_j are spin variables on sublattices A and B, respectively, and the superscript AF denotes the antiferromagnetic system. After performing the trace over the selected spin s^A_i on the right-hand side of the relation (4), applying the differential operator technique, and using the van der Waerden identity for the two-state Ising spin system, one finds

$$m_A \equiv \langle s^A_i \rangle = \left\langle \prod_{i_1=1}^{3} (A_1 + B_1 s^B_{i_1}) \prod_{i_2=1}^{6} (A_2 + B_2 s^A_{i_2}) \right\rangle \tanh(\beta x)\Big|_{x=0}, \tag{7}$$

where $A_\nu = \cosh(J_\nu D_x)$, $B_\nu = \sinh(J_\nu D_x)$ $(\nu = 1, 2)$, and $D_x = \partial/\partial x$ is the differential operator.

To proceed further, one has to approximate the thermal multiple correlation functions occurring on the right-hand side of Eq. (7) as follows:

$$\langle s^B_{i_1} s^B_{i'_1} \cdots s^A_{i_2} \rangle \approx \langle s^B_{i_1} \rangle \langle s^B_{i'_1} \rangle \cdots \langle s^A_{i_2} \rangle, \tag{8}$$

which means that nn and nnn of site i are assumed to be completely independent of each other. It should be noted here that the approximation (8) is quite superior to the standard mean-field theory since even though it neglects correlations between different spins but takes the single-site kinematic relations exactly into account through the van der Waerden identity. Based on this approximation, Eq. (7) reduces to

$$m_A = (A_1 + B_1 m_B)^3 (A_2 + B_2 m_A)^6 \tanh(\beta x)\Big|_{x=0}, \tag{9}$$

where m_α $(\alpha = A, B)$ are the sublattice magnetizations per site. At this place, in order to solve the problem generally, we need to evaluate the sublattice magnetization m_B. It can be derived in the same way as m_A by the use of (4) for the selected spin s_j on B

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