Specific Features of Phase States of a Diluted 2D Magnet with Frustration

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The properties of a dilute Ising magnet are studied using a two-dimensional spin–pseudospin model with charged impurities and a frustration caused by the competition of the charge and magnetic orderings. Based on the classical Monte Carlo method, the ground state phase diagram has been obtained and also unusual phase states appeared at finite temperatures have been studied. The regions in which order–order phase transitions and also reentrant phase transition are observed have been found.

Keywords: dilute Ising magnet, classical Monte Carlo method, frustration, phase transitions

1 Introduction

At present, the study of the properties of disordered and frustrated magnets and also diluted systems is of significant interest from both fundamental and practical points of view. Such systems have a rich ground state phase diagram and exhibit high sensitivity to external actions, demonstrating various types of phases and phase transitions at finite temperatures [1, 2, 3]. The interest in unusual phase states of such systems is particularly topical taking into account their close connection with spin liquids [3].

The spin–pseudospin model considered in this work belongs to a wide class of the pseudospin Blume–Emery–Griffiths-type models [5] which are widely used for description of the properties of quantum and classical liquids, binary and ternary al-
loys, metamagnets, dilute magnets, cold atoms, and many other physical systems [6]. The spin–pseudospin model was proposed in [7] for the description of the competition between magnetic and charge orderings in HTSC cuprates in normal state. In this model for the cuprate CuO$_2$ plane along with [CuO$_4$]$^{6-}$ centers with spin 1/2, we consider the interacting [CuO$_4$]$^{5-}$ and [CuO$_4$]$^{7-}$ centers with spin 0 in the ground state. The more detailed justification of the model and the possibility of its using for describing the physical properties of cuprates and also the results obtained in the mean-field approximation are presented in [8, 9]. The model Hamiltonian includes the on-site ($\Delta$) and intersite ($V$) density–density correlations for nonmagnetic centers which have the form of single-ion anisotropy and the Ising exchange coupling in the language of pseudospin operators, and also the conventional spin exchange interaction in the Ising form ($J$):

$$H = \Delta \sum_i S^2_{iz} + V \sum_{\langle ij \rangle} S_{iz}S_{jz} + \tilde{J} \sum_{\langle ij \rangle} \sigma_{iz} \sigma_{jz} - \mu \sum_i S_{iz}. \quad (1)$$

Here, $\sigma_{iz} = (1 - S^2_{iz}) s_{iz}$, $\tilde{J} = Js^2$, and $\mu$ is the chemical potential that is necessary to take into account the constant charge constrain

$$n = \frac{1}{N} \sum_i \hat{S}_{iz} = const, \quad (2)$$

where $n$ is the charge density. The states corresponding to two pseudospin projections $S_z = \pm 1$ belong to two nonmagnetic [CuO$_4$]$^{5-}$ and [CuO$_4$]$^{7-}$ states with charges $\pm 1$, which are counted from the charge of the magnetic [CuO$_4$]$^{6-}$ states with $S_z = 0$. The magnetic state with $S_z = 0$ is the spin doublet $s = 1/2$. The summation is performed over the sites of a two-dimensional square lattice, $\langle ij \rangle$ denotes the nearest neighbors).

The term “frustration” can have various meanings; thus, it should be refined in this work. The systems with nonzero entropy of the ground state can be called frustrated systems [10]. In the system considered in this work, nonzero entropy of
the ground state is observed over a wide range of parameters due to the existence of strongly interacting impurities [11]. In this work, we call the frustration point the values of the model parameters at which the ordering type is changed from the charge ordering to the magnetic ordering in the ground state. It is the classical analog of the quantum critical point.

A feature of our model is the existence of both the disorder (annealed charged impurities) and also the frustration related to the competition of various-type interactions. In [12, 13], it was shown that the introduction of impurities and various structural defects in the system substantially influences the phase states and the critical behavior, and also extends the possibilities of applying this model for the description of real physical systems. Thus, it is interesting to study the influence of charged impurities on the phase states of our system near the frustration point.

2 Methods

The numerical simulation was performed using the classical Monte Carlo (MC) method. The charge constraint (2) is provided by the modification of the Metropolis algorithm [14]. The calculations were carried out on a square lattice with periodic boundary conditions, linear sizes \( L \), and the number of sites \( N = L \times L \), where \( a \) is the lattice constant taken to be 1. All the calculations were carried out for the lattice \( L = 64 \) with annealing of \( 1 \cdot 10^6 \) MC steps per site, and the data were averaged over 100 copies of the system. All the effects and results discussed in this report were checked for \( L = 256 \).

The temperature dependences of the specific heat and the susceptibility are determined using fluctuation relations

\[
C = \frac{1}{N} \frac{\langle E^2 \rangle - \langle E \rangle^2}{k_B T^2}; \quad \chi = \frac{1}{N} \frac{\langle O^2 \rangle - \langle O \rangle^2}{k_B T}
\]

where \( k_B \) is the Boltzmann constant and \( E \) is the energy of the system with Hamil-
Order parameters $O$ for the checkerboard antiferromagnetic and charge-ordered phases were determined as follows:

$$O = \begin{cases} 
  m_1 - m_2, \\
  M_1 - M_2.
\end{cases}$$

(4)

Here, $m_\lambda = \sum_{i \in \lambda} s_{iz}$ is the magnetization of a sublattice $\lambda = 1, 2$, and $M_\lambda = \sum_{i \in \lambda} S_{iz} -$ is the summary charge of a sublattice $\lambda$ (pseudo-magnetization).

The charge and spin structure factors were calculated using the following relations:

$$S(\vec{q}) = \frac{1}{N^2} \sum_{lm} e^{i\vec{q} \cdot (\vec{r}_l - \vec{r}_m)} \langle S_{lz} S_{mz} \rangle,$$

$$s(\vec{q}) = \frac{1}{N^2} \sum_{lm} e^{i\vec{q} \cdot (\vec{r}_l - \vec{r}_m)} \langle s_{lz} s_{mz} \rangle,$$

(5)

The critical phase transition temperatures were determined by the maxima of the specific heat and the susceptibilities. In this case, the error of determination of the critical temperatures was no higher than 1% in comparison with the critical temperatures found by the Binder cumulant method. The existence of the charge and antiferromagnetic orders (both long-range and short-range orders) was determined using the values of the structure factors in point $a\vec{q} = (\pi, \pi)$.

### 3 Results and discussion

In [15], it was shown that, in the mean-field approximation (MFA), a change in the relation of parameters $V$ and $J$ leads to two qualitatively different ground state phase diagrams. In this work we have restricted ourselves to the case of a weak spin exchange ($V = 4.7J$). In this case, in MFA, four phases with the checkerboard-type charge orderings (CO) form in the ground state (Fig. 1a). COI phase corresponds to the charge order without spin centers; COII and COIII are the phases diluted with spin centers distributed only over one sublattice. In COII phase at $|n| \geq 0.5$, one sublattice is completely filled with charge centers of one type. In MFA, both
phases have a magnetic ordering that evidently is not observed during numerical MC calculations. MFA predicts the ferromagnetic ordering for FIM phase; however, the numerical calculation showed the existence of a dilute antiferromagnetic (AFM) ordering at small $n$ and the short-range AFM ordering at $0.33 \lesssim n < 0.5$. In addition, the ground state phase diagram obtained in terms of the MC method (Fig. 1b) differs in the existence of a large region of the short-range charge ordering (SRO) of one or other type. The asterisks denote the phases obtained in terms of MFA.

Figure 1: Ground state phase diagrams for the weak spin exchange limit obtained (a) in MFA and (b) using the MC method.

Studying the phase states at finite temperatures is of specific interest. The total diagram of possible phase states for $V = 4 \tilde{J}$ is shown in Fig. 2. Near the frustration point $\Delta^*/J = 1.5$, there are three regions labeled by numerals 1, 2, and 3 in frames in which the ordering type is changed as the temperature decreases.

Figures 3–5 show the temperature phase diagrams for $n = 0.1$, $n = 0.15$, and $n = 0.225$ corresponding to the horizontal lines in regions 1, 2, and 3 in Fig. 2 respectively. At the right of the phase diagrams, there are the snapshots of lattice fragments of $16 \times 16$ sites. Different projections of pseudospin $S_z = \pm 1$ (two charge states) and spin $s_z = \pm 1/2$ (two magnetic states) are indicated by different gradations of the grey color. In region 1 for $n = 0.1$ (Fig. 3), a decrease in temperature leads to the phase transition from the nonordered state (NO) to the AFM phase and then, at lower temperatures, another order–order phase transition
Figure 2: Diagram of possible phase states. Near the frustration point $\Delta^*/J = 1.5$, there are regions 1, 2, and 3, in which the types of ordering are changed as the temperature decreases. The horizontal dash–dot lines correspond to the temperature phase diagrams shown in Figs. 3–5. The vertical dash–dot line corresponds to the dependences of the structure factors on the charge density $n$ in Fig. 6.

with a change of the AFM ordering to the COIII phase takes place. The change in the ordering type is observed up to the value $\Delta/J = 1.5$.

In region 2 (“bridge”), such a change in the orderings takes place twice as temperature decreases. This situation is shown in Fig. 4 for $n = 0.15$. Thus, there are three sequential phase transitions: from the high-temperature NO phase to the ordered AFM state; then, the change to the COIII charge ordering, and the reentrant phase transition to the AFM phase. In the line for $n = 0.225$ (Fig. 5), we also observe the change of one type of ordering to another, namely of COIII to AFM at $\Delta/J > \Delta^*/J = 1.5$.

Figure 6 shows the dependence of the maximum values of the charge and spin structure factors in point ($\pi, \pi$) on charge concentration $n$. This picture corresponds to vertical line $\Delta/J = 1.52$ in Fig. 2. The value of the maximum of the spin (charge)
Figure 3: Temperature phase diagram for $n = 0.1$ near the frustration point. As temperature decreases, the second phase transition accompanied by changing the AFM ordering to the COIII phase, takes place.

Figure 4: Temperature phase diagram for $n = 0.15$ near the frustration point. A double change in the ordering type is observed with an increase in temperature; i.e. the reentrant phase transition to AFM takes place.
Figure 5: Temperature phase diagram for $n = 0.225$ near the frustration point. As temperature decreases, another phase transition from COIII to AFM is observed.

The structure factor in point ($\pi, \pi$) allows us to judge the existence of the AFM (CO) ordering and to determine the boundary between the long-range and short-range orders. In this case, we determined this boundary from the structure factor value equal to 0.1. It is important to note that the certain structure factor can reach its maximum value not in the ground state but at finite temperatures due to the change in the ordering types. As shown in Fig. 6 at small $n$, a long-range order forms in the system. As $n$ increases (regions 2 and 3), CO and AFM ordering "coexist" and change to one another. The condition of conservation of the charge (2) formally corresponds to the existence of an external field acting to the pseudospin subsystem. In the case of a weak exchange at large $n$, the charge ordering minimizes the energy of the density–density correlations. In this sense, the charge ordering is induced by the charge constraint. In the FIM phase, one sublattice is completely filled with various magnetic centers and another sublattice is filled with charge states of one type diluted with small number of magnetic centers. Thus, the FIM phase appears as the COII-type order diluted with the shortrange AFM order. It conserves up to
Figure 6: Dependence of the maxima of the charge and spin structure factors in point $(\pi, \pi)$ on charge concentration $n$ for $\Delta/J = 1.52$.

$n = 0.5$; in this case, at $n \gtrsim 0.42$, the peak height of the spin structure factor in point $(\pi, \pi)$ is no higher than 0.002.

4 Conclusions

Using the classical MC method, we studied the two-dimensional spin–pseudospin model for the Ising magnet diluted with charged impurities and frustrated by the competition of the charge and magnetic orderings. The particular attention was focused on the influence of annealed charged impurities on the phase states of the system near to the frustration point in the case of a weak spin exchange.

It is shown that the competition between the charge and magnetic ordering leads to the formation of unusual phase states at finite temperatures. The MC-method simulation enabled us to refine the ground state phase diagram obtained in MFA before and to determine the boundary between the long-range and short-range orders. We also built the diagram of possible phase states that takes into account
their evolution with an increase in temperature. Near the frustration point $\Delta^*/J = 1.5$, we found three regions, in which the changes in the types of orderings and also reentrant phase transitions take place at finite temperatures. This effect is caused by the combination of the following factors. In the case of a weak spin exchange, the substantial concentration of charged impurities leads to the charge ordering, unlike the case of strong spin exchange [8], at which we observe the phase separation into macroscopic regions consisting of charge and magnetic centers. In addition, in the case of a weak exchange in the frustration point, the ground state is degenerate in energy for two various ordering types, namely, the charge and antiferromagnetic orderings. As a result, at finite temperatures near the frustration point, we can observe orderings that do not correspond to the minimum energy at $T = 0$.

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