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Frustration in an exactly solvable mixed-spin Ising model with bilinear and three-site four-spin interactions on a decorated square lattice ☆

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ABSTRACT

Competitive effects of so-called three-site four-spin interactions, single ion anisotropy and bilinear interactions is studied in the mixed spin-1/2 and spin-1 Ising model on a decorated square lattice. Exploring the decoration–iteration transformation, we have obtained exact closed-form expressions for the partition function and other thermodynamic quantities of the model. From these relations, we have numerically determined ground-state and finite-temperature phase diagrams of the system. We have also investigated temperature variations of the correlation functions, internal energy, entropy, specific heat and Helmholtz free energy of the system. From the physical point of view, the most interesting result represents our observation of a partially ordered ferromagnetic or phase in the system with zero bilinear interactions. It is remarkable, that due to strong frustrations disordered spins survive in the system even at zero temperature, so that the ground state of the system becomes macroscopically degenerate with non-zero entropy. Introduction of arbitrarily small bilinear interaction completely removes degeneracy and the entropy always goes to zero at the ground state.

1. Introduction

The investigation of multi-spin interactions has been initiated several decades ago in order to clarify their influence on phase transitions and magnetic properties in various physical systems. In order to investigate basic aspects of multi-spin interactions the authors have utilized various theoretical methods including exact calculations [1–15], series expansions [16–18], renormalization-group techniques [19–22], Monte Carlo simulations [23–26], mean-field and effective-field theory [27–30].

On the other hand, from the experimental point of view, the models with multi-spin interactions have been widely used to explain the thermodynamic properties of various physical systems, such as binary alloys [23], classical fluids [31], solid He_3 [32], lipid bilayers [33], metamagnets [34], rare gases [35] or hydrogen bonded ferroelectrics $PbHPO_4$ and $PbDPO_4$ [36]. One should also mention here that the models with multi-spin interactions have been successfully used to describe the first-order phase transition in the squaric acid crystal $H_2C_2O_4$ [27,37,38] and some co-polymers [39]. Moreover, the cycling four-spin exchange interactions have been adopted to explain experimental results on spin gaps [40–42], Raman peaks [43] and optical conductivity of the cuprate ladder $La_2Ca_{14-x}Cu_{24}O_{41}$ [44]. The four-spin interactions have been taken into account also in the study of two-dimensional antiferromagnet La_2CuO_4, the parent material of high-T_c superconductors [45,46]. The effects of so called three-site four-spin interactions on magnetic properties and phase transitions in various model systems have been widely studied by Iwashita and Uryu [47–50]. Finally, let us mention a series of works by Köbler et al. [51–54] in which the authors have very carefully investigated the role of higher-order spin interactions in a wide class of real magnetic materials.

As far as it concerns of magnetic properties, the models with multi-spin interactions may exhibit some peculiarities, for example, the non-universal critical behavior [1,2,17,18] or deviations from the Bloch's $T^{3/2}$ law at low temperatures [51–54]. Here it is worth emphasizing that some of these phenomena are not yet well understood and clarified even at the present time. In fact, the investigation of many-body interactions is of tremendous importance in all branches of physics, since such studies may discover new physical phenomena that do not appear in the systems with pair interactions only. However, it is necessary to recall that the investigation of the systems with many-body interactions is as a rule much more complex than those with pair interactions only. Nonetheless, we have recently demonstrated [11–15] that various

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versions of the Ising model represent a very good theoretical ground for an accurate treatment of multi-spin interactions.

The main aim of this work is to extend our recent research in this field in order to investigate in detail the role of so-called three-site four-spin interactions in crystalline systems with localized magnetic moments. For this purpose, we will study the mixed-spin 1/2 and 1 Ising model with the single-ion anisotropy, pair and three-site four spin interactions on a decorated square lattice. The outline of the present work is as follows. In Sections 2 and 3 we derive exact equations for all physical quantities applying a generalized form of decoration–iteration transformation. The ground-state and finite-temperature phase diagrams are discussed in detail in Section 4 along with thermal variations of other physical quantities. Finally some conclusions are sketched in the last section.

2. Theory

In this work we will investigate the mixed spin-1/2 and spin-1 Ising model on a decorated square lattice depicted in Fig. 1. The system is described by the Hamiltonian

$$\mathcal{H} = -\frac{J}{2}\sum_{i,j}\mu_i^z S_j^z - \frac{J'}{2}\sum_{i,j}\mu_i^z\mu_j^z - J_4\sum_k \mu_{k1}^z (S_k^z)^2\mu_{k2}^z - D\sum_k (S_k^z)^2 \tag{1}$$

where J and J' respectively denote the nearest-neighbor and next-nearest-neighbor bilinear exchange interactions, J_4 is the three-site four-spin exchange interaction and D represents the single-ion anisotropy parameter. The summations in the first and second term in (1) run over all relevant pairs on the decorated square lattice, while in the third and fourth term the summations are over all decorating spins, i.e. $k = 1, \ldots, 2N$, where N represents the total number of spin-1/2 atoms.

In order to apply the decoration–iteration transformation to the present model, we at first express the total Hamiltonian in the form

$$\mathcal{H} = \sum_k \mathcal{H}_k, \tag{2}$$

where the Hamiltonian $\mathcal{H}_k$ includes all interaction terms within the k-th bond of the lattice and it is given by

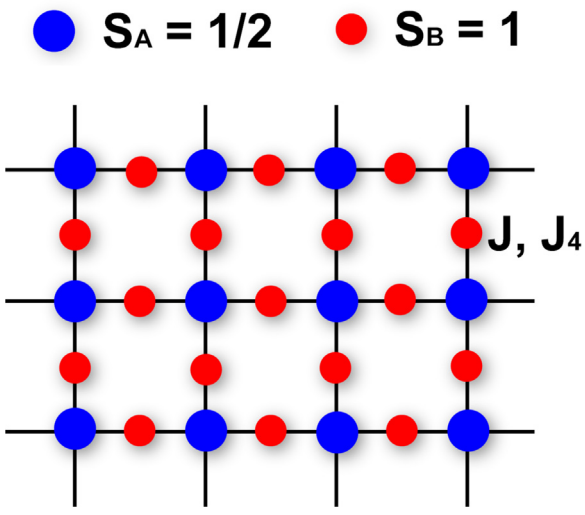

Fig. 1. Part of a mixed spin decorated square lattice. Blue circles located on the original square lattice nodes denote the spin-1/2 atoms and the red ones represent decorating atoms with spin 1 located at each bond of the square lattice. (For interpretation of the references to color in this figure legend, the reader is referred to the web version of this article.)

$$\mathcal{H}_k = -J(\mu_{ki}^z + \mu_{kj}^z)S_k^z - J'\mu_{ki}^z\mu_{kj}^z - J_4\mu_{ki}^z\mu_{kj}^z(S_k^z)^2 - D(S_k^z)^2 \tag{3}$$

Now, using (2), the partition function of the model can be expressed as

$$\begin{aligned}\mathcal{Z} &= \sum_{\{\mu_{k\gamma}^z=\pm 1/2\}}\sum_{\{S_k^z=\pm 1,0\}} \exp(-\beta\mathcal{H}) \\ &= \sum_{\{\mu_{k\gamma}^z=\pm 1/2\}}\prod_{k=1}^{2N}\sum_{S_k^z=\pm 1,0} \exp(-\beta\mathcal{H}_k),\end{aligned} \tag{4}$$

where the curled brackets denote the fact that relevant summation concerns all spin variables of the lattice.

Introducing the following decoration–iteration transformation [55–57]

$$\sum_{S_k^z=\pm 1,0} \exp(-\beta\mathcal{H}_k) = A\exp(\beta R\mu_{ki}^z\mu_{kj}^z) \tag{5}$$

one rewrites Eq. (4) as follows

$$\mathcal{Z} = A^{2N}\mathcal{Z}_0(\beta R). \tag{6}$$

In the last equation $\mathcal{Z}_0(\beta R)$ represents the partition function of conventional Ising model on a square lattice described by the Hamiltonian $\mathcal{H}_0 = -R\sum_k \mu_{ki}^z\mu_{kj}^z$. This partition function has been exactly calculated in a seminal Onsager's work [58] and it will be used in this paper to obtain exact results for thermodynamic properties of the model under investigation. Of course, to complete the calculation of $\mathcal{Z}$ we have also to determine the unknown functions A and R. Fortunately, this evaluation may be straightforwardly performed by substituting $\mu_{ki}^z = \pm 1/2$ and $\mu_{kj}^z = \pm 1/2$ into Eq. (5) and in this way one gets

$$A = \sqrt{w_1 w_2}, \quad \beta R = \beta J' + 2\ln\left(\frac{w_1}{w_2}\right), \tag{7}$$

where

$$w_1 = 1 + 2e^{\beta D + \frac{\beta J_4}{4}}\cosh(\beta J) \tag{8}$$

$$w_2 = 1 + 2e^{\beta D - \frac{\beta J_4}{4}}. \tag{9}$$

3. Ground-state and thermodynamic properties

The ground-state phase diagram can be determined investigating the internal energy of the system at $T=0$. Since we do not consider any external field, the internal energy of the system can be evaluated as a mean value of the Hamiltonian (1), i.e. $U = \langle\mathcal{H}\rangle$ and it takes the following form

$$\begin{aligned}\frac{U}{2N} = &-J\left\langle(\mu_{k1}^z + \mu_{k2}^z)S_k^z\right\rangle - J'\left\langle\mu_{k1}^z\mu_{k2}^z\right\rangle - J_4\left\langle\mu_{k1}^z(S_k^z)^2\mu_{k2}^z\right\rangle \\ &- D\left\langle(S_k^z)^2\right\rangle,\end{aligned} \tag{10}$$

where the angular brackets denote the standard canonimathcal averaging using the density matrix $\rho = \exp(-\beta\mathcal{H})/\mathcal{Z}$. For further progress in calculation it is of crucial importance that all correlation functions entering previous equation can be mathcalculated using the generalized Callen–Suzuki identities [59,60] which in our case take the form