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Research articles

Anomalous spin frustration enforced by a magnetoelastic coupling in the mixed-spin Ising model on decorated planar lattices

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ABSTRACT

The mixed spin-1/2 and spin-*S* Ising model on a decorated planar lattice accounting for lattice vibrations of decorating atoms is treated by making use of the canonical coordinate transformation, the decoration-iteration transformation, and the harmonic approximation. It is shown that the magnetoelastic coupling gives rise to an effective single-ion anisotropy and three-site four-spin interaction, which are responsible for the anomalous spin frustration of the decorating spins in virtue of a competition with the equilibrium nearest-neighbor exchange interaction between the nodal and decorating spins. The ground-state and finite-temperature phase diagrams are constructed for the particular case of the mixed spin-1/2 and spin-1 Ising model on a decorated square lattice for which thermal dependencies of the spontaneous magnetization and specific heat are also examined in detail. It is evidenced that a sufficiently strong magnetoelastic coupling leads to a peculiar coexistence of the antiferromagnetic long-range order of the nodal spins with the disorder of the decorating spins within the frustrated antiferromagnetic phase, which may also exhibit double reentrant phase transitions. The investigated model displays a variety of temperature dependencies of the total specific heat, which may involve in its magnetic part one or two logarithmic divergences apart from one or two additional round maxima superimposed on a standard thermal dependence of the lattice part of the specific heat.

1. Introduction

A complete thermodynamic description of magnetic, vibrational and elastic properties of insulating solid-state materials remains a long-standing problem of particular research interest, because considerable computational difficulties arise when magnetic and lattice degrees of freedom are coupled together through a magnetoelastic interaction. Owing to this fact, the magnetoelastic coupling is often completely disregarded in order to preserve a capability of treating magnetic and lattice degrees of freedom of magnetic solids independently of each other. A substantial progress in this research area has been recently made by Balcerzak and co-workers when developing a phenomenological theory based on a self-consistent variational approach, which combines different approximations for individual subsystems as for instance a mean-field approximation for a magnetic subsystem, Debey approximation for a lattice subsystem, etc. [1–3].

It is notorious that the leading-order interaction term between localized spins of insulating magnetic solids is an indirect superexchange coupling, which according to the Kramers-Anderson mechanism basically depends on an overlap of atomic wave functions [4,5]. The superexchange coupling (further referred to as the exchange coupling) thus strongly depends on an instantaneous distance between the magnetic atoms, which are subject to a perpetual temperature-dependent lattice vibrations. Hence, it follows that the lattice vibrations of magnetic atoms can fundamentally influence a magnetic spin ordering and vice versa. This effect might be especially marked in a close vicinity of phase transitions connected with a breakdown of a spontaneous long-range order [6–11]. It is worth mentioning that the mixed-spin Ising models display in general a more diverse critical behavior than their single-spin counterparts, but most of exactly solved mixed-spin systems neglect vibrational and elastic degrees of freedom when considering spins situated on a perfectly rigid lattice [12–19].

The main goal of the present work is to examine an effect of the magnetoelastic coupling on a full thermodynamics of the mixed spin-1/

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2 and spin-S Ising model on decorated planar lattices, which are constituted by nodal atoms placed at rigid lattice positions and decorating atoms capable of lattice vibrations treated within the harmonic approximation. To this end, we will generalize the calculation procedure developed in our previous work for the analogous spin-1/2 Ising model on decorated planar lattices [20]. Interestingly, the same local canonical transformation can be applied to decouple magnetic and lattice degrees of freedom [21], but the relevant decoupling gives rise to an effective three-site four-spin interaction and a shift of uniaxial single-ion anisotropy in contrast to the previous case with an effective next-nearest-neighbor interaction [20]. The magnetoelastic coupling may thus enforce a remarkable spin frustration of the decorating atoms, which has been comprehensively studied in the mixed-spin Ising model with the three-site four-spin interaction on decorated planar lattices [22,23] with the help of exact mapping transformation method [24–29].

The organization of this paper is as follows. The investigated mixed-spin Ising model is defined in Section 2, where the basic steps of the calculation procedure are also explained. The most interesting results for the ground-state and finite-temperature phase diagrams, the spontaneous magnetization and the specific heat are presented in Section 3. Finally, some conclusions and future outlooks are mentioned in Section 4.

2. Model and method

Let us consider a two-dimensional decorated lattice as schematically illustrated in Fig. 1 on the particular example of a decorated square lattice, the nodal sites of which are occupied by the spin-1/2 atoms and the decorating sites of which are occupied by the spin-S ($S \geqslant 1$) atoms. It is assumed that the spin-1/2 nodal atoms are placed at rigid lattice positions in contrast to the spin-S decorating atoms, which may oscillate around their equilibrium lattice positions. This approximation is justified because the relaxation of the nodal atoms from their equilibrium lattice positions would cost a greater amount of the elastic energy in comparison with the one of the decorating atoms due to a deformation of greater number of lattice bonds. Under these assumptions, the total Hamiltonian of the mixed-spin Ising model on decorated

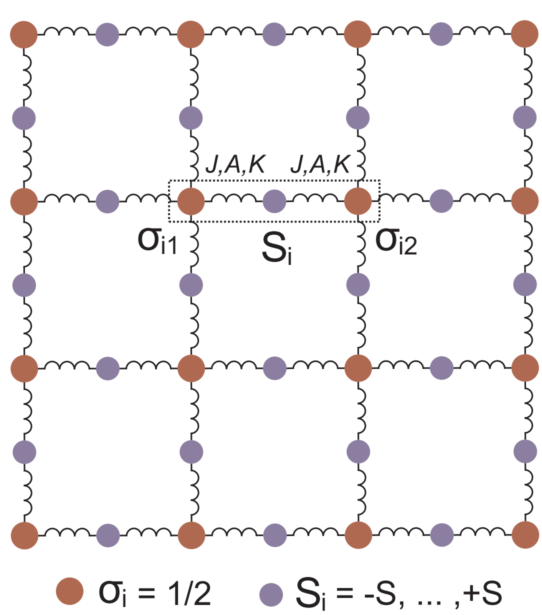

Fig. 1. A cross-section from a decorated square lattice. Nodal lattice sites (red circles) are occupied by the spin-1/2 atoms ($\sigma_i = \pm 1/2$), while decorating lattice sites (blue circles) are occupied by the spin-S atoms ($S_i = -S, -S+1, ..., S$) being subject to lattice vibrations. (For interpretation of the references to colour in this figure legend, the reader is referred to the web version of this article.)

planar lattices can be defined as a sum over bond Hamiltonians $\hat{\mathscr{H}}_i$ involving all interaction terms of the ith decorating atom

$$\hat{\mathscr{H}} = \sum_{i=1}^{Nq/2} \hat{\mathscr{H}}_i = \sum_{i=1}^{Nq/2} (\hat{\mathscr{H}}_i^m + \hat{\mathscr{H}}_i^e), \tag{1}$$

which are further split into the magnetoelastic part $\hat{\mathscr{H}}_i^m$ and the pure elastic part $\hat{\mathscr{H}}_i^e$ (N labels the total number of the spin-1/2 nodal atoms and q is their coordination number). The magnetoelastic part of the bond Hamiltonian $\hat{\mathscr{H}}_i^m$ takes into account the uniaxial single-ion anisotropy D acting on the decorating spin S_i as well as the exchange interaction between the decorating spin S_i and its two nearest-neighbor nodal spins σ_{i1} and σ_{i2}

$$\hat{\mathscr{H}}_i^m = -(J - A\hat{\rho}_i)S_i\sigma_{i1} - (J + A\hat{\rho}_i)S_i\sigma_{i2} - DS_i^2, \tag{2}$$

which depends on an instantaneous distance between the relevant spins through the local coordinate operator $\hat{\rho}_i$ assigned to a displacement of the ith decorating atom from its equilibrium lattice position placed at a midpoint in between its two nearest-neighbor nodal atoms. The exchange constant J marks a size of the nearest-neighbor interaction between the decorating and nodal spins on assumption that the decorating atom takes its equilibrium position (i.e. $\rho_i = 0$), whereas the magnetoelastic coupling constant A determines an increase (decrease) of the nearest-neighbor interaction owing to a contraction (elongation) of the respective atomic distance. The magnetoelastic coupling constant A thus crucially connects the magnetic (spin) degrees of freedom with the vibrational ones.

The purely elastic part of the bond Hamiltonian $\hat{\mathscr{H}}_i^e$ incorporates the kinetic energy of the ith decorating atom with the mass M and the elastic energy penalty, which is in the harmonic approximation connected to a square of the displacement operator of the ith decorating atom from its equilibrium lattice position

$$\hat{\mathscr{H}}_i^e = \frac{\hat{p}_i^2}{2M} + K\hat{\rho}_i^2. \tag{3}$$

The spring stiffness constant K emerging in the elastic part of the bond Hamiltonian (3) characterizes a vibrational energy of the decorating atoms and it can be alternatively viewed as a bare elastic constant of two harmonic springs attached to each decorating atom. The spring stiffness constant K is thus inversely proportional to a deformation of the lattice bonds.

It is evident from Eq. (2) that the magnetic and lattice degrees of freedom are coupled together through the magnetoelastic constant A, which usually makes solution of the respective Ising models refined with a magnetoelastic coupling more complex. However, the magnetoelastic interaction can be decoupled through a local canonical coordinate transformation [20,21]

$$\hat{\rho}_i = \hat{\rho}_i' - \frac{A}{2K}S_i(\sigma_{i1} - \sigma_{i2}), \tag{4}$$

which eliminates from the magnetoelastic part of bond Hamiltonian (2) dependence on a displacement operator

$$\hat{\mathscr{H}}_i^{m'} = -JS_i(\sigma_{i1} + \sigma_{i2}) + J'S_i^2\sigma_{i1}\sigma_{i2} - D'S_i^2. \tag{5}$$

After implementation of the canonical coordinate transformation (4) the magnetoelastic part of the bond Hamiltonian (5) actually involves the effective three-site four-spin interaction $J' = A^2/2K$ and the rescaled uniaxial single-ion anisotropy $D' = D + A^2/8K$ besides the equilibrium nearest-neighbor bilinear interaction J. Recently, it has been demonstrated that the mixed-spin Ising models on a decorated square lattice with the nearest-neighbor bilinear interaction, three-site four-spin interaction and uniaxial single-ion anisotropy may exhibit striking frustrated states due to competing effects arising from the three-site four-spin interaction [22,23]. On the other hand, the elastic part of the bond Hamiltonian (3) remains invariant under the canonical coordinate transformation (4)