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The ternary alloy with a structure of Prussian blue analogs in a transverse field

J. Dely, A. Bobák*

Department of Theoretical Physics and Astrophysics, Faculty of Science, P.J. Šafárik University, Park Angelinum 9, 041 54 Košice, Slovak Republic

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Abstract

The effects of applied transverse field on transition and compensation temperatures of the AB_pC_{1-p} ternary alloy consisting of spins $S^A = \frac{3}{2}$, $S^B = 2$, and $S^C = \frac{5}{2}$ are investigated by the use of a mean-field theory. The structure and the spin values of the model correspond to the Prussian blue analog of the type $(Fe^{II}_pMn^{II}_{1-p})_{1.5}[Cr^{III}(CN)_6]\cdot nH_2O$. We find that two or even three compensation points may be induced by a transverse field for the system with appropriate values of the parameters in the model Hamiltonian. In particular, the influence of a transverse field on the compensation point in the ground state is examined.

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1. Introduction

The emerging field of molecular magnetism constitutes a new branch of material science that deals with the magnetic properties of molecules, or assemblies of molecules, that contain magnetic centers [1–3]. The growing interest in understanding of the origin of the magnetic ordering in these materials is to obtain novel molecular magnetic materials with high transition temperature. For this purpose several families of molecule-based magnets have been under consideration in the past two decades [4–8].

Recently much interest has focused on the family of multi-metal Prussian blue analogs with the general formula $A_k[B(CN)_6]_l\cdot nH_2O$ [9], where A and B are 3d transi tion-metal ions with various oxidation and spin states. The large-scale choice of A and B ions allows to modify the nature of the coupling constants and thereby the magnetic properties of the system. Up to date, various fascinating phenomena have been observed in Prussian blue analogs [10]. In particular, the class members $(X^{II}_pMn^{II}_{1-p})_{1.5}$ $[Cr^{III}(CN)_6]\cdot nH_2O$ $(X^{II} = Ni^{II}, Fe^{II})$ [11,12] or $(Ni^{II}_pMn^{II}_qFe^{II}_r)_{1.5}[Cr^{III}(CN)_6]\cdot nH_2O$ [13], which include both ferromagnetic $(J_{XCr} > 0)$ and antiferromagnetic $(J_{MnCr} < 0)$ superexchange interactions between the neighbouring metal ions through the cyanide bridging ligands, may exhibit one or even two compensation temperatures, respectively. We note that the existence of a compensation temperature T_k, at which the total magnetization vanishes below its transition temperature T_c, is an interesting phenomenon with important technological applications in the field of thermomagnetic recording. This behaviour is possible due to the fact that the magnetic moments of the sublattices compensate each other completely at $T = T_k$, owing to the different temperature dependencies of the sublattice magnetizations.

On the other hand, we have very recently found within the standard mean-field theory (MFT) that depending on the values of the parameters in the model Hamiltonian the mixed ferro-ferrimagnetic ternary alloy of the type AB_pC_{1-p} with a structure of the Prussian blue analog may exhibit two or even three compensation points [14]. In consequence of the multicompensation behaviour appearing in the mixed ferro-ferrimagnetic ternary alloy, it is

*Corresponding author. Fax: +421 55 6222124.
E-mail address: abobak@upjs.sk (A. Bobák).

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interesting now to study such the ternary alloy in the presence of an applied transverse field. As has been pointed out in Refs. [15,16], the application of a weak transverse field to the binary ferrimagnetic system can control the compensation points. However, the role of a transverse field in the mixed ferro-ferrimagnetic ternary alloy has not been examined yet. Therefore, the purpose of this work is to investigate the effects of an applied transverse field (i.e. the field is applied perpendicularly to the spontaneous magnetization axis) on phase diagrams and compensation temperature of the AB_pC_{1-p} ternary alloy corresponding to the Prussian blue analog of the type $(Fe^{II}_pMn^{II}_{1-p})_{1.5}[Cr^{III}(CN)_6]\cdot nH_2O$ [11]. To simulate the structure of this Prussian blue analog, we consider that the A and X ($X=B$ or C) magnetic ions are alternately connected and have different spins $S^A=\frac{3}{2}, S^B=2$, and $S^C=\frac{5}{2}$, respectively. The model is described by the Ising Hamiltonian to which is added a term which represents the effects of transverse field part. Owing to the requisite non-commutativity of operators in the Hamiltonian, deriving the eigenvalues of the Hamiltonian is very difficult. Fortunately, the predictions of the MFT up to now for such a complex system in the zero transverse field turned out to be in satisfactory agreement with the experiment [10,17]. Moreover, it is well known that as far as the exchange interaction between sublattices is greater than the exchange interaction within sublattices, which is the case, the necessary condition for the MFT applicability is satisfied [18]. Taking this into account, in the present paper we exploit the MFT for the study of magnetic properties of the AB_pC_{1-p} ternary alloy in the presence of a transverse field.

An outline of the remainder of this paper is as follows. A formulation of the problem within the MFT is presented in Section 2. In Section 3, the effects of transverse field on phase diagrams and compensation temperature of the ternary alloy are numerically and analytically studied. Finally, brief conclusions are presented in Section 4.

2. Formulation

We consider a mixed ferro-ferrimagnetic ternary alloy model of the type AB_pC_{1-p} consisting of three kinds of magnetic ions A, B, and C with different Ising spins $S_{iA}=\frac{3}{2}$, $S_{jB}=2$, and $S_{jC}=\frac{5}{2}$, respectively. To be consistent with a structure of the Prussian blue analog [11], we assume that the S_{iA} and either S_{jB} or S_{jC} spins, which are randomly distributed in the lattice, are linked in an alternating fashion. Restricting the interactions to nearest-neighbours, the general transverse Ising model is described by the Hamiltonian

$$H = -\sum_{(i,j)} S^z_{iA}[J_{AB}S^z_{jB}\xi_j + J_{AC}S^z_{jC}(1-\xi_j)] - \Omega\left\{\sum_{i=1}^{N_A} S^x_{iA} + \sum_{j=1}^{N_X}[S^x_{jB}\xi_j + S^x_{jC}(1-\xi_j)]\right\}, \quad (1)$$

where the first summation is carried out only over nearest-neighbour pairs of spins on different sublattices and J_{AB} ($J_{AB}=J_{BA}, J_{AB}>0$) and J_{AC} ($J_{AC}=J_{CA}, J_{AC}<0$) are the nearest-neighbour exchange interactions. S^v_{iA}, S^v_{jB}, and S^v_{jC} ($v=x$ or z) are components of the spin operators on sublattices A, B, and C, respectively, and Ω is the transverse field applied perpendicularly to the spontaneous magnetization axis (or the z-axis). N_A and N_X are the numbers of sites occupied by the A and X ($X=B$ or C) ions, respectively, with $N_A+N_X=N$ the total number of sites of the lattice. $\{\xi_j\}$ is a set of independent, uniformly distributed random variables which take values of unity or zero, depending on whether the site j is occupied by an ion of the type B or C, respectively.Therefore, the probability distribution function of ξ_j is given by

$$P(\xi_j) = p\delta(\xi_j - 1) + q\delta(\xi_j), \quad (2)$$

where p is the concentration of B ions and $q=1-p$ is the concentration of C ions.

For N_A and N_X in the Hamiltonian (1) of the present system, one can require the following general relation:

$$z_1N_A = z_2N_X, \quad (3)$$

where z_1 and z_2 are the numbers of the nearest neighbours of the A and X ($X=B$ or C) ions, respectively. The values of z_1 and z_2 are fixed and controlled by the stoichiometry of the mixed-spin system. In the case of the above-mentioned Prussian blue analog, which for X/A displays a 3:2 stoichiometry, there is $z_1=6$ and $z_2=4$ (Refs. [10,12]).

Our aim in this work is to use the spin Hamiltonian given by Eq. (1) to investigate the effects of the concentration p, the interaction ratio $R=|J_{AC}|/J_{AB}$, and the transverse magnetic field Ω on the magnetic properties of the system. To this end, we develop the MFT that is based on the following single-site effective Hamiltonians:

$$H^A_i = -z_1[J_{AB}m^z_B + J_{AC}m^z_C]S^z_{iA} - \Omega S^x_{iA}, \quad (4)$$

$$H^B_j = -z_2J_{AB}m^z_A\xi_jS^z_{jB} - \Omega\xi_jS^x_{jB}, \quad (5)$$

$$H^C_j = -z_2J_{AC}m^z_A(1-\xi_j)S^z_{jC} - \Omega(1-\xi_j)S^x_{jC}. \quad (6)$$

Here, m^z_α ($\alpha=A,B$ or C) are the averaged longitudinal sublattice magnetizations per site defined by

$$m^z_A = \langle\langle S^z_{iA}\rangle_0\rangle_c, \quad m^z_B = \langle\langle S^z_{jB}\rangle_0\xi_j\rangle_c, \quad m^z_C = \langle\langle S^z_{jC}\rangle_0(1-\xi_j)\rangle_c, \quad (7)$$

where $\langle\cdots\rangle_0$ and $\langle\cdots\rangle_c$ denote thermal and configurational averaging, respectively. Then the averaged value of a general function of spin operator components A_n, at the lattice site n, is given by

$$\langle\langle A_n\rangle_0\rangle_c = \left\langle \frac{\mathrm{Tr}_n A_n \exp(-\beta H^\alpha_n)}{\mathrm{Tr}_n \exp(-\beta H^\alpha_n)} \right\rangle_c, \quad (8)$$

where Tr_n denotes a partial trace with respect to the lattice site n and $\beta = 1/k_BT$.

The single-site Hamiltonians (4)–(6) can readily be diagonalized by using a rotation transformation (see, e.g., Ref. [19]). Then, by the use of Eq. (8), the averaged longitudinal and transverse sublattice magnetizations per