acta physica slovaca vol. 46 No. 2, 113 – 116 April 1996

EFFECTIVE-FIELD ANALYSIS OF FERRIMAGNETIC MIXED SPIN ISING SYSTEMS WITH SITE DILUTION[1]

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Received 31 July 1995, accepted 8 February 1996

Using an effective-field theory with correlations we study a diluted mixed two-sublattice Ising ferrimagnetic system consisting of spin-$\frac{1}{2}$ and spin-1. The phase diagrams (transition temperature and compensation temperature) and magnetization curves for a square lattice with coordination number $z = 4$ are obtained. We find a number of interesting phenomena in these quantities, such as the possibility of two compensation points in the total magnetization curve and magnetization curves not predicted in the Néel theory.

1. Introduction

In recent years approximation schemes have been developed which represent remarkable improvements of the traditional mean field theory as applied to spin systems. In particular, we refer to the effective-field theory with correlations which is based on the use of some extensions of the Callen identity [1]. This theory has been successfully applied to a variety of spin-$\frac{1}{2}$ Ising problems as well as the higher-spin Ising models [2]. Its application to ferrimagnetism in a diluted mixed spin-$\frac{1}{2}$ and spin-1 Ising system on a honeycomb lattice [3] exhibits two compensation points in the total magnetization curve and magnetization curves not predicted in the Néel theory.

The purpose of this paper is to present an extension of the referred effective-field approach to a diluted mixed spin Ising system (spin-$\frac{1}{2}$ and spin-1) in a square lattice ($z =$ 4) and to clarify whether the existence of more than one compensation point depends on the lattice structure. We note that mixed Ising systems have less translational symmetry than their single spin counterparts and are well adopted to study a certain type of ferrimagnetism [4].

[1] Presented at 9$^{\text{th}}$ Czech and Slovak conference on magnetism, Košice, Slovakia, August 28-30 1995

2. Theory

We consider a site diluted mixed spin-$\frac{1}{2}$ and spin-1 Ising ferrimagnetic system on the square lattice ($z = 4$) described by the Hamiltonian

$$H = -J \sum_{<i,j>} s_i^A s_j^B \xi_i^A \xi_j^B, \tag{1}$$

where s_i^A takes, on sublattice A, the values of $\pm\frac{1}{2}$, s_j^B on sublattice B, can be ± 1 and 0, and the summation is carried out only over nearest-neighbour pairs of spins. The $J (J < 0)$ is the nearest-neighbour exchange interaction and $\xi_i^A (\xi_j^B)$ is a random variable which takes the value of unity or zero, depending on whether the site $i(j)$ is occupied by a magnetic atom of type $A(B)$ or not.

Within the formulation of the effective-field theory [3],the sublattice magnetizations m_A and m_B of the system with $z = 4$ are given by

$$m_A \equiv < \xi_i^A < s_i^A >>_c = p_A[1 - q + q\cosh(JD) + m_B \sinh(JD)]^4 f(x)|_{x=0}, \tag{2}$$

$$m_B \equiv < \xi_j^B < s_j^B >>_c = p_B[1 - p_A + p_A\cosh(\frac{1}{2}JD) + 2m_A \sinh(\frac{1}{2}JD)]^4 F(x)|_{x=0}, \tag{3}$$

where $< ... >$ $(< ... >_c)$ denotes the thermal (configurational) average, $D = \partial/\partial x$ is a differential operator, $p_\alpha = < \xi_i^\alpha >_c$ is the concentration of magnetic α atoms ($\alpha = A$ or B) and the parameter q is determined by

$$q \equiv < \xi_j^B < (s_j^B)^2 >>_c = p_B[1 - p_A + p_A\cosh(\frac{1}{2}JD) + 2m_A \sinh(\frac{1}{2}JD)]^4 G(x)|_{x=0}. \tag{4}$$

The functions $f(x), F(x)$ and $G(x)$ are defined by

$$f(x) = \frac{1}{2}\tanh(\frac{1}{2}\beta x), \tag{5}$$

$$F(x) = \frac{2\sinh(\beta x)}{2\cosh(\beta x) + 1}, \tag{6}$$

$$G(x) = \frac{2\cosh(\beta x)}{2\cosh(\beta x) + 1}, \tag{7}$$

where $\beta = 1/k_B T$. The averaged total magnetization per site is then given by

$$M = \frac{1}{2}(m_A + m_B). \tag{8}$$

In order to determine the transition temperature T_c , we expand the right-hand side of equations (2), (3) and (4) and we obtain the polynomial equations of m_A, m_B and q. The second-order line is then given by substituting equations (3) and (4) in (2) and linearizing the latter. On the other hand, the compensation temperature $T_k (T_k < T_c)$, at which the total magnetization vanishes, can be evaluated by requiring the condition $M = 0$ in the coupled equations (2) and (3).

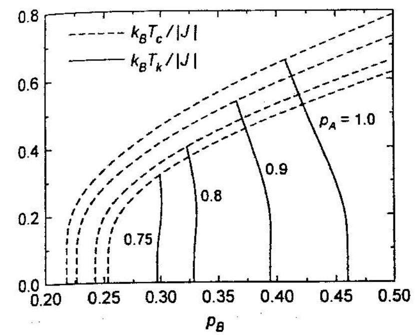

Fig. 1. Phase diagrams in the (T, p_B) plane for the diluted mixed ferrimagnetic system on a square lattice, when the concentration of magnetic atoms p_A in the sublattice A is changed. The dashed and solid curves represent the transition temperature T_c and compensation temperature T_k, respectively.

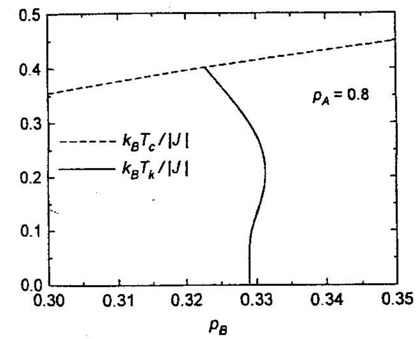

Fig. 2. The same as in Fig. 1 for the curves T_c and T_k with $p_A = 0.8$ on an enhanced scale.

3. Numerical results and discussion

Some typical phase diagrams in the (T, p_B) plane for different values of p_A are shown in Fig.1. The solid and dashed lines represent the variations of compensation temperature T_k and transition temperature T_c, respectively. The figure shows that two compensation points may exist in the system with a certain concentration of p_A (see curves with $p_A = 0.9$; 0.8 and 0.75), although the scale of Fig.1 does not allow to see it. In Fig.2 we therefore show on an enlarged scale one such curve $T_k(p_A = 0.8)$ where for a very small range of concentration p_B two values of T_k are obtained. From our detailed numerical investigations we have found that the system exhibits two compensation points in the (T, p_B) plane for $0.7227 \leq p_A < 1.0$ while in the (T, p_A) plane for $0.2848 \leq p_B < 0.4597$. These concentration ranges may be compared with those of $0.9333 \leq p_A \leq 1.0$ and $0.3562 \leq p_B \leq 0.3988$ respectively, recently reported by us for the honeycomb lattice [3]. Thus, the concentration ranges where two compensation points occur are increased with increasing the coordination number value.

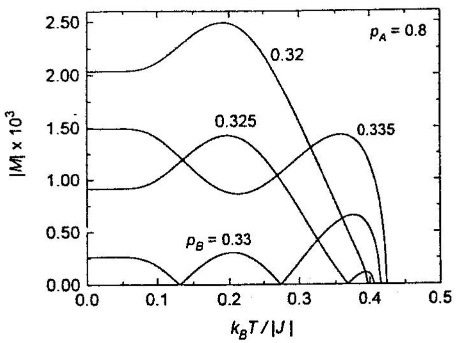

Fig. 3 Temperature dependences of the total magnetization $|M|$ for the diluted mixed ferrimagnetic system on a square lattice with $p_A = 0.8$, when the value of p_B is changed from $p_B = 0.32$ to $p_B = 0.335$.

In order to confirm the prediction for the existence of two compensation points, let us study the thermal dependence of the total magnetization $|M|$. Figure 3 shows the behaviour of $|M|$ as a function of T for the system with $p_A = 0.8$, when value of p_B is changed from $p_B = 0.32$ to 0.335. That is to say they are obtained by changing p_B from the right-hand side to the left-hand side in Fig.1 and crossing the curve of T_k for $p_A = 0.8$. For $p_B = 0.335$, the magnetization curve shows a minimum and maximum in the temperature region below T_c. On the other hand, the curve labeled $p_B = 0.325$ exhibits only the maximum with one compensation point at $T \neq 0$. However, when $p_B = 0.33$, as predicted in Fig.1, two compensation points are found. Note that these phenomena have not been predicted in the Néel theory of ferrimagnetism [5]. We hope that the results obtained in this work may be helpful when the experimental data of ferrimagnetic materials are analysed.

Finally, it is worth mentioning that the single-site approach used in this work is not able to reflect the details of the lattice geometry beyond its coordination number. Therefore, the results presented apply also withount any changes to all lattices with coordination number $z = 4$ (e.g. diamond lattice).

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