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Ferrimagnetism in Diluted Mixed Spin-1/2 and Spin-3/2 Ising Systems

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Abstract. Using an effective field theory with correlations we study a diluted mixed spin-1/2 and spin-3/2 Ising ferrimagnetic system with a crystal field interaction $D(D < 0)$ on a honeycomb lattice. We find that the system may exhibit two compensation points in the total magnetization curve, although the corresponding system in the absence of dilution or with $D = 0$ never exhibits any compensation point at $T \neq 0K$.

1. INTRODUCTION

Ferrimagnetism has been intensively investigated in the past both experimentally and theoretically. From a theoretical point of view, the two-sublattice mixed-spin Ising system consisting of spins $s_A = 1/2$ and $s_B (s_B > 1/2)$ has been introduced as a simple model showing a certain type of ferrimagnetism. In particular, it was shown for the case $s_B = 1$ that this model with site-dilution on a honeycomb lattice may exhibit two compensation points [1], although the same system consisting of $s_A = 1/2$ and $s_B = 3/2$ never exhibits any compensation point [2].

On the other hand, for Ising systems with $s_B > 1/2$, one has to expect an appreciable crystal-field splitting of the energy levels, which could strongly influence the physical properties of the system. The purpose of this work is thus to clarify the effects of crystal field interaction on a compensation temperature in the diluted mixed spin Ising ferrimagnetic system when the values of s_A and s_B are selected as $s_A = 1/2$ and $s_B = 3/2$ on a honeycomb lattice.

2. FORMULATION

We consider a site-diluted mixed spin-1/2 and spin-3/2 Ising ferrimagnetic system in the presence of a crystal field interaction D described by the Hamiltonian

$$H = -J \sum_{\langle i,j \rangle} s_i^A s_j^B \xi_i^A \xi_j^B - D \sum_j \xi_j^B (s_j^B)^2, \tag{1}$$

where s_i^A takes, on sublattice A, the values $\pm 1/2$, and s_j^B on sublattice B, can be $\pm 1/2$ and $\pm 3/2$. $J (J < 0)$ is the exchange interaction and $\xi_i^A (\xi_j^B)$ is the site occupancy number 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.

To evaluate the averaged sublattice magnetizations m_A, m_B and the parameters q, r , defined by

$$m_A = \langle \xi_i^A \langle s_i^A \rangle \rangle_c, \quad m_B = \langle \xi_j^B \langle s_j^B \rangle \rangle_c, \quad q = \langle \xi_j^B \langle (s_j^B)^2 \rangle \rangle_c, \quad r = \langle \xi_j^B \langle (s_j^B)^3 \rangle \rangle_c, \tag{2}$$

where $\langle \dots \rangle$ ($\langle \dots \rangle_c$) denotes the thermal (configurational) average, the effective-field theory with correlation [3] can be applied to this problem. By using a similar calculation as in [1,3], one finds

$$m_A = p_A \{1 + p_B [K_0(\gamma) - 1] + m_B K_1(\gamma) + q K_2(\gamma) + r K_3(\gamma)\}^z f(x)|_{x=0}, \tag{3}$$

$$\langle \xi_j^B \langle (s_j^B)^k \rangle \rangle_c = p_B \{1 + p_A [\cosh(\gamma/2) - 1] + 2m_A \sinh(\gamma/2)\}^z F_k(x)|_{x=0} \quad (k = 1, 2, 3), \tag{4}$$

where $p_\alpha = \langle \xi_i^\alpha \rangle_c$ is the concentration of magnetic α atoms ($\alpha = A$ or B), z is the coordination number and

$$K_0(\gamma) = \frac{1}{8} [9 \cosh(\gamma/2) - \cosh(3\gamma/2)], \quad K_1(\gamma) = \frac{1}{12} [27 \sinh(\gamma/2) - \sinh(3\gamma/2)],$$

$$K_2(\gamma) = \frac{1}{2} [\cosh(3\gamma/2) - \cosh(\gamma/2)], \quad K_3(\gamma) = \frac{1}{3} [\sinh(3\gamma/2) - 3\sinh(\gamma/2)],$$

with $\gamma = J\nabla$ and $\nabla = \partial/\partial x$ is the differential operator. The functions $f(x)$ and $F_k(x)$ are given by

$$f(x) = \frac{1}{2} \tanh(\beta x/2), \quad F_1(x) = \frac{1}{2} \frac{3 \sinh(3\beta x/2) + \exp(-2D\beta) \sinh(\beta x/2)}{\cosh(3\beta x/2) + \exp(-2D\beta) \cosh(\beta x/2)},$$

$$F_2(x) = \frac{1}{4} \frac{9 \cosh(3\beta x/2) + \exp(-2D\beta) \cosh(\beta x/2)}{\cosh(3\beta x/2) + \exp(-2D\beta) \cosh(\beta x/2)}, \quad F_3(x) = \frac{1}{8} \frac{27 \sinh(3\beta x/2) + \exp(-2D\beta) \sinh(\beta x/2)}{\cosh(3\beta x/2) + \exp(-2D\beta) \cosh(\beta x/2)},$$

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

$$M = \frac{1}{2} (m_A + m_B). \quad (5)$$

The second-order line is then given by substituting equations (4) in (3) 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 $m_B = -m_A$ in the coupled equations (3) and (4).

3. RESULTS AND DISCUSSIONS

Figure 1 a) shows some typical phase diagrams in the (T, p_B) plane for the ferrimagnet with $z = 3$ and $p_A = 1$, when the value of $D/|J|$ is changed. The solid and dashed lines represent the variations of the compensation temperature T_k and transition temperature T_c , respectively. The results clearly show that the compensation point at $T \neq 0K$ may exist in the system with $p_A = 1$ and $p_B < 1$ for an appropriate negative D value. Notice that the curve labelled $D/|J| = -0.4$ exhibits even two compensation points, although this is not sufficiently extensive to be seen on the scale of figure 1 a). The appearance of the compensation point (or points) in this system comes from both the dilution of the sublattice B and the negative crystal field interaction. Indeed, the corresponding system in the absence of dilution ($p_A = p_B = 1$) [4] or with $D = 0$ [2] does not exhibit any compensation point at $T \neq 0K$.

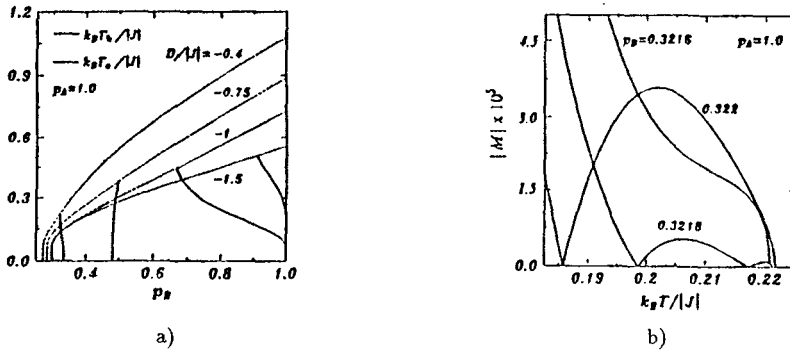


Figure 1: a) Transition temperature T_c (dashed lines) and compensation temperature T_k (solid lines) versus the concentration of agnetic atoms (p_B) in the sublattice B for the system with $z = 3$ and $p_A = 1$, when the value of $D/|J|$ is changed. b) $M - T$ curves for the system with $p_A = 1$ and $D/|J| = -0.4$, when p_B is changed.

In order to confirm the prediction of two compensation points, let us examine the total magnetization $|M|$ as a function T especially for the system with $p_A = 1$ and $D/|J| = -0.4$, when the value of p_B is changed. As seen from figure 1 b), the $M - T$ curve labelled $p_B = 0.322$ shows only one compensation point, however, the curve with $p_B = 0.3218$ exhibits two compensation points. We hope that the results obtained in this work may be helpful when the experimental data of ferrimagnetic materials are analysed.

References

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