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Random single-ion anisotropy in an Ising bilayer film with non-magnetic inter-layers

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ABSTRACT

The magnetic properties (phase diagrams and magnetizations) of an Ising bilayer film with non-magnetic inter-layers are investigated by the use of the effective field theory with correlations. The system is consisted of two magnetic layers where upper and lower layers are respectively consisted from spin-1/2 atoms and spin-1 atoms with a single-ion anisotropy D_i. The value of D_i is randomly distributed by a bimodal distribution function. The possibility of multi-compensation points and the reentrant phenomena are obtained.

1. Introduction

In the previous works [1–3], we have investigated the magnetic properties (phase diagram and magnetizations) of various bilayer Ising films on graphene-like honeycomb lattice with nonmagnetic inter-layers. The aim of this work is, by the use of the same formulation as that in the previous works, to investigate the effects of random single-ion anisotropy on the magnetic properties in the same system as that of [3], which is consisted of spin-1/2 upper layer and spin-1 lower layer with a single-ion anisotropy D_i at each site. In this work, however, the single-ion anisotropy D_i is randomly distributed according to the bimodal distribution function, instead of $D_i = D$ (constant value) in the previous work.

The spin-1 Ising model with a single-ion anisotropy and its variants have been used to simulate many physical systems, in order to clarify the first-order phase transition in various magnetic systems. The model is often called as the Blume-Capel (BC) model. The spin-1 Ising model with a random single-ion anisotropy and its variants have also been examined for long time by using a variety of theoretical techniques. In these systems, there exists a tricritical point at which the second-order phase transition may change to the first-order phase transition, when the value of single-ion anisotropy takes a large negative value. In general, the value (- D_T and $D_T > 0.0$) of tricritical point in the BC model is given by $D_T/z\ J = 0.47$, where z is the coordination number and J is the nearest-neighbor exchange interaction ($J > 0.0$) in the system. As discussed in the previous work [3], we have shown that the bilayer Ising film with nonmagnetic inter-layers exhibit the tricritical point, when the exchange interaction in the spin-1 (lower) layer is larger than that in the spin-1/2 (upper) layer. As far as we know, what phenomena are obtained in the bilayer Ising film with non-magnetic interlayers has not been investigated theoretically, when the value of D_i is randomly distributed by a bimodal distribution function. For recent development of theoretical research in a variety of systems with a random single-ion anisotropy, one can consult the references in [4].

In Section 2, the model and formulation are briefly given within the theoretical framework of the effective-field theory with correlations (EFT). In section 3, the phase diagrams are obtained and discussed. In section 4, the temperature dependences of magnetizations are obtained. The possibility of multi-compensation points and the reentrant phenomena have been obtained. The last section is devoted to conclusion.

2. Model and formulation

We consider the system consisting of two graphene-like honeycomb lattices with n non-magnetic inter-layers, as depicted in Fig. 1. The white and black circles represent respectively the magnetic atoms with spin-1/2 and the magnetic atoms with spin-1 and a crystal field D_i. The spins (white and black circles) are coupled by the nearest-neighbor exchange interactions J_A and J_B ($J_A > 0.0$ and $J_B > 0.0$). In Fig. 1, each Ising spin on upper layer is coupled to the corresponding spin on the lower layer with an indirect exchange interaction – J_R ($J_R > 0.0$). The Hamiltonian of Fig. 1 is given by

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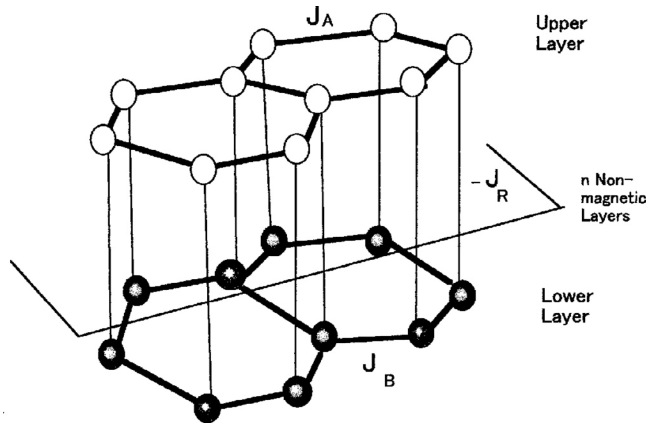

Fig. 1. Schematic representation of a bilayer Ising film on graphene-like honeycomb lattices, which are consisted of spin-1/2 (white circle) and spin-1 (black circle) atoms with a randomly distributed single-ion anisotropy. They are coupled by the nearest-neighbor exchange interactions J_A (in the upper layer) and J_B (in the lower layer). There exist n non-magnetic layers between the two layers. Each Ising spin on upper layer is coupled to the corresponding spin on the lower layer with an indirect exchange interaction $-J_R$ ($J_R > 0.0$).

$$H = -J_A\sum_{(ij)}\sigma_i^Z\sigma_j^Z - J_B\sum_{(mn)}S_m^Z S_n^Z + J_R\sum_{(im)}\sigma_i^Z S_m^Z - \sum_{(m)} D_m\left(S_m^Z\right)^2, \tag{1}$$

where σ_i^Z represents the spin-1/2 operator with $\sigma_i^Z = \pm 1/2$ and S_J^Z is the spin-1 operator with $S_m^Z = \pm 1$ and 0. The first and the second terms in (1) represent the contributions from the intra-layer interactions. The indirect exchange interaction J_R is given by

$$J_R/J = \exp(-\lambda(n+1))/(n+1)^{\delta}, \tag{2}$$

when the non-magnetic layers between the two layers are arranged by the equal distance a. J is the direct exchange interaction between two magnetic layers, when they are coupled directly. The crystal field D_m is randomly distributed according to the bimodal distribution function $P(D_m)$, namely

$$P(D_m) = [\delta(D_m - D(1.0+h)) + \delta(D_m - D(1.0-h))]/2.0 \tag{3}$$

In general, the parameter δ in (2) depends on the dimensionality of the system. From recent discussions on magnetic graphene systems, it is assumed that the value of δ is larger than the value of dimensionality of the system. The magnetic properties in graphene systems have been often discussed by the use of the indirect exchange interaction in which the distance-dependent oscillation can be neglected [1–3]. In the following discussions, accordingly, let us take the value of δ as $\delta = 3.0$. In (2), furthermore, we have assumed the following facts; When n = 0.0, it represents the fact that the two magnetic layers are coupled by the direct exchange interaction $-J$. Otherwise, it represents the indirect exchange interaction between the two layers. From this procedure, we can compare the differences of results between n = 0.0 and $n \neq 0.0$ cases systematically, as discussed in [1–3].

The total magnetization ($m_T = m_T^Z$) per site in the system is defined as

$$m_T = [m_A + m_B]/2.0, \tag{4}$$

where $m_A = m_A^Z = \langle\sigma_i^Z\rangle$ and $m_B = m_B^Z = \langle\langle S_m^Z\rangle\rangle_r$. $\langle A\rangle_r$ expresses the random average of D_m. Within the EFT [5,6], the m_A and m_B in the system are given by

$$m_A = [\cos h(A/2.0) + 2.0\, m_A \sin h(A/2.0)]^3 \quad [q_B\{\cos h(R) - 1.0\} + 1.0 - m_B \sin h(R)] f(x)|_{x=0} \tag{5}$$

and

$$m_B = [q_B\{\cos h(B) - 1.0\} + 1.0 + m_B \sin h(B)]^3 \quad [\cos h(R/2.0) - 2.0\, m_A \sin h(R/2.0)] F(x)|_{x=0} \tag{6}$$

$$q_B = [q_B\cos h(B) - 1.0 + 1.0 + m_B \sin h(B)]^3 \quad [\cos h(R/2.0) - 2.0 m_A \sin h(R/2.0)] G(x)|_{x=0} \tag{7}$$

where $q_B = \langle\langle(S_m^Z)^2\rangle\rangle_r$, A = J_A O, B = J_B O and R = J_R O. O = $\partial/\partial x$ is the differential operator. Here, the functions f (x), F(x) and G (x) are defined by

$$f(x) = \tan h(\beta x/2.0)/2.0 \tag{8}$$

$$F(x) = \sin h(\beta x)/[2.0\cos h(\beta x) + \exp(-D\beta(1.0+h))] + \sin h(\beta x)/[2.0\cos h(\beta x) + \exp(-D\beta(1.0-h))] \tag{9}$$

$$G(x) = \cos h(\beta x)/[2.0\cos h(\beta x) + \exp(-D\beta(1.0+h))] + \cos h(\beta x)/[2.0\cos h(\beta x) + \exp(-D\beta(1.0-h))], \tag{10}$$

where $\beta = 1.0/k_BT$. The transition temperature T_C of the system can be obtained from the relation

$$[6.0K_1 - 1.0][3.0K_2 - 1.0] - 2.0K_3K_4 = 0.0, \tag{11}$$

where the coefficients K_n (n = 1–4) are given by

$$\begin{aligned} K_1 &= \sin h(A/2.0)\cos h^2(A/2.0)[q_B\{\cos h(R) - 1.0\} + 1.0]^2 f(x)|_{x=0} \\ K_2 &= \sin h(B)\cos h(R/2.0)[q_B\{\cos h(B) - 1.0\} + 1.0]^2 F(x)|_{x=0} \\ K_3 &= \cos h^3(A/2.0)\sin h(R) F(x)|_{x=0} \\ K_4 &= \sin h(R/2.0)[q_B\{\cos h(B) - 1.0\} + 1.0]^3 F(x)|_{x=0} \end{aligned} \tag{12}$$

The value of q_B in (12) can be given by solving the following equation

$$q_B = \cos h(R/2.0)[q_B\{\cos h(B) - 1.0\} + 1.0]^3 G(x)|_{x=0}. \tag{13}$$

In the following sections, the magnetic properties of the system are examined by solving the relations given in this section numerically. For the aim, let us here introduce the reduced parameters, t, a, b, r and d as

$$\begin{aligned} t &= k_BT/J, \\ a &= J_A/J, \\ b &= J_B/J, \\ r &= J_R/J \text{ and} \\ d &= D/J \end{aligned} \tag{14}$$

Before doing the numerical works, one should notice the following facts; When the value of h in (9) and (10) is given by h = 0.0, the present formulation given in this section is completely equivalent to those in the previous work [3]. Accordingly, we can use the numerical results obtained in the work as the starting and guide points. Furthermore, when h = 1.0, it represents the following physical result; With the probability of p = 1/2, the dilution of the single-ion anisotropy is done.

3. Phase diagrams

Selecting the system with a = 1.0 and b = 0.5, just like the results of Fig. 2 in [3], let us examine the phase diagrams ($t_C = k_BT_C/J$ versus d plot) of the present system. In Fig. 2(A), the effects of h on the T_C value are given by taking the values of n = 1.0 and $\lambda = 0.0$, where the dashed curve labeled h = 0.0 is equivalent to the corresponding one in Fig. 2(A) of [3]. When the value of h is larger than h = 1.0, the t_C curve (the curve labeled h = 3.5 or h = 5.0) shows a