Vol 15 No 6, June 2006
1009-1963/2006/15(06)/1346-05

Chinese Physics

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Magnetic properties of a three layer superlattice with a crystal field*

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(Received 25 January 2006; revised manuscript received 13 February 2006)

In this paper the magnetic properties of a three layer superlattice with the crystal field on the honeycomb and square lattice have been studied based on the effective-field theory with self-spin correlations and the differential operator technique. The effects of the crystal field and longitudinal magnetic field on the susceptibility are discussed in detail. A number of interesting phenomena, originating from the competition between the longitudinal magnetic field, crystal-field, and coordination number, have been found.

Keywords: three-layer superlattice, longitudinal magnetic field, magnetic properties
PACC: 7510H

1. Introduction

Because of the syntheses of many new magnetic materials, such as the thin-film magnet, the molecular-based magnet and superlattice magnet, the emphasis has been laid on the theoretical study of the layered Ising model.[1−4] Layered composite materials have become of great interest, since the physical properties of these composite materials may be different from those of the corresponding bulk systems. The effect-field theory (EFT) concerning the correlations between spins is a more advanced method in dealing with the Ising model than the mean-field theory method. The EFT method has been applied to the investigation of interesting physical systems, such as surface magnetism,[5] thin films,[6] superlattices[7] and molecular magnetism.[8] The nonlinear magnetization dynamics of the classical ferromagnet with biaxial anisotropies in an external magnetic field and magnetization dynamics in thin films with stripe structures induced by spin-polarized current have been investigated.[9,10] Experimentally, a three layer superlattice has been widely studied owning to the advancements of experimental techniques making well-characterized samples possible. [11,12] However, less attention has been devoted theoretically to the three layer superlattice spin system with the crystal field in a longitudinal field, owing to mathematical complexities. In this paper, the three layer superlattice system consists of three magnetic bilayer (AA, BB and CC) with different spins ($S_A = S_C$=1/2 and S_B=3/2) in presence of the crystal field of the bilayer BB. The Hamiltonian of the three layer superlattice is described by

$$\begin{aligned} H = & - J_{a(c)} \sum_{i,j} \sigma^z_{i(k)} \sigma^z_{j(l)} - J_b \sum_{mn} S^z_m S^z_n \\ & - \sum_{jn} J_{ij} \sigma^z_j S^z_n - D \sum_m (S^z_m)^2 \\ & - h \sum_i \sigma^z_i - h \sum_m S^z_m, \end{aligned} \tag{1}$$

where σ^z_i, σ^z_k and S^z_m are the components of spin-1/2 and spin-3/2 operator in AA, CC and BB bilayer respectively. The first three sums are carried out only over nearest-neighbour pairs. J_a, J_b and J_c are the exchange interaction constant between two nearest-neighbour magnetic atoms in the bilayer AA, BB and CC respectively. J_{ij} is J_{ab}, J_{bc} and J_{ac} between the A and B,B and C, A and C respectively. In order to relate the system to some experimental data for RE/TM (rare-earth/transit metal) multilayer systems, we presume that AA and CC bilayers consist of TM atoms

*Project supported by the Natural Science Foundation of Liaoning Province (Grant No 20041021) and the Scientific Research Foundation of the Educational Department of Liaoning Province (Grant No 2004C006).

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and BB bilayer are made of RE atoms. J_{ab} (J_{bc}) (or 3d-4f indirect interaction) is taken to be positive for light RE or negative for heavy RE. D is the crystal-field in the bilayer BB. h represents the external longitudinal magnetic field.

This paper is organized as follows. We shall study the magnetic properties of the three layer superlattice with crystal-field systems in a longitudinal magnetic field. The formulation is based on the EFT with the differential operator technique. In Section 2, we shall introduce briefly the basic framework of the EFT theory with correlations and give the formulation for the systems. In Section 3, numerical results for the susceptibility will be presented in detail. Finally, we shall give the summary in Section 4.

2. Formulation

We can investigate the magnetization for the present system with a coordination number z. We will study the honeycomb (z=3) and square (z=4) lattices. For obtaining the detailed expression of each layer magnetization, according to the EFT and using the differential operator technique, we can get the each layer magnetization as

$$M_i = \langle \sigma_i^z \rangle = \langle \exp(E_i \nabla) \rangle F_i(x) \,|_{x=0} \,, \tag{2}$$

$$M_j = \langle S_m^z \rangle = \langle \exp(E_j \nabla) \rangle F_j(x) \,|_{x=0} \,, \tag{3}$$

$$\eta_j^2 = \langle (S_m^z)^2 \rangle = \langle \exp(E_j \nabla) \rangle G_j(x) \,|_{\mathrm{x=0}} \,. \tag{4}$$

where $\nabla = \partial / \partial x$ is differential operator, $E_{i(j)}$ (i=1, 2, 5, 6 and j=3, 4) is the effective field, and the functions $F_{i(j)}(x)$ and $G_j(x)$ are expressed as

$$F_i(x) = \frac{1}{2} \tanh \left[\frac{1}{2} \beta (x+h) \right], \tag{5}$$

$$F_j(x) = \frac{3 \sinh \left[\frac{3}{2} \beta (x+h) \right] + \exp(-2D\beta) \sinh \left[\frac{1}{2} \beta (x+h) \right]}{2 \cosh \left[\frac{3}{2} \beta (x+h) \right] + 2 \exp(-2D\beta) \cosh \left[\frac{1}{2} \beta (x+h) \right]}, \tag{6}$$

$$G_j(x) = \frac{9 \cosh \left[\frac{3}{2} \beta (x+h) \right] + \exp(-2D\beta) \cosh \left[\frac{1}{2} \beta (x+h) \right]}{4 \cosh \left[\frac{3}{2} \beta (x+h) \right] + 4 \exp(-2D\beta) \cosh \left[\frac{1}{2} \beta (x+h) \right]}, \tag{7}$$

where, $\beta = 1/k_{\mathrm{B}}T$, k_{B} is the Boltzmann constant and T is the absolute temperature.

In order to treat Eqs.(2)–(4) further, we can use the van der Waerden identity and the decoupling approximation[13]

$$\exp(aS) = \cosh(\eta a) + \frac{S}{\eta} \sinh(\eta a), \tag{8}$$

$$\langle S_i (S_j)^2 \ldots S_n \rangle = \langle S_i \rangle \langle (S_j)^2 \rangle \ldots \langle S_n \rangle. \tag{9}$$

Using Eqs.(8) and (9), we can get the magnetization for each layer as follows

$$\begin{aligned} M_1 =& \left[\cosh \left(\frac{1}{2} J_a \nabla \right) + 2M_1 \sinh \left(\frac{1}{2} J_a \nabla \right) \right]^z \\ & \times \left[\cosh \left(\frac{1}{2} J_a \nabla \right) + 2M_2 \sinh \left(\frac{1}{2} J_a \nabla \right) \right] \times \left[\cosh \left(\frac{1}{2} J_{ac} \nabla \right) + 2M_6 \sinh \left(\frac{1}{2} J_{ac} \nabla \right) \right] F_1(x)|_{x=0}, \end{aligned} \tag{10}$$

$$\begin{aligned} M_2 =& \left[\cosh \left(\frac{1}{2} J_a \nabla \right) + 2M_2 \sinh \left(\frac{1}{2} J_a \nabla \right) \right]^z \\ & \times \left[\cosh(J_{ab} \eta_3 \nabla) + \frac{M_3}{\eta_3} \sinh(J_{ab} \eta_3 \nabla) \right] \times \left[\cosh \left(\frac{1}{2} J_a \nabla \right) + 2M_1 \sinh \left(\frac{1}{2} J_a \nabla \right) \right] F_2(x)|_{x=0}, \end{aligned} \tag{11}$$

$$\begin{aligned} M_3 =& [\cosh(J_b \eta_3 \nabla) + \frac{M_3}{\eta_3} \sinh(J_b \eta_3 \nabla)]^z \\ & \times \left[\cosh(J_b \eta_4 \nabla) + \frac{M_4}{\eta_4} \sinh(J_b \eta_4 \nabla) \right] \times \left[\cosh \left(\frac{1}{2} J_{ab} \nabla \right) + 2M_2 \sinh \left(\frac{1}{2} J_{ab} \nabla \right) \right] F_3(x)|_{x=0}, \end{aligned} \tag{12}$$

$$M_4 = \left[\cosh(J_b\eta_4\nabla) + \frac{M_4}{\eta_4}\sinh(J_b\eta_4\nabla)\right]^z \times \left[\cosh(J_b\eta_3\nabla) + \frac{M_3}{\eta_3}\sinh(J_b\eta_3\nabla)\right] \times \left[\cosh\left(\frac{1}{2}J_{bc}\nabla\right) + 2M_5\sinh\left(\frac{1}{2}J_{bc}\nabla\right)\right] F_4(x)|_{x=0}, \quad (13)$$

$$M_5 = \left[\cosh\left(\frac{1}{2}J_c\nabla\right) + 2M_5\sinh\left(\frac{1}{2}J_c\nabla\right)\right]^z \times \left[\cosh(J_{bc}\eta_4\nabla) + \frac{M_4}{\eta_4}\sinh(J_{bc}\eta_4\nabla)\right] \times \left[\cosh\left(\frac{1}{2}J_c\nabla\right) + 2M_6\sinh\left(\frac{1}{2}J_c\nabla\right)\right] F_5(x)|_{x=0}, \quad (14)$$

$$M_6 = \left[\cosh\left(\frac{1}{2}J_c\nabla\right) + 2M_6\sinh\left(\frac{1}{2}J_c\nabla\right)\right]^z \times \left[\cosh\left(\frac{1}{2}J_{ac}\nabla\right) + 2M_1\sinh\left(\frac{1}{2}J_{ac}\nabla\right)\right] \times \left[\cosh\left(\frac{1}{2}J_c\nabla\right) + 2M_5\sinh\left(\frac{1}{2}J_c\nabla\right)\right] F_6(x)|_{x=0}. \quad (15)$$

Applying the mathematical relation $e^{\alpha\nabla} f(x) = f(x+\alpha)$, we can expand the right-hand side of Eqs.(10)–(15) and solve the above coupled equations by numerical calculation. The average total magnetization per site is given by

$$M = (M_1 + M_2 + M_3 + M_4 + M_5 + M_6)/6. \quad (16)$$

The longitudinal susceptibility for the system can be determined from the relation

$$\chi = \partial M/\partial h. \quad (17)$$

3. Numerical results and discussions

In this section, at first we shall study magnetization of a three layer superlattice with a single-ion anisotropy on the honeycomb (z=3) and square (z=4) lattice by solving the coupled equations given in Section 2 numerically. In the figures of this paper, the exchange interaction constant are fixed as $J_a = J_b$=1.0, J_c=0.8, $J_{ab} = J_{bc}$=–0.5, J_{ac}=0.5 respectively. The magnetizations are functions of temperature, exchange interaction, crystal field and longitudinal magnetic field and depend on the value of temperature, longitudinal magnetic field and coordination number. The numerical results are plotted in Fig.1(a) for the case of the honeycomb lattice and Fig.1(b) for the case of the square lattice without applying the longitudinal magnetic field. The solid and dashed lines are the case of the crystal field $D/J_a = -1.2$ and $D/J_a = -3.5$ respectively. The curves a, b, c, d are plotted for the average magnetization of bilayer sublattice AA $((M_1 + M_2)/2)$, BB $((M_3 + M_4)/2)$, CC $((M_5 + M_6)/2)$ and the total average M respectively.

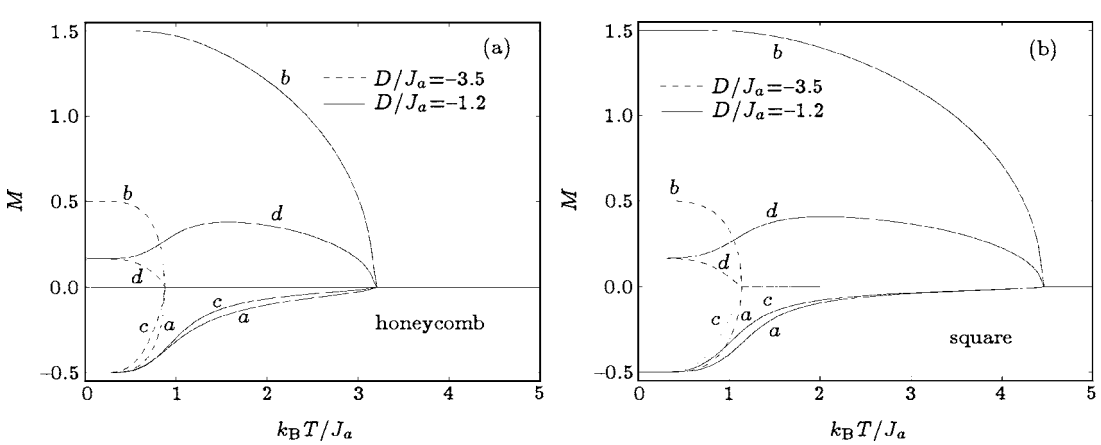


Fig.1. The temperature dependence of magnetization for the three layer superlattice when the crystal fields are selected as $D/J_a = -1.2$ (solid lines) and $D/J_a = -3.5$ (dashed lines). The curves a, b, c, d for the average magnetization of bilayer sublattice AA $((M_1 + M_2)/2)$, BB $((M_3 + M_4)/2)$, CC $((M_5 + M_6)/2)$ and the total average M respectively. (a) For the case of the honeycomb lattice. (b) For the case of the square lattice.

From the figures, we can see that the absolute value of bilayer CC average magnetization (c curves) is smaller than that of AA (a curves), which results in the case that the exchange interaction constant J_a=1.0 is bigger than J_c=0.8. When the crystal field changes from D/J_a=–1.2 to D/J_a=–3.5, the saturation magnetization at T=0K of bilayer sublattice BB changes from 3/2 to 1/2. This result is in agreement with that of Ref.[14]. The saturation magnetization at T=0K may change from 3/2 to 1/2 when the critical value of D is given $D/J_a = -z/2$ for the case of the honeycomb lattice $D/J_a = -1.5$ and square lattice $D/J_a = -2$. Comparing with Figs.1(a) and 1(b), one can find that the phase temperature of the honeycomb lattice is smaller than that of the square lattice.

In Figs.2(a), 2(b) and Figs.3(a), 3(b), we plot the numerical results of the susceptibility of a three layer superlattice with a single-ion anisotropy on the honeycomb (z=3) and square (z=4) lattice respectively, with and without the longitudinal magnetic field. It can be seen that the curves of susceptibility rapidly increase and express the peak at the transition temperature and then rapidly decrease with the increase of temperature. The peak of susceptibility is increasing with the decrease of the longitudinal magnetic field. From Figs.2(a), 2(b), it is clearly seen that the transition temperature at which the curve appears maximum for the case of the honeycomb lattice is lower than that of the square lattice. In Figs.3(a) and 3(b), one can find that there exist two peaks, which means that the first peak results from the spin-1/2 of bilayer sublattice AA and CC and the second peak results from the spin-3/2 of bilayer sublattice BB. Comparing with Figs.3(a) and 3(b), we find that the temperature at which the susceptibility shows the peak for the honeycomb lattice is also lower than that of the square lattice.

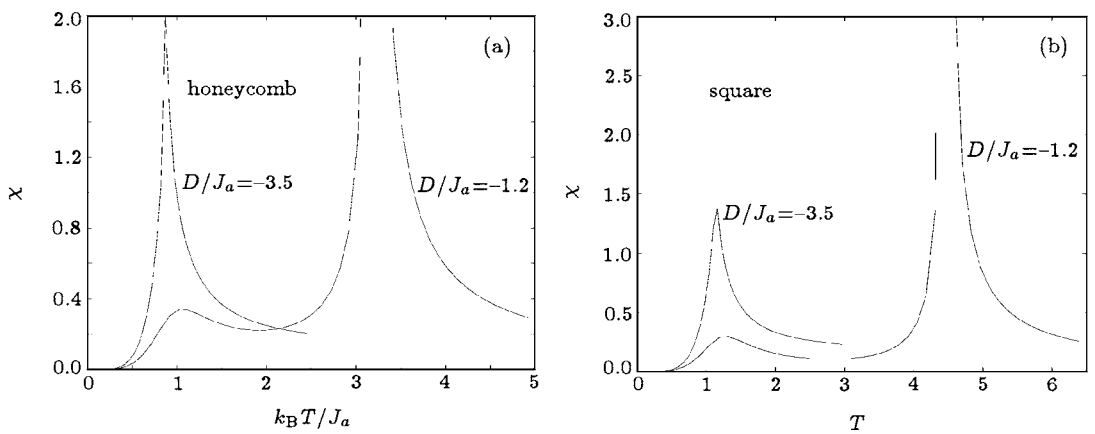


Fig.2. The temperature dependence of susceptibility for the three layer superlattice without applying the longitudinal magnetic field, when the crystal field are selected as $D/J_a = -1.2$ and –3.5, respectively. (a) For the case of the honeycomb lattice. (b) For the case of the square lattice.

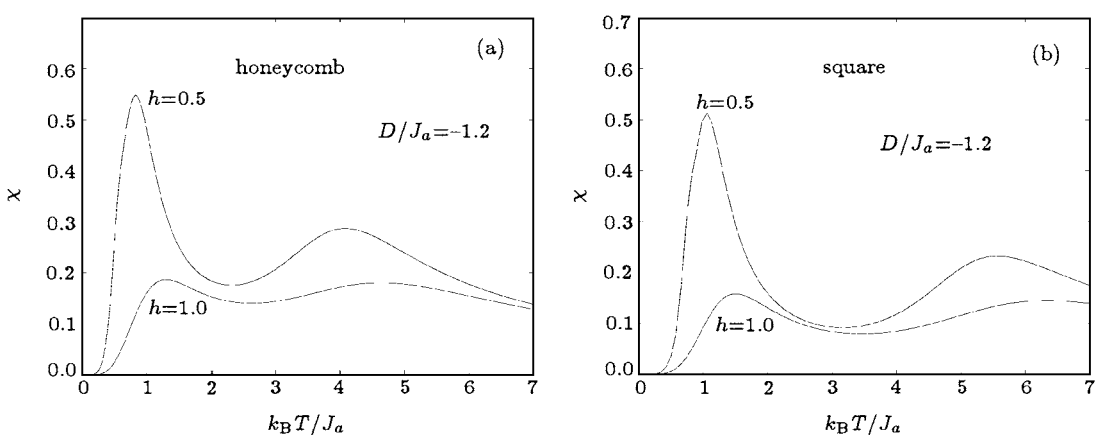


Fig.3. The temperature dependence of susceptibility for the three layer superlattice, when the crystal field is selected as $D/J_a = -1.2$. The numbers represent the values of the longitudinal magnetic field h=0.5 and h=1 respectively. (a) For the case of the honeycomb lattice. (b) For the case of the square lattice.

4. Conclusion

Within the framework of EFT based on the differential technique, we have discussed in detail the influence with and without the longitudinal magnetic field on the susceptibilities for the honeycomb and square lattice. The crystal field plays an important role in magnetization. The peak of susceptibility is increasing with the decrease of the longitudinal magnetic field. The temperature at which the susceptibility shows the peak for the honeycomb lattice is lower than that of the square lattice.

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