VNU Journal of Science: Mathematics – Physics, Vol. 35, No. 1 (2019) 76-82

VNU Journal of Science: Mathematics - Physics

Journal homepage: https://js.vnu.edu.vn/MaP

Original Article

Effect of Next Nearest Neighbor Interaction on Thermodynamic Properties of Ultrathin Magnetic Films

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Received 15 January 2019
Revised 07 March 2019; Accepted 15 March 2019

Abstract: This work studies on the thermodynamic properties of the ultra-thin magnetic films within the framework of a transverse Ising model. Equations for free energy, entropy and specific heat of spin system are obtained by using the mean field approximation. We also analyze the effect of the next nearest neighbor interaction on critical temperature, layer magnetization and specific heat of the thin films.

Keywords: Magnetic ultra-thin films, transverse Ising model, next nearest neighbor interaction, critical temperature.

1. Introduction

Recently the ultra-thin magnetic films have been used more and more in memory and microwave devices. Many researches on the magnetic ultra-thin films have been carried out both experimentally and theoretically [1, 2]. The magnetic ultra-thin films have magnetic properties which are different from those of the bulk [3, 4]. Several models have been used to investigate the features of the films such as: Heisenberg model, transverse Ising model, XY model… Among them, the transverse Ising model (TIM) is often used because of its simplicity and usefulness. There are many works has applied TIM to investigate magnetic thin films within the framework of the mean field theory and effective field theory [4-7]. In a previous work [8], we investigated the dependence of the order-disorder phase transition temperature on the transversal field and obtained the explicit equation for this temperature. However, we only consider the nearest- neighbor (n.n) exchange interaction between spins in [8]. In the real magnetic ultra-thin films, the next nearest- neighbor (n.n.n) exchange interaction may affect strongly on

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https//doi.org/ 10.25073/2588-1124/vnumap.4314

properties of the films. Therefore, in this paper we use the transverse Ising model to calculate the thermodynamic properties of the ultra-thin magnetic film in which the n.n.n exchange interaction is taken into account. All calculations are carried out by using the mean field approximation.

2. Film model and formulation

We consider a transverse Ising magnetic thin film which has simple cubic symmetry composed of *n* spin layers. Each layer is defined on the *xOy* plane and contains *N* spins (see [8]). The *z*-direction is perpendicular to the film surface. The Hamiltonian of the system has the form:

$$H = -h\sum_{\nu j} S^z_{\nu j} - \Omega \sum_{\nu j} S^x_{\nu j} - \tfrac{1}{2}\sum_{\nu j,\nu' j'} J_{\nu\nu'}\left(\mathbf{R}_j - \mathbf{R}_{j'}\right) S^z_{\nu j} S^z_{\nu' j'} . \tag{1}$$

h and Ω represent the external longitudinal and transverse fields given in energy unit (effective dipole moment is included in the field h). $S^z_{\nu j}$ and $S^x_{\nu j}$ are the *z* and *x* components of a spin operator $\mathbf{S}_j$ at site *j* in the *Oxyz* coordinate; $J_{\nu\nu'}$ is the strength of the exchange interaction between spin at site j^{th} and j'^{th}, ν is the layer index (ν =1,2,...,n), $\mathbf{R}_j$ is the two-component vector denoting the position of j^{th} spin in this layer.

Following our previous work [8], when taking into account the n.n.n exchange interaction between spins, we obtain the expression for the free energy of the film in the mean field approximation:

$$F_0 = \frac{N}{2}\sum_{\nu\nu'}(J_s(0) + J_p(0))\langle S^z_\nu\rangle\langle S^z_{\nu'}\rangle - \frac{N}{\beta}\sum_\nu \ln\frac{sh(s+1/2)Y_\nu}{sh\frac{Y_\nu}{2}} \tag{2a}$$

$$Y_\nu = \beta\gamma_\nu \cdot \gamma_\nu = \sqrt{h_\nu^2 + \Omega^2}\ ;\ \beta^{-1} = k_B T \tag{2b}$$

where $J_s(0)$ is the exchange strength between in-plane spins and given by:

$$J_{11}(0) = J_{\nu\nu}(0) = J_{nn}(0) = J_s(0) = \sum_j J_s(\mathbf{R}_j)\ , \tag{2c}$$

$J_p(0)$ is the exchange strength between out-of-plane spinsand

$$J_{\nu,\nu-1}(0) = J_{\nu,\nu+1}(0) = J_p(0) = \sum_j J_p(\mathbf{R}_j) \tag{2d}$$

The critical temperature and the critical transversal field of the film can be obtained as:

$$\begin{vmatrix} a & c & 0 & 0 & \cdots & 0 & 0 \\ c & a & c & 0 & \cdots & 0 & 0 \\ 0 & c & a & c & \cdots & 0 & 0 \\ . & . & . & . & \cdots & . & . \\ 0 & 0 & 0 & 0 & \cdots & a & c \\ 0 & 0 & 0 & 0 & \cdots & c & a \end{vmatrix} = 0, \tag{3a}$$

where

$$a = 1 - \frac{b_s(\beta_c\Omega)}{\Omega} J_s(0) \text{ and } c = -\frac{b_s(\beta_c\Omega)}{\Omega} J_p(0) . \tag{3b}$$

$$b_s(x) = (s+\frac{1}{2})coth(s+\frac{1}{2})x - \frac{1}{2}coth\frac{x}{2}$$ is the Brillouin function. (3c)

The longitudinal and transversal magnetization of the films are given by:

$$m_{z\nu} = \frac{h_\nu}{\gamma_\nu} b_s(Y_\nu);\ m_{x\nu} = \frac{\Omega_\nu}{\gamma_\nu} b_s(Y_\nu) \tag{4}$$

Specific heat is derived from (2a) as:

$$C = \frac{1}{n}\sum_{\nu=1}^{n}\left(\frac{\gamma_\nu}{\theta}\right)^2 b_S'(Y_\nu)\left\{\frac{1-\frac{\Omega^2 b_S(Y_\nu)}{(\gamma_\nu)^3}\left(\sum_{\nu'=1}^{n}\left(J_s(0)+J_p(0)\right)\right)}{1-\left[\frac{\Omega^2 b_S(Y_\nu)}{(\gamma_\nu)^3}+\beta b_s'(Y_\nu)\frac{h_\nu^2}{\gamma_\nu^2}\right]\left(\sum_{\nu'=1}^{n}\left(J_s(0)+J_p(0)\right)\right)}\right\} \text{with } \theta = k_B T = \beta^{-1} \tag{5a}$$

and $b_S'(x) = \frac{1}{4sh^2\left(\frac{x}{2}\right)} - \frac{\left(s+\frac{1}{2}\right)^2}{sh^2\left[\left(s+\frac{1}{2}\right)\frac{x}{2}\right]}$ is the 1st derivative of Brillouin function. (5b)

From (5a) one sees that specific heat C tend to zero in the limit $T \to 0$.

3. Numerical result and discussion

In this section, we carry out the numerical calculations for the properties of the magnetic ultra-thin film. The numerical calculations for the cubic spin lattice is done when the n.n.n exchange is taken into account. We define following parameters:

$$\xi = \frac{J_s^{(2)}}{J_s^{(1)}},\ \eta_1 = \frac{J_p^{(1)}}{J_s^{(1)}},\ \eta_2 = \frac{J_p^{(2)}}{J_s^{(1)}} \tag{6}$$

$J_s^{(1)}$ ($J_p^{(1)}$) denote the exchange strength between in-plane (out-of-plane) n.n spins. $J_s^{(2)}$ ($J_p^{(2)}$) denote the exchange strength between in-plane (out-of-plane) n.n.n spins.

ξ is the strength of the competition between the surface interactions of the in-plane n.n spins and the in-plane n.n.n spin; η_2 is the parameter for the difference between the exchange interactions of the out - of plane n.n.n spins and the in-plane n.n spins. Ratio η_1 is the anisotropic parameter that shows the difference between the exchange interactions of the in-plane and out-of plane n.n spins. We suppose that the interactions of the n.n.n spins is smaller than the interactions of the n.n spins (that means $J_s^{(2)} < J_s^{(1)}, J_p^{(1)}$ and $J_p^{(2)} < J_s^{(1)}, J_p^{(1)}$).

Firstly, we consider the results which are depicted in Fig.1 where the critical temperature is plotted as a function of η_2 and ξ with different values of the transversal field. As shown in the figure, we can found that the critical temperature T_C increases with the increase of η_2 and ξ . For the film, we find that the transversal field has a limited value Ω_l. When Ω is smaller than Ω_l, the film can change from ferromagnetic phase into paramagnetic phase with all values of ξ and η_2, but when Ω is larger than Ω_l we can only observe the transition from ferromagnetic phase into paramagnetic phase with some values of ξ and η_2 .

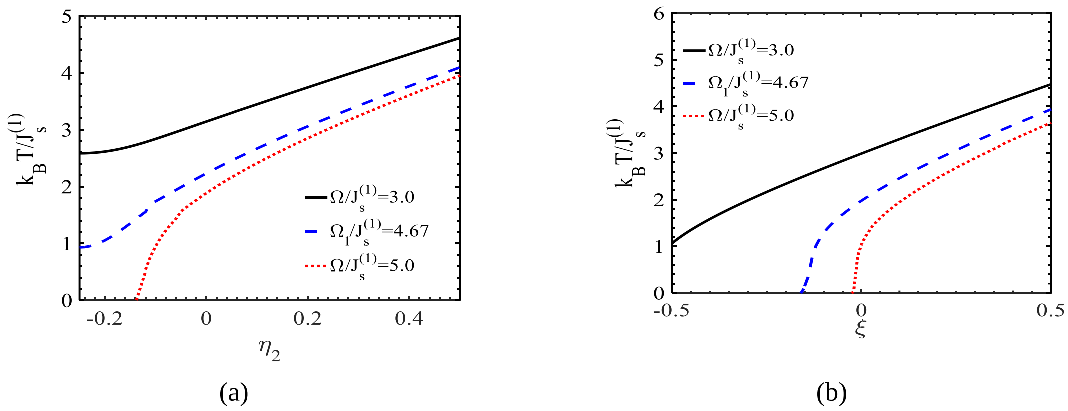


Fig 1. The dependence of the critical temperature of 3-layer film on the strength of the competition between the interactions of the n.n spins and the then.n.n spins out-of plane $\eta_2 = J_p^{(2)} / J_s^{(1)}$ (a) and in-plane $\xi = J_s^{(2)} / J_s^{(1)}$ (b) with various transversal fields.Here $\eta_1 = J_p^{(1)} / J_s^{(1)} = 0.5$ and s=1.

Fig. 2 shows the effect of n.n.n exchange interaction on the critical temperature. The dotted line is plotted with $\eta_2 = 0.05$.The dashed line is plotted with $\eta_2 = -0.1$. It is obvious that there is a great difference of the critical of the films when n.n.n exchange interaction is taken account.

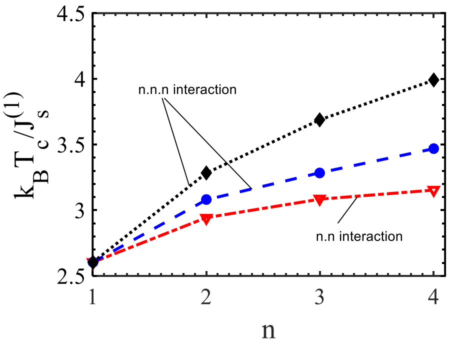


Fig. 2. The effect of then.n.n exchange interaction on Tc for differenent thickness of the film. Here $\Omega = 1.0$, $\eta_1 = 0.5$, $\xi = 0.1$, s=1.

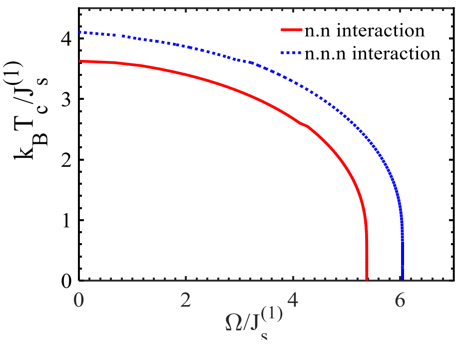


Fig. 3. The effect of then.n.n exchange interaction on the phase diagram of 4-layer film. Here $\eta_1 = 0.5$, $\eta_2 = 0.05$, $\xi = 0.1$, s=1.

Comparing between dash dotted line with dotted linein Fig.2, we see that the critical temperature of the films with the n.n.n interaction increases more rapidly than that with the n.n interaction. Besides, if $\eta_2 < 0$, we also see that the critical temperature of the film with n.n.n interaction is much smaller than that when $\eta_2 > 0$. It is obvious that strength of the n.n.n interaction affects quite strongly on the critical temperature T_C of the film. Fig.3 indicates the dependence of the phase diagram on the strength of the n.n.n exchange interaction of the films with 4 layers. Obviously, when taking into the n.n.n exchange interaction, the range of the ferromagnetic phase in the phase diagram is larger.

Next we investigate the nature of the magnetization components with the existence of the n.n.n exchange. For simplicity, in the numerical calculations we note that the film is symmetric. Fig.4a.

presents dependence on temperature of the magnetization components of the symmetric two layer film for a given transversal field. The existence of the n.n.n exchange leads to the extension of the longitudinal magnetization m_z but the reduction of transversal magnetization m_x. At a given temperature, the larger η_2 leads to the decrease of m_z more rapidly as shown in Fig.4b.

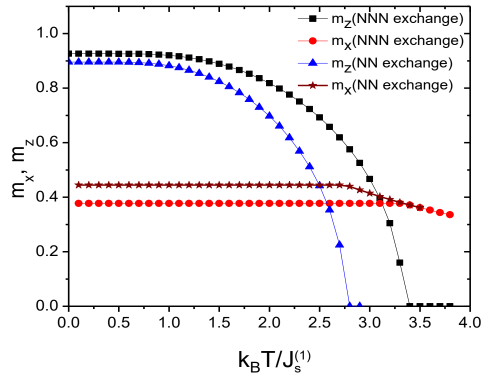


Fig. 4a. The thermal variation of the spin components for symmetric double layer thin film. Here ξ=0.1, s=1, $\eta_1 = 0.5$.

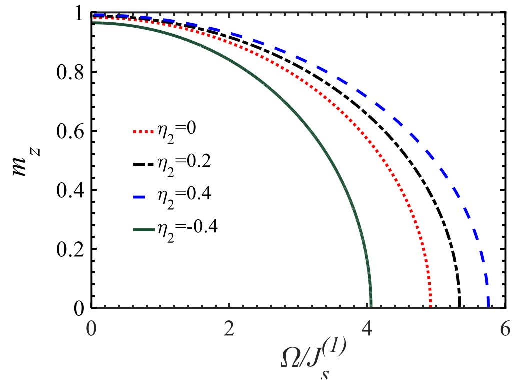
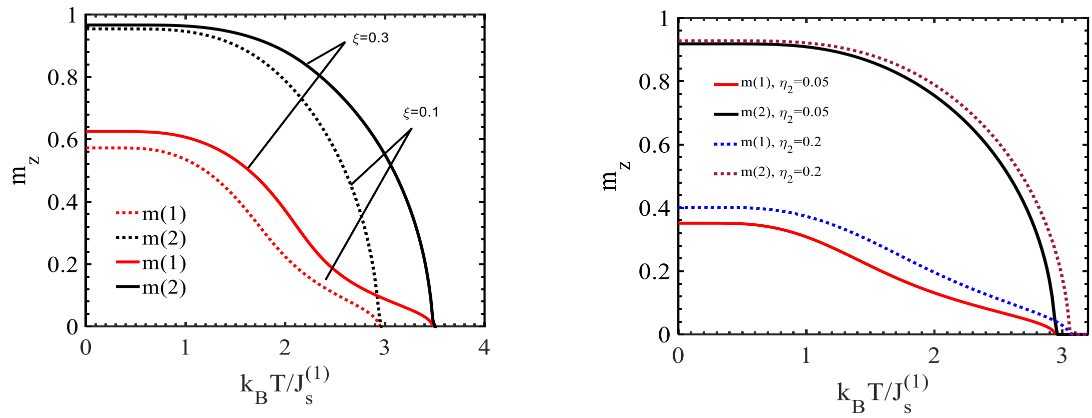


Fig. 4b. The dependence of the longitudinal spin of symmetric double layer thin film on the transversal field with different η_2 at given temperature $k_B T / J_s^{(1)} = 1.8$, ξ=0.1, s=1, $\eta_1 = 0.5$.

The influence of ξ and η_2 on the temperature dependence of the longitudinal magnetization and the specific heat of the symmetric three layer film is shown in Fig.5 and Fig.6. m(1), m(2) and m(3) are longitudinal magnetizations of the first layer (the surface), the second layer, and the third layer (the surface). Because the film is symmetric, m(1) is equal to m(3).



(a) (b)

Fig. 5. The thermal variation of the longitudinal magnetization of three-layer thin film with different values of ξ for $\eta_1 = 0.5,\ \eta_2 = 0.01$ (a) and different values of η_2 for $\eta_1 = 0.5,\ \xi = 0.1$ (b). Parameters is chosen: s=1; $\Omega / J_s^{(1)} = 1.5$

It can be seen from Fig. 5 and Fig. 6 that the layer magnetization and peak of the specific heat increase with the increase of the n.n.n exchange interaction. We find that the layer magnetizations are m(2) > m(1) for a fixed value of η_2 and ξ, namely the inner layer magnetization is larger than the surface magnetization. Fig.6 also reveals the effect of η_2 and ξ on the peak of the specific heat. The increase of ξ leads to the shift of the peak of the specific heat toward the higher temperature (Fig. 6a), while the increase of η_2 only leads to the increase of the value of the specific heat of the film (Fig. 6b).

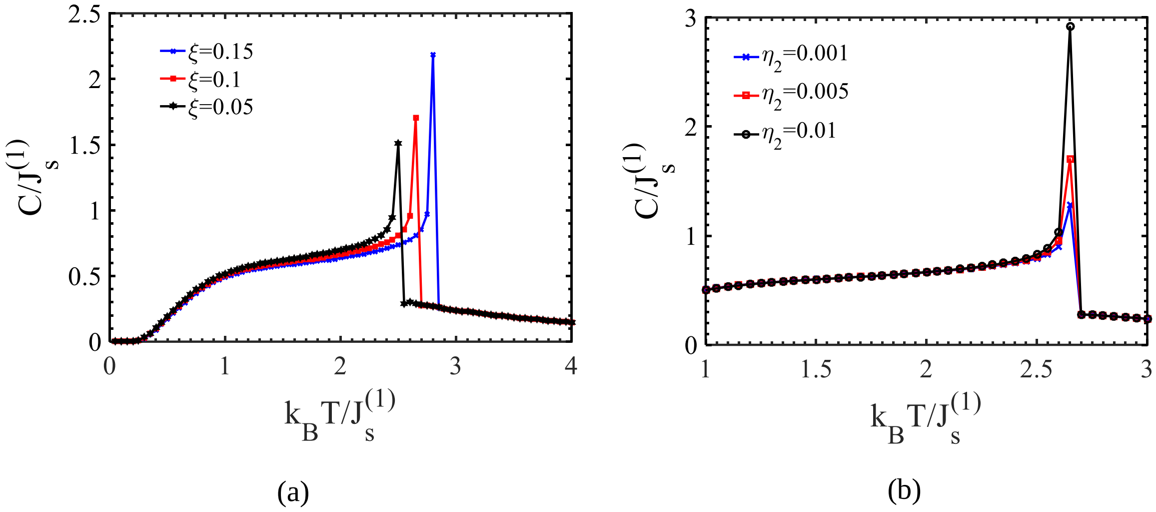


Fig. 6. The thermal variation of the specific heat of three-layer thin film with different values of ξ for $\eta_1 = 0.3,\ \eta_2 = 0.01$ (a) and different values of η_2 for $\eta_1 = 0.3,\ \xi = 0.1$ (b). All the curves are plotted with s=1; $\Omega / J_s^{(1)} = 2.0$.

4. Conclusion

In conclusion, we have considered features of the magnetic ultra-thin film with the n.n.n interaction. The contribution of the n.n.n interaction causes the increase of the critical temperature, the transversal field, the longitudinal magnetization and the specific heat. The numerical calculations imply that the n.n.n interaction has an influence quite clearly on the magnetic properties of the thin films.

Acknowledgements

This research is funded by the VNU University of Science under project number TN.17.04.

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