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Short communication

Critical behaviour of magnetic thin film with Heisenberg spin-S model

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ABSTRACT

The magnetic properties of a ferromagnetic thin film of face centered cubic (FCC) lattice with Heisenberg spin-S are examined using the high-temperature series expansions technique extrapolated with Padé approximations method. The critical reduced temperature of the system τ_c is studied as function of thickness of the film and the exchange interactions in the bulk, and within the surfaces J_b, J_s and $J_\perp$ respectively. A critical value of surface exchange interaction above which surface magnetism appears is obtained. The dependence of the reduced critical temperature on the film thickness L has been investigated.

1. Introduction

During the last decade, the magnetic properties of thin films have been extensively investigated experimentally and theoretically. Within the advance of modern vacuum sciences, and in particular epitaxial techniques, it is now possible to grow in very controlled way, magnetic films with few atomic layers or even monolayer atop nonmagnetic substrate. A number of theoretical works have been devoted to the magnetic and phase transition properties of magnetic film. Mean-field theories have been used, which are particularly simple to apply for complicated systems. Hu and Kawazoe [1] have treated the magnetic reorientation of the system and mean-field-like expressions for the magnetization density. Saber et al. [2] have examined the phase to phase transition of a diluted spin-1/2 Ising film using the effective field theory with a probability distribution technique that accounts for the single-site spin correlations. Lin et al. [3] have developed an analytical method based on the variational cumulant expansion to calculate the critical temperature of the Ising film as a function of the film thickness. Diep [4–6] has analyzed the dependence of the surface magnetisation and the critical temperature of ferromagnetic T_F with free surfaces, on the surface exchange integrals. Some authors have investigated the effects of quantum fluctuations on the layer magnetizations in the vicinity of the surface at an arbitrary temperature in bcc antiferromagnetic thin film (1 0 0) surfaces. The stochastic series expansion quantum Monte Carlo method is used to study thin ferromagnetic films, described by a Heisenberg model including local anisotropies [7]. They examined many interesting properties, of which we only mentioned the reorientation effect, in which the magnetization changes from out of plane to in plane. The magnetic phase transition in Heisenberg ferro-antiferromagnetic films with cubic lattices has been studied by high-temperature series expansions [8,9] and by application of a mean field approximation as well as by a many-body Green's function theory [10]. The effects of frustration in an antiferromagnetic film of FCC lattice with Heisenberg spin model including an Ising-like anisotropy [11] and the critical behaviour of magnetic thin films as a function of the film thickness [12] are study by the Monte Carlo (MC) simulations.

Stanley [13] has suggest a phase transition ($T_c \neq 0$) for some two-dimensional lattices with nearest-neighbor ferromagnetic interactions for the plane square and triangular lattices, using the high-temperature series expansions (HTSE) method and using a diagrammatic representation [14]. He argued that the magnetic order of many occurs at low-temperature state with

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zero spontaneous magnetization but with an infinite zero field susceptibility. In fact, the general expression of spin–spin correlation obtained by the HTSE semiclassical method [14] takes into accounts the influence of the others neighbour spins. Then, the spin–spin correlation becomes different from the bulk to the surfaces and lead to an anisotropic behaviour, which may be found in thermodynamic functions such as the magnetic susceptibility χ. The consideration of the some neighbouring spins in the calculation of the correlation functions in the HTSE method can be understood as long-range interaction, which depress the effect of quantum and thermal fluctuations, and contributes to the ordered phase in the system with low dimensionality [15].

The purpose of this work is to study critical magnetic properties of thin film using the HTSE method extrapolated with Padé approximants method (PA) [16]. The series expansions for the magnetic susceptibility have been derived to order six the reciprocal temperature including nearest-neighbour exchange couplings in the bulk and within the surfaces. The technique of HTSE extrapolated with PA method have been widely developed and applied to various magnetic systems [17]. This method is fundamental than usual molecular field approach as it partially takes into consideration spin–spin correlations.

2. Methods and model

The theoretical method used in this work has been developed in previous papers [14,18] here we give only a brief description of the essentials of the method. The starting point of the semiclassical HTSE technique is the expansion of the zero-field static correlation function, between spins at site i and j, in power of the $\beta(\beta = 1/_{K_BT})$

$$\langle \vec{S}_i\vec{S}_j\rangle = \frac{Tr\,\vec{S}_i\vec{S}_j e^{-\beta H}}{Tr\, e^{-\beta H}} = \sum_{l}^{\infty}\frac{(-1)^l}{l!}\alpha_l\beta^l \tag{1}$$

where Tr means the trace over spin configurations and K_B being the Boltzmann's constant. The Heisenberg Hamiltonian is given by $H = -2\sum_{ij}J_{ij}\vec{S}_i\cdot\vec{S}_j$, where J_{ij} is the exchange coupling between spin at site i and spin at site j, and $\vec{S}$ is the spin operator with the magnitude S.

The calculation of the coefficients α_l leads to a diagrammatic representation [18], which involves two separate stages:

(a) The finding and cataloguing of all diagrams or graphs which can be constructed from one dashed line connecting the site i and j, and l straight lines, and the determination of diagrams whose contribution is nonvanishing. This step has already been accomplished in the Stanley work.
(b) Counting the number of times that each diagram can occur in the magnetic system.

In our case, we have to deal with nearest-neighbour coupling J_{ij}. The coefficient α_l may be expressed for each topological graph as [17]

$$\alpha_l = \vec{S}^2(-2\vec{S}^2)^l(J^{m_1}_{ik_1}J^{m_2}_{k_2k_3}\ldots J^{m_v}_{k_wj})[\alpha_l] \tag{2}$$

with the condition $\sum_{r=1}^{v} m_r = l$ for $m_r = 0, 1, \ldots, l$. The "weight" $[\alpha_l]$ of each graph is tabulated and given in Ref. [14] and $k_1, k_2, \ldots, k_w$ represent the sites surrounding the sites i and j.

In this paper, we consider a ferromagnetic thin film of face centred cubic lattice composed of L layers. The free surfaces are considered to be parallel to (1 0 0) planes. The exchange coupling between spins at sites i and j takes the value J_s if both spins are nearest neighbours within the surface layers, $J_\perp$ if it is between a spin on the surface and its nearest neighbour in the next layer, and the value J_b, for nearest neighbour interactions within the bulk.

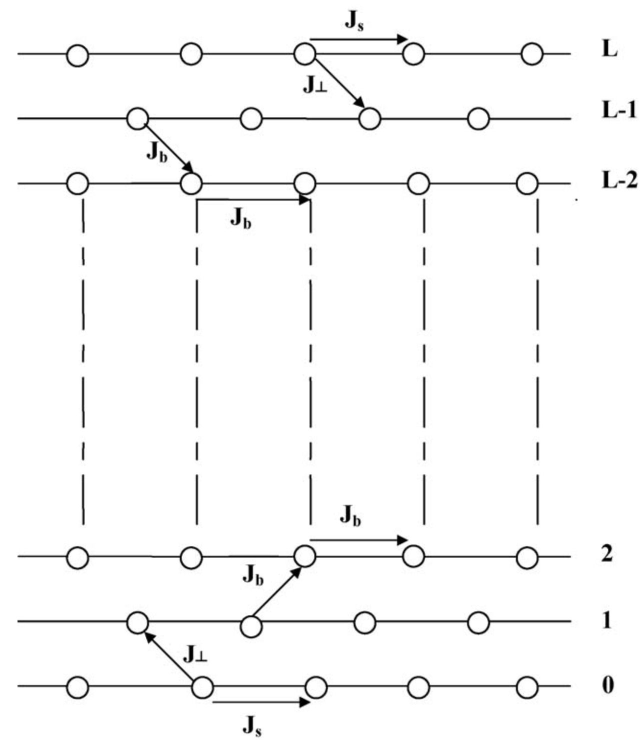

Fig. 1. Two-dimensional cross-section of the ferromagnetic thin film of the face centered cubic lattice.

The HSTE of the magnetic susceptibility $\chi(T)$ have been derived to order six in the reciprocal temperature including nearest-neighbour exchange couplings in the bulk and within the surfaces J_b, J_S and $J_\perp$, respectively (see Fig. 1). For the thin film with thickness L, we obtain the following function:

$$\chi(T) = \frac{g\mu_B^2\beta S(S+1)}{NL}\sum_{ij}\langle\vec{S}_i\cdot\vec{S}_j\rangle = \frac{g\mu_B^2\beta S(S+1)}{NL}\sum_{n=0}^{6}\left(\sum_{p=0}^{n}\sum_{q=0}^{n}a(p,q,n)R_1^pR_2^q\right)\tau^{-n} \tag{3}$$

avec: $R_1 = \frac{J_\perp}{J_b}$ and $R_2 = \frac{J_s}{J_b}$, with $\tau_c = \frac{K_BT_c}{2S(S+1)J_b}$ and the condition $p+q \le n$.

μ_B is the Bhor magneton, g the gyromagnetic ratio and N is the number of magnetic ion in each plane.

The nonzero coefficients $a(p, q, n)$ are computed till order $n = 6$, for some of thickness (L = 7, 11, 20 and 26) and are gathered in Table 1 (see Appendix). It should be noted that for the specific case where $R_1 = R_2 = 1$ and $L = 1$, we obtain the coefficients of the magnetic susceptibility $\chi(T)$, up to the order 6 in β for Heisenberg model: $a_0 = 1$, $a_1 = 8.0000$, $a_2 = 58.6667$, $a_3 = 413.8667$, $a_4 = 2855.3481$, $a_5 = 19415.8527$, $a_6 = 130694.4263$. These coefficients are similar to those computed by Stanley [13] for the face centred cubic lattice with Heisenberg model. In order to estimate the reduced critical temperature, τ_c at which the magnetic susceptibility diverges, we use the well-known Padé approximants method [16].

3. Results and discussion

The calculations were carried out to investigate the effects of the thickness and the ratios of exchange parameters R_1 and R_2,