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**EFFECTS OF SURFACE AND BULK TRANSVERSE FIELDS  
ON CRITICAL BEHAVIOUR OF FERROMAGNETIC FILMS**

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**Abstract**

The influence of surface and bulk transverse fields on the critical behaviour of a ferromagnetic Ising film is studied using the effective field theory based on a single-site cluster method. Surface exchange enhancement is considered and a critical value is obtained. The dependence of the critical uniform transverse field on film thickness, phase diagrams in the fields, critical surface transverse field versus the bulk one, and exchange coupling ratio are presented.

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# 1 Introduction

The recent advances of modern vacuum science, and in particular epitaxial growth techniques, have made possible the preparation of a large variety of magnetic layered structures, whose properties differ drastically from the bulk ones. This theoretical activity has been devoted to the study of Ising thin films. Among the more recent investigations has been the study of thin magnetic films having enhanced (or reduced) surface exchange, both by mean-field theory [1,2] and within an effective field theory treatment that accounts for the self-spin correlations [3,4]. Both the thickness dependence of the Curie temperature [1-4] and the magnetization properties [4] have been studied. The influence of surface and bulk transverse fields on the critical behaviour of Ising thin films has been studied but in the spin-1/2 case, see [5, 6]. Other studies on this problem have been reported [7-8] but only for the situation where the surface and bulk transverse fields are equal. In this work, we examine the critical behaviour of a spin-one Ising films under a surface and bulk transverse fields.

The article is organized as follows. In the next section the basic points of the effective field theory with a probability distribution technique that accounts for the single-site spin correlation, as applied to the present model, are briefly reviewed. This is followed by a presentation of numerical results, and their discussion, in Section 3. A short conclusion is given in Section 4.

## 2 Formalism

The spin-one Ising Hamiltonian of a simple cubic ferromagnetic thin film composed of  $L$  atomic layers and in the presence of a transverse field is given by

$$H = - \sum_{i,j} J_{ij} \sigma_i^z \sigma_j^z - \sum_i \Omega_i \sigma_i^x, \quad (1)$$

where  $\sigma_i^z$  and  $\sigma_i^x$  are the  $z$  and  $x$  components of a quantum spin  $\vec{\sigma}_i$  of magnitude  $\sigma_i = 1$  at the site  $i$ .  $J_{ij}$  is the nearest-neighbour exchange interaction between spins at site  $i$  and  $j$ , that takes the value  $J_s$  if both spins lie on the surface of the thin film and  $J_b$  otherwise,  $\Omega_i = \Omega_b$  and  $\Omega_s$  represent transverse fields in the bulk and on the surface of the film, respectively.

The statistical properties of the system are studied using an effective field theory that employs the probability distribution technique, which is based on a simple site cluster comprising just a simple selected spin labeled  $i$ , and the neighbour spins with which it directly interacts. To this end, the total Hamiltonian is split into two parts,  $H = H_i + H'$ . The part  $H_i$  includes all those terms in the Hamiltonian,  $H$  associated with the lattice site  $i$  and  $H'$  is the remainder.

The starting point of the effective field theory is a set of formal identities of the type

$$\langle\langle (\sigma_i^\alpha)^p \rangle_c \rangle = \left\langle \frac{Tr_i [(\sigma_i^\alpha)^p \exp(-\beta H_i)]}{Tr_i [\exp(-\beta H_i)]} \right\rangle \quad (2)$$

where  $\alpha = z, x$ ,  $p = 1, 2$ ,  $\langle (\sigma_i^\alpha)^p \rangle_c$  denotes the mean value of  $(\sigma_i^\alpha)^p$  for a given configuration  $c$  of all other spins,  $\langle \dots \rangle$  denotes the average over all spin configurations  $\sigma_j$ ,  $Tr_i$  means the trace performed over  $(\sigma_i^\alpha)^p$  only,  $\beta = 1/k_B T$  with  $k_B$  the Boltzmann constant and  $T$  the absolute temperature. For a fixed configuration of neighbouring spins of the site  $i$  the longitudinal and the transverse magnetizations and quadrupolar moments of any spin at site  $i$  are given by,

$$m_{i\alpha} = \langle \sigma_i^\alpha \rangle = \langle f_{1\alpha}(s, t) \rangle \quad (3)$$

$$q_{i\alpha} = \langle (\sigma_i^\alpha)^2 \rangle = \langle f_{2\alpha}(s, t) \rangle \quad (4)$$

where  $\alpha = z, x$  for the longitudinal and transverse magnetizations and quadrupolar moments respectively and

$$f_{1z}(s, t) = \frac{s}{[s^2 + t^2]^{1/2}} \frac{2 \sinh(\beta [s^2 + t^2]^{1/2})}{1 + 2 \cosh(\beta [s^2 + t^2]^{1/2})} \quad (5)$$

$$f_{2z}(s, t) = \frac{1}{[s^2 + t^2]} \frac{t^2 + (2s^2 + t^2) \cosh(\beta [s^2 + t^2]^{1/2})}{1 + 2 \cosh(\beta [s^2 + t^2]^{1/2})} \quad (6)$$

and

$$f_{1x}(s, t) = f_{1z}(t, s) \quad (7)$$

$$f_{2x}(s, t) = f_{2z}(t, s) \quad (8)$$

with

$$s = \sum_j J_{ij} \sigma_j^z, \quad (9)$$

$$t = \Omega_i \quad (10)$$

where  $\beta = 1/k_B T$ ,  $\langle \dots \rangle$  indicates the usual canonical ensemble thermal average for a given configuration and the first and second sums run over all possible configurations of atoms environing or lying on the  $i$  site, respectively. Each of these configurations can be characterized by numbers of magnetic atoms in the planes  $i - 1, i, i + 1$ .

To perform thermal averaging on the right-hand side of equations (3) and (4) one now follows the general approach described in [8]. Thus with the use of the integrable representation method of Dirac  $\delta$ -distribution, equations (3) and (4) can be written in the form

$$\langle \sigma_i^\alpha \rangle = \int d\omega f_{1\alpha}(\omega, B) \frac{1}{2\pi} \int dt \exp(i\omega t) \prod_j \langle \exp(-it J_{ij} \sigma_j^z) \rangle \quad (11)$$

$$\langle (\sigma_i^\alpha)^2 \rangle = \int d\omega f_{2\alpha}(\omega, y) \frac{1}{2\pi} \int dt \exp(i\omega t) \prod_j \langle \exp(-it J_{ij} \sigma_j^z) \rangle \quad (12)$$

In the derivation of the equations (10) and (11), the commonly used approximation has been made according to which the multi-spin correlation functions are decoupled into products of the

spin averages. We introduce the longitudinal magnetization and the longitudinal quadrupolar moment of the  $i$ -th layer, on the basis of equations (2) and (3), with the use of the probability distribution of the spin variables [9]

$$P(\sigma_i^z) = \frac{1}{2} [(q_{iz} - m_{iz}) \delta(\sigma_i^z + 1) + 2(1 - q_{iz}) \delta(\sigma_i^z) + (q_{iz} + m_{iz}) \delta(\sigma_i^z - 1)] \quad (13)$$

Allowing for the site magnetizations and quadrupolar moments to take different values in each atomic layer parallel to the surfaces of the film, and labeling them in accordance with the layer number in which they are situated, the application of Eqs. (3), (11) and (15) yields the following set of equations for the layer longitudinal magnetizations

$$\begin{aligned} m_{i\alpha} = & 2^{-N-2N_0} \sum_{\mu=0}^N \sum_{\nu=0}^{N-\mu} \sum_{\mu_1=0}^{N_0} \sum_{\nu_1=0}^{N_0-\mu_1} \sum_{\mu_2=0}^{N_0} \sum_{\nu_2=0}^{N_0-\mu_2} 2^{\mu+\mu_1+\mu_2} C_{\mu}^N C_{\nu}^{N-\mu} \\ & C_{\mu_1}^{N_0} C_{\nu_1}^{N_0-\mu_1} C_{\mu_2}^{N_0} C_{\nu_2}^{N_0-\mu_2} (1 - 2q_{iz})^{\mu} (q_{iz} - m_{iz})^{\nu} (q_{iz} + m_{iz})^{N-\mu-\nu} \\ & (1 - 2q_{i-1,z})^{\mu_1} (q_{i-1,z} - m_{i-1,z})^{\nu_1} (q_{i-1,z} + m_{i-1,z})^{N_0-\mu_1-\nu_1} \\ & (1 - 2q_{i+1,z})^{\mu_2} (q_{i+1,z} - m_{i+1,z})^{\nu_2} (q_{i+1,z} + m_{i+1,z})^{N_0-\mu_2-\nu_2} f_{1\alpha}(y_i, \Omega_i) \end{aligned} \quad (14)$$

where

$$y_i = \begin{cases} J_s(N - \mu - 2\nu) + J_b[2N_0 - (\mu_1 + \mu_2) - 2(\nu_1 + \nu_2)] & \text{for } i = 1, L \\ J_b[N + 2N_0 - (\mu + \mu_1 + \mu_2) - 2(\nu + \nu_1 + \nu_2)] & \text{for } i = 2, 3 \dots L - 1 \end{cases} \quad (15)$$

$N$  and  $N_0$  are the numbers of nearest neighbours in the plane and between adjacent planes respectively ( $N = 4$  and  $N_0 = 1$  in the case of a simple cubic lattice which is considered here) and  $C_k^l$  are the binomial coefficients,  $C_k^l = \frac{l!}{k!(l-k)!}$ .

The equations of the longitudinal and transverse quadrupolar moments are obtained by substituting the function  $f_{1\alpha}$  by  $f_{2\alpha}$  in the expressions of the layer longitudinal and transverse magnetizations respectively. This yields

$$q_{i\alpha} = m_{i\alpha} [f_{1\alpha}(y_i, \Omega_i) \rightarrow f_{2\alpha}(y_i, \Omega_i)] \quad (16)$$

In this work we are interested with the calculation of the ordering near the transition Curie temperature. The usual argument that  $m_{iz}$  tends to zero as the temperature approaches its critical value, allows us to consider only terms linear in  $m_{iz}$  because higher order terms tend to zero faster than  $m_{iz}$  on approaching a Curie temperature. Consequently, all terms of the order higher than linear terms in eqs. (14) that give the expressions of  $m_{iz}$  can be neglected.

This leads to the set of simultaneous equations

$$m_{iz} = A_{i,i-1} m_{i-1,z} + A_{i,i} m_{iz} + A_{i,i+1} m_{i+1,z} \quad (17)$$

or

$$A \vec{m}_z = \vec{m}_z \quad (18)$$

where  $\vec{m}_z$  is a vector of components  $(m_{1z}, m_{2z}, \dots, m_{iz}, \dots, m_{Lz})$  and the matrix  $A$  is symmetric and tridiagonal with elements

$$A_{i,j} = A_{i,i}\delta_{i,j} + A_{i,j}(\delta_{i,j-1} + \delta_{i,j+1}) \quad (19)$$

The system of eqs. (18) is of the form

$$M \vec{m}_z = \vec{0} \quad (20)$$

where

$$M_{i,j} = (A_{i,j} - 1)\delta_{i,j} + A_{i,j}(\delta_{i,j-1} + \delta_{i,j+1}) \quad (21)$$

The only non zero elements of the matrix  $M$  are given by

$$\begin{aligned} M_{i,i-1} &= 2^{-N-2N_0} \sum_{\mu=0}^N \sum_{\nu=0}^{N-\mu} \sum_{\mu_1=0}^{N_0} \sum_{\nu_1=0}^{N_0-\mu_1} \sum_{\mu_2=0}^{N_0} \sum_{\nu_2=0}^{N_0-\mu_2} \sum_{i=0}^{\nu_1} \sum_{j=0}^{N_0-(\mu_1+\nu_1)} (-1)^i 2^{\mu+\mu_1+\mu_2} \delta_{1,i+j} \quad (22) \\ & C_{\mu}^N C_{\nu}^{N-\mu} C_{\mu_1}^{N_0} C_{\nu_1}^{N_0-\mu_1} C_{\mu_2}^{N_0} C_{\nu_2}^{N_0-\mu_2} C_i^{\nu_1} C_j^{N_0-(\mu_1+\nu_1)} (1-r_i)^{\mu} \\ & (1-r_{i-1})^{\mu_1} (1-r_{i+1})^{\mu_2} r_i^{N-\mu} r_{i-1}^{(N_0-\mu_1)-(i+j)} r_{i+1}^{N_0-\mu_2} f_{1z}(y_i, \Omega_i) \end{aligned}$$

$$\begin{aligned} M_{i,i} &= 2^{-N-2N_0} \sum_{\mu=0}^N \sum_{\nu=0}^{N-\mu} \sum_{\mu_1=0}^{N_0} \sum_{\nu_1=0}^{N_0-\mu_1} \sum_{\mu_2=0}^{N_0} \sum_{\nu_2=0}^{N_0-\mu_2} \sum_{i=0}^{\nu_1} \sum_{j=0}^{N_0-(\mu_1+\nu_1)} (-1)^i 2^{\mu+\mu_1+\mu_2} \delta_{1,i+j} \\ & C_{\mu}^N C_{\nu}^{N-\mu} C_{\mu_1}^{N_0} C_{\nu_1}^{N_0-\mu_1} C_{\mu_2}^{N_0} C_{\nu_2}^{N_0-\mu_2} C_i^{\nu_1} C_j^{N_0-(\mu_1+\nu_1)} (1-r_i)^{\mu} \\ & (1-r_{i-1})^{\mu_1} (1-r_{i+1})^{\mu_2} r_i^{N-\mu-(i+j)} r_{i-1}^{(N_0-\mu_1)} r_{i+1}^{N_0-\mu_2} f_{1z}(y_i, \Omega_i) - 1 \quad (23) \end{aligned}$$

$$\begin{aligned} M_{i,i+1} &= 2^{-N-2N_0} \sum_{\mu=0}^N \sum_{\nu=0}^{N-\mu} \sum_{\mu_1=0}^{N_0} \sum_{\nu_1=0}^{N_0-\mu_1} \sum_{\mu_2=0}^{N_0} \sum_{\nu_2=0}^{N_0-\mu_2} \sum_{i=0}^{\nu_1} \sum_{j=0}^{N_0-(\mu_2+\nu_2)} (-1)^i 2^{\mu+\mu_1+\mu_2} \delta_{1,i+j} \\ & C_{\mu}^N C_{\nu}^{N-\mu} C_{\mu_1}^{N_0} C_{\nu_1}^{N_0-\mu_1} C_{\mu_2}^{N_0} C_{\nu_2}^{N_0-\mu_2} C_i^{\nu_1} C_j^{N_0-(\mu_2+\nu_2)} (1-r_i)^{\mu} \\ & (1-r_{i-1})^{\mu_1} (1-r_{i+1})^{\mu_2} r_i^{N-\mu} r_{i-1}^{(N_0-\mu_1)} r_{i+1}^{N_0-\mu_2-(i+j)} f_{1z}(y_i, \Omega_i) \quad (24) \end{aligned}$$

where

$$\begin{aligned} r_i &= 2^{-N-2N_0} \sum_{\mu=0}^N \sum_{\nu=0}^{N-\mu} \sum_{\mu_1=0}^{N_0} \sum_{\nu_1=0}^{N_0-\mu_1} \sum_{\mu_2=0}^{N_0} \sum_{\nu_2=0}^{N_0-\mu_2} 2^{\mu+\mu_1+\mu_2} C_{\mu}^N C_{\nu}^{N-\mu} \\ & C_{\mu_1}^{N_0} C_{\nu_1}^{N_0-\mu_1} C_{\mu_2}^{N_0} C_{\nu_2}^{N_0-\mu_2} (1-2r_i)^{\mu} r_i^{N-\mu} (1-r_{i-1})^{\mu_1} r_{i-1}^{(N_0-\mu_1)} \\ & (1-2r_{i+1})^{\mu_2} r_{i+1}^{N_0-\mu_2} f_{2z}(y_i, \Omega_i) \quad (25) \end{aligned}$$

In a general case, for arbitrary values of these parameters, the evaluation of the Curie temperature relies on the numerical solution of the system of linear equations (20).



### 3 Results and discussion

In this paper, we take  $J_b$  as the unit of the energy, the length is measured in units of the lattice constant and we introduce the reduced exchange couplings  $p = J_s/J_b$ .

From equation (30) we can obtain the phase diagrams of the film. In Fig. 1, we show the phase diagram ( $p, k_B T_c/J_b$ ) plane for different numbers of layers and when ( $\Omega = \Omega_s = \Omega_b$ ). The solid and dotted lines correspond respectively to  $\Omega/J_b = 0$  and 2. For each value of  $\Omega/J_b$ , we see that all curves intersect at the same abscissa point  $p_c = 1.2937$  (parameter  $p$  at which  $k_B T_c/J_b$  being greater than the bulk Curie temperature  $k_B T_c^B/J_b$  is independent of the film thickness and is equal to one coordinate of the multicritical point of the surface bulk transition in the semi-infinite case), see [9]. In Fig. 2 we have plotted the critical parameter  $p_c$  versus the uniform transverse field. Notice that  $p_c$  is weakly sensitive to  $\Omega/J_b$  but its dependence is significant near the infinite bulk critical transverse field  $(\Omega/J_b)_{crit} = 5.259$ .

The dependence of the critical uniform transverse field on film thickness is shown in Fig. 3. In the presence of surface exchange enhancement,  $\Omega_c(L)/J_b$  naturally exhibits the same qualitative dependence on  $L$  as exhibited by  $k_B T_c(L)/J_b$  [13] (see Fig. 3 of that reference). The characteristic properties of the curves refer to  $p > p_c$  as indicated in the figure, is a decrease of the film critical field  $\Omega_c(L)/J_b$  when the film thickness increases. We see that for an enhanced value of  $p$  the film critical transverse field exceeds  $(\Omega/J_b)_{crit} = 5.259$  despite the reduced number of nearest neighbours. In this case,  $\Omega_c(L)/J_b$  exhibits a maximum for small film thickness  $L$ .

On the other hand, for curves referring to  $p < p_c$ , we note just the opposite tendency. For  $p = p_c$ , the film critical transverse field  $\Omega_c(L)/J_b$  is equal to the bulk one regardless of the film thickness (dotted horizontal line).

Fig. 4a-b shows the phase diagrams ( $\Omega_s/J_b, k_B T_c/J_b$ ) under different values of  $p$  for various layers of the films and for  $\Omega_b/J_b = 0$  and 2. When  $p = 1$ , as shown in Fig. 4a, the Curie temperature  $k_B T_c(\Omega_s/J_b)/J_b$  of the films was lower than  $k_B T_c^B(\Omega/J_b)/J_b$  for the bulk (dotted horizontal lines). Upon increasing the layer number,  $k_B T_c(\Omega_s/J_b)/J_b$  approaches asymptotically  $k_B T_c^B(\Omega/J_b)/J_b$ .  $L$  and  $\Omega_{s(b)}/J_b$  are fixed, the Curie temperature of the film increases with a decrease in  $\Omega_{b(s)}/J_b$  as expected. When  $p = 1.5$ , as shown in Fig. 4b,  $k_B T_c/J_b$  changed from  $T_c < T_c^B$  to that of  $T_c > T_c^B$ . This means that there exists a critical value of the surface transverse field,  $(\Omega_s/J_b)_{crit} = 3.519$  and 4.0139 at  $\Omega_b/J_b = 0$  and 2 respectively. The variation of the critical surface transverse field with the bulk one of the film is shown in Fig. 5 for a fixed value of  $p = 1.5$ .  $(\Omega_s/J_b)_{crit}$  rises with increasing  $\Omega_b/J_b$  to reach its maximum value  $(\Omega_s/J_b)_{crit} = 6.0635$  at the infinite bulk critical transverse field  $(\Omega/J_b)_{crit} = 5.259$ .

In Fig. 6, we represent the critical ratio  $p_c$  against the surface transverse field  $\Omega_s/J_b$  for different values of the bulk transverse field  $\Omega_b/J_b$ . We can see clearly that  $p_c$  increases (decreases)

with the increase of  $\Omega_{(s)b}/J_b$  for a fixed value of  $\Omega_{(b)s}/J_b$ . Such behaviour is similar to that obtained in the surface behaviour of the transverse spin-1/2 Ising model [5, 6].

In order to complete this work, we study the variation of the critical ratio  $p_c$  with the bulk transverse field strength for different values of  $\Omega_s/J_b$ , Fig. 7. The effect of the bulk transverse field is to lower the value of the Curie temperature and at the same time,  $p_c$  shifts to lower values.  $p_c$  reaches its minimum value at the infinite bulk critical transverse field. The surface and bulk transverse fields act in opposite ways see Figs. 6-7. Above  $\Omega/J_b)_{crit}$ , even the infinite bulk Curie temperature goes to zero, a film of a finite size can still exhibit a phase transition for sufficiently large values of  $p_c$ .

## 4 Conclusion

Using the effective field with a probability distribution technique, we studied critical properties of magnetic Ising film in the presence of transverse fields, both at the surface, and within the bulk of the film. A critical value  $p_c = J_s/J_b)_{crit}$  of the ratio of the exchange interactions that lead to a Curie temperature higher than that for the infinite bulk material is obtained. It is shown that  $p_c$  is weakly sensitive to the strength of the uniform field. The dependence of the critical uniform transverse field on the film thickness and phase diagrams in the fields are examined. A critical value  $\Omega_s/J_b)_{crit}$  of the surface transverse field, and exchange interaction ratio  $p_c$  are presented. These two critical parameters  $p_c$  and  $\Omega_s/J_b)_{crit}$  influenced the transition.

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## Figure Captions

Fig 1. Variation of the Curie temperature with surface exchange enhancement  $p$  for a transverse field  $\Omega/J_b = 2$  (dotted curves). The solid curves refer to the pure Ising model. The number accompanying each curve denotes the film thickness  $L$ . The dotted horizontal line is the infinite bulk Curie temperature.

Fig 2. Variation of the critical ratio  $p_c$  with the transverse field when  $(\Omega = \Omega_b = \Omega_s)$ .

Fig 3. Dependence of the critical transverse field strength on film thickness when  $(\Omega_b/J_b = \Omega_s/J_b)$ . The number accompanying each curve denotes the values of  $p$ . The dotted line is that for the infinite bulk  $(\Omega/J_b)_{crit} = 5.259$ .

Fig. 4. Surface transverse field dependence of the Curie temperature for different thickness  $L$  indicated by numbers 4, 8 and 12 and two values of  $\Omega_b/J_b = 0$  (solid curves) and 2. (dashed curves).  $p = 1$  (a) and for  $p = 1.5$  (b). The dotted horizontal lines correspond to the bulk Curie temperature when  $\Omega_b/J_b = 0$  and 2.

Fig. 5. The variation of the critical surface transverse field with the bulk transverse field of the film when  $p = 1.5$ .

Fig. 6. Dependence of the critical ratio  $p_c$  with the surface transverse field strength for three values of  $\Omega_b/J_b = 0, 1$  and 2.

Fig. 7. The critical ratio  $p_c$  versus the bulk transverse field strength for three values of  $\Omega_s/J_b = 1, 2$  and 3.