Layering Transitions in a Random Variable Transverse Field

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The effect of a random surface transverse magnetic field (TMF) on the order-disorder layering transitions of a spin-$1/2$ Ising model is investigated using the finite cluster (FC) approximation. Each layer k ($k = 1, 2, \ldots, N$) of the film (formed with N layers) is subject to the transverse magnetic field $_k = {}_s/k^{\alpha}$, α being a constant. $_s$ is the surface transverse magnetic field distributed according to a probability law given in the body of the text. The order-disorder layering transitions of a layer k depend strongly on the concentration p of the surface transverse magnetic field, and there exists a critical probability p_c, below which the film is always ordered at very low temperatures for any values of the surface transverse magnetic field $_s$. Above this critical probability, we show the existence of a sequence of probabilities $p_c(k)$ at which the first k layers will be disordered at a sequence of critical surface transverse magnetic field values $^c_s(k)$. We show that $p_c(k)$ and $^c_s(k)$ depend on the exponent α and on the film thickness N. The behaviour of the longitudinal and transverse magnetisations as well as the critical exponents are also investigated for several values of film thickness and exponent α.

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I. Introduction

Phase transitions in Ising spin systems, driven entirely by quantum fluctuations, have been getting a lot of attention lately [1]. The simplest of such systems is the Ising model in a transverse field which can be exactly solved in one dimension. This model has been introduced to explain the phase transitions of hydrogen-bonded ferroelectrics such as KH_2PO_4 [2]. Since then, this model has been applied to several physical systems like $DyVO_2$ and studied by a variety of sophisticated techniques. Recently, many experimental studies have shown that magnetisation enhancement exists in multilayered films consisting of magnetic layers. The development of the molecular beam epitaxy technique and its application to the growth of thin metallic films have stimulated renewed interest in thin film magnetism. The fabrication of thin metallic films has led to a surge of experimental activity [3-6]. The thickness dependence of the critical temperature of thin Ising magnetic films having surface exchange enhancement has been studied by Hong [7], by Aguilera-Granja and Moran Lopez [8] within the mean field approximation, and by Hai and Li [9] and Wiatrowski *et al.* [10] within an effective field treatment that accounts for the self-spin correlations. Several authors have described ferroelectric films using an Ising model in a transverse field [11-13]. By modifying the interaction constants and the transverse fields at the surface, Wang *et al.* [14] have successfully extended the transverse Ising model to the study of surface and size effects in ferroelectric films. It is found that when the film becomes very thick its properties are those of a semi-infinite Ising system [15-17]. The most commonly studied magnetic multilayers are those of a ferromagnetic transition metal, such as Fe/Ni, where coupling can exist between magnetic layers [18-20].

Surface magnetism is a rich problem for study on both theoretical and experimental grounds. Indeed, considerable effort has been devoted to investigating its various applications in information storage catalysis and its relevance to problems of corrosion, among others. More recently, the development of the molecular beam epitaxy technique and its application to the growth of thin metallic films has simulated renewed interest in thin film magnetism. The fabrication of thin magnetic films has led to a surge of experimental activity [21-24] and references therein.

From the experimental point of view, the effects of the surface on the ferroelectric phase transitions have been investigated for many years, but, due to the variety of ferroelectric materials and the difficulty of preparing high quality single-crystal samples, it is difficult to make useful general statements. A brief review of some of the experimental results is given in [25].

Using the mean field theory, we have studied in a previous work [26] the effect of a uniform transverse magnetic field on the layering and wetting transitions of a spin$-1/2$ Ising model in a longitudinal magnetic field. We showed the existence of layering and wetting transitions above a critical transverse magnetic field, which is a function of the temperature and the surface magnetic field. Karevski *et al.* [27] have studied the random transverse Ising spin chain according to a distribution of the transverse field governed by a law of type $k^{-\alpha}$ (k being the distance from the surface and α being a constant). More recently, we have shown the existence of order-disorder layering transitions in the pure case of a variable transverse magnetic field, using both the mean field theory and the finite cluster approximation [28]. As far as we know, no investigation has been made of order-disorder layering transitions in a random surface transverse magnetic field.

Our aim in this paper is to study the effects of a random surface transverse magnetic field $_s$ distributed according to a probability law on such a model, using the finite cluster approximation. The phase diagrams and the behaviour of the longitudinal and transverse magnetisations are investigated. This paper is organised as follows. Section 2 describes the model and the methods. In section 3 we present our results and a discussion.

II. Model and method

We consider N coupled ferromagnetic square layers in the presence of a transverse magnetic field. The Hamiltonian for a layer k is given by

$$\mathcal{H} = -\sum_{<i,j>} J_{ij} S_i^z S_j^z - \sum_i \ {}_i S_i^x, \tag{1}$$

where (S_i^σ, ($\sigma = x, z$) are the Pauli matrices; the spin interactions are assumed to be constant $J_{ij} = J$. The transverse magnetic field $_i$ applied to each site 'i' of the layer 'k' is defined by

$${}_i = {}_k = {}_s/k^\alpha. \tag{2}$$

$_s$ is the applied transverse magnetic field on the surface ($k = 1$). The values of the parameter α will be discussed in the following. In particular $\alpha = 0$ corresponds to a uniform transverse magnetic field applied to each layer. The surface transverse magnetic field $\ _s$ is governed by the probability law

$$\mathcal{P}(\ _i) = p\delta(\ _s - \ _i) + (1-p)\delta(\ _i), \tag{3}$$

where $\ _i$ is the transverse magnetic field applied to a site 'i' and p is the probability. The situation $p = 1$ indicates that the surface transverse magnetic field is acting on each spin, whereas $p = 0$ denotes the absence of the surface transverse magnetic field.

The model we are studying should provide a reasonable description of the experimental system [29] $LiHo_xY_{1-x}F_4$ and may also be able to describe non-fermi liquid behaviour [30]. Naturally, the random transverse field Ising model has been quite extensively studied and many surprising analytical results are available for the case of dimension $d = 1$ [31-33].

For disordered Ising models, the mean field approximation, which neglects all spin correlations, is not satisfactory. Hence, to compute the average over all spin configurations, we will use the finite cluster approximation with an expansion technique for the spin-$1/2$ cluster identities. Within the framework of this technique one uses a single site cluster approximation [34-36], in which attention is focused on a cluster comprising just a single selected spin and the neighbouring spins with which it directly interacts. The starting point of the single-site cluster approximation is a set of formal identities of the type

$$<< S_0^\sigma >_c >=< \frac{\mathrm{Tr}_0[S_0^\sigma \exp(-\beta H_0)]}{\mathrm{Tr}_0[\exp(-\beta H_0)]} >, \tag{4}$$

where $S_0^\sigma(\sigma = z, x)$ is the σ-component of the spin operator S_0. $< S_0^\sigma >_c$ denotes the mean value of S_0^σ for a given configuration c of all other spins. $< ... >$ denotes the average over all other spin configurations. Tr_0 means the trace performed over S_0 only. $\beta = 1/k_BT$, T is the absolute temperature and k_B is the Boltzmann constant.

Eq. (4) is not exact for the transverse Ising model. Nevertheless, it has been accepted as a starting point in many studies [34-36].

The magnetizations m^σ $(\sigma = z, x)$ are given by

$$m^\sigma =<< S_0^\sigma >_c> . \tag{5}$$

The finite cluster approximation has been designed to treat all spin self-correlations exactly while still neglecting correlations between different spins, using the Zernike approximation: $< S_iS_j...S_k >=< S_i >< S_j > ... < S_k >$. To calculate m^σ, $(\sigma = z, x)$ we must average the right-hand sides of Eq. (4).

To calculate the longitudinal and transversal layer magnetisations, in the spirit of the finite cluster approximation [34, 35], we expand Eq. (4) in the set $\{1, \sigma_1, ..., \sigma_N, \sigma_1\sigma_2, ..., \sigma_1\sigma_2...\sigma_N\}$, which contains all the products of different spins. This set forms an orthonormal basis for the inner product defined by

$$< f_1|f_2 >= \frac{1}{2^N}\mathrm{Tr}_{\sigma_1...\sigma_N} f_1(\sigma_1, ..., \sigma_N) f_2(\sigma_1, ..., \sigma_N). \tag{6}$$

* For longitudinal magnetisations

$$f_k^z(\sigma_1, ..., \sigma_N) = \frac{(h_k + \lambda_k)^2 - \ _k^2}{(h_k + \lambda_k)^2 + \ _k^2} \tanh(\beta\lambda_k), \tag{7}$$

* for transverse magnetisations

$$f_k^x(\sigma_1, ..., \sigma_N) = \frac{2 \quad _k(h_k + \lambda_k)}{(h_k + \lambda_k)^2 + \quad _k^2} \tanh(\beta \lambda_k), \tag{8}$$

where $h_k = J(\sum_{i=1}^N \sigma_i)$ and $\lambda_k = \sqrt{h_k^2 + \quad _k^2}$.

The longitudinal magnetisations m_k^z, for a plane 'k' $(k = 1, ..., N)$ are given by:

$$\begin{aligned} m_k^z = & A_0 + A_1(m_{k-1}^z + 4m_k^z + m_{k+1}^z) + A_2(4m_{k-1}^z mk^z + 4m_k^z m_{k+1}^z + 6(m_k^z)^2 \\ & + m_{k-1}^z m_{k+1}^z) + A_3(6m_{k-1}^z (m_k^z)^2 + 4m_{k-1}^z m_k^z m_{k+1}^z + 6(m_k^z)^2 m_{k+1}^z \\ & + 4(m_k^z)^3) + A_4(4m_{k-1}^z (m_k^z)^3 + 4(m_k^z)^3 m_{k+1}^z + 6m_{k-1}^z (m_k^z)^2 m_{k+1}^z \\ & + (m_k^z)^4) + A_5(m_{k-1}^z (m_k^z)^4 + m_{k+1}^z (m_k^z)^4 + 4m_{k-1}^z m_{k+1}^z (m_k^z)^3) \\ & + A_6(m_{k-1}^z m_{k+1}^z (m_k^z)^4), \end{aligned} \tag{9}$$

where the coefficients $A_k, (k = 0, 1, ..., 6)$ are calculated in the Appendix.

To evaluate the transverse magnetisations m_k^x, the same method is valid, provided that one expands the function f_x in the basis set $\{1, \sigma_1, ..., \sigma_N, \sigma_1\sigma_2, ..., \sigma_1\sigma_2 ... \sigma_N\}$ and calculates the corresponding coefficients: $A_k^{'}, (k = 0, 1, ..., 6)$.

III. Results and discussion

We consider a film formed with N square layers, under a random variable transverse magnetic field defined by Eq. (2) and distributed according to the probability law Eq. (3). Unless otherwise specified, the results established in this manuscript have been obtained for a film formed with $N = 20$ layers. The notation $O^k D^{N-k}$ will be used to denote that the first k layers are ordered while the remaining $N - k$ layers are disordered. In particular, O^N corresponds to an ordered film, whereas D^N denotes a totally disordered film.

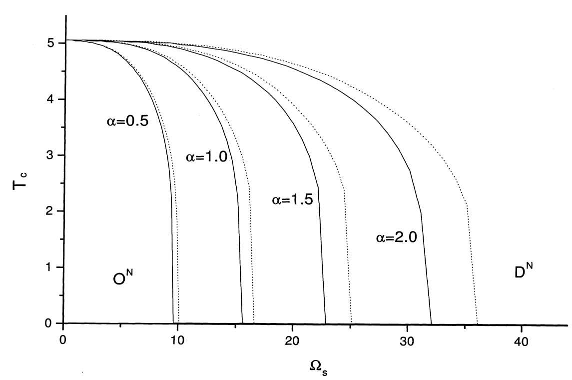

FIG. 1. The dependence of the critical temperature T_c on the surface transverse magnetic field $\quad_s$, for $p = 1.0$ (solid line) and $p = 0.9955$ (dashed line) with different values of α: $0.5, 1.0, 1.5$ and 2.0. The notations $O^{N-k}D^k$ are defined in the body of the text. In particular O^N and D^N denote the totally ordered and disordered films, respectively.

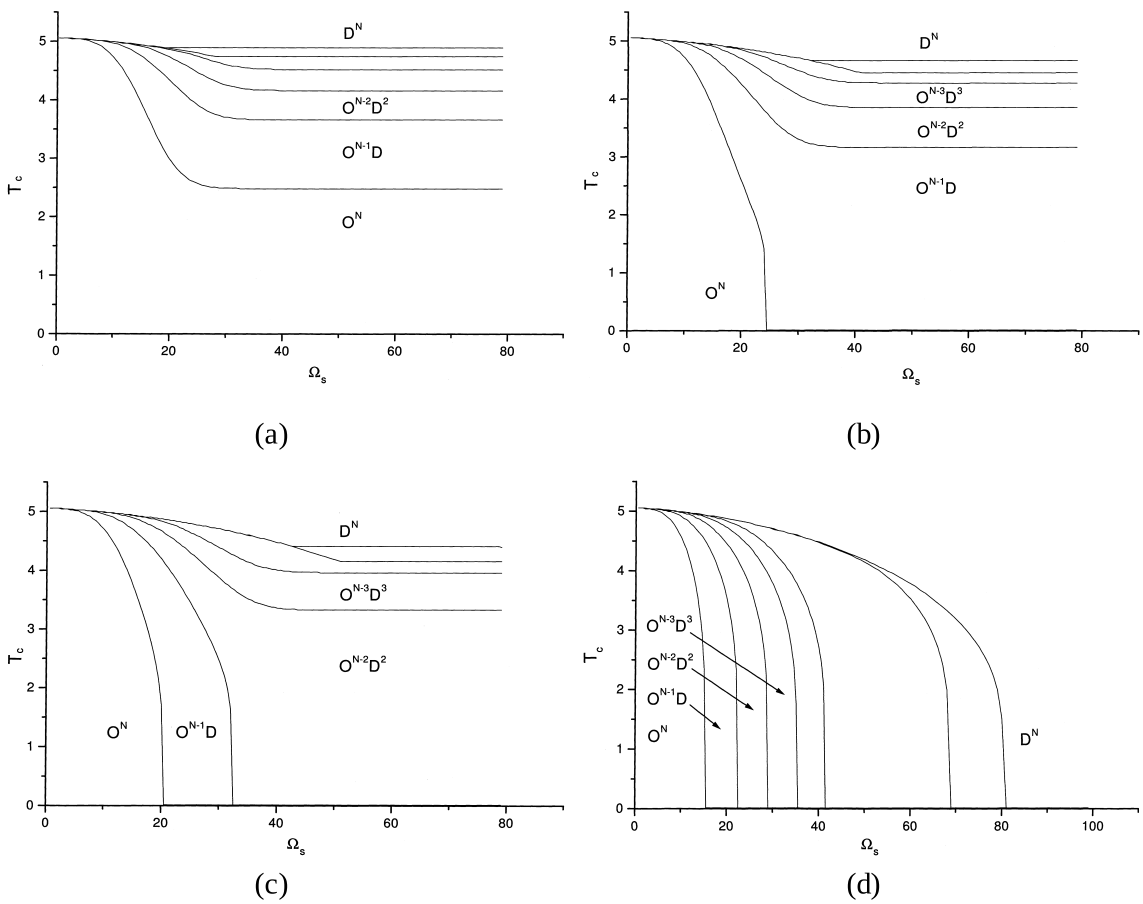

FIG. 2. The dependence of the critical temperature T_c on the surface transverse magnetic field for $\alpha = 1.0$ and different values of the probability: $p(= 0.9945) < p_c(= 0.9949)$ (a), $p_c < p \quad p_c(k = 1) = 0.9950$ (b), $p_c(k = 1) < p \quad p_c(k = 2) = 0.9955$ (c) and $p = 1.0$ (d).

In order to show the effect of the dilution, we plot in Fig. 1 the critical temperature of the surface ($k = 1$) as a function of the surface transverse field $\ _s$ for two probabilities: $p = 1.0$ and $p = 0.9955$ and several values of the parameter α. It arises that when comparing the pure case ($p = 1.0$, solid line) with the presence of a probability ($p = 0.9955$, dashed line), the dilution effect increases the transverse field values needed to disorder the system. Furthermore, for a fixed value of α it is found that there exists a critical probability above which the surface ($k = 1$) becomes disordered at a critical value of the surface transverse magnetic field $\ ^c_s(k = 1)$. For $\alpha = 1.0$ this critical probability is found to be close to $p_c(k = 1) = 0.9949$. Fig. 1 shows also that, in the absence of the surface transverse magnetic field ($\ _s$=0), and for arbitrary values of α and p, the film is totally ordered (O^N) for $T < T_c = 5.073$ but becomes completely disordered (D^N) for $T > T_c$. This is in good agreement with our previous work [28], corresponding to the pure case $p = 1.0$. The behaviour of the other layers ($k > 1$) was found to be similar to that one established in Fig. 1 for the surface ($k = 1$). On the other hand, it is shown that for a fixed α and very low temperatures, each layer k becomes disordered at a critical probability $p_c(k)$ corresponding to a critical surface transverse magnetic field $\;^c_s(k)$. Indeed, as shown in Fig. 2 for $\alpha = 1.0$, the film is ordered at $p \quad p_c = 0.9949$, even for very large surface transverse magnetic field vallues (Fig. 2a). The first surface becomes disordered for a probability greater than the critical value, $p_c < p \quad p_c(k = 1) = 0.9950$ (Fig. 2b). The second layer becomes disordered at $p_c(k = 1) < p \quad p_c(k = 2) = 0.9955$ (Fig. 2c), and so on. Finally the film becomes totally disordered when the applied surface transverse magnetic field acts on all the surface sites: this is the case when $p = 1.0$ (Fig. 2d). It arises that a sequence of order-disorder layering transitions occurs when the probability decreases from the value $p = 1.0$, which corresponds to a totally ordered film at very low temperatures.

In order to illustrate the phenomenon shown in Fig. 2, we plot in Fig. 3 the longitudinal magnetisations m_k^z as a function of the surface transverse magnetic field, for the probability classes considered above. Indeed, for low values of the probability, $p \quad p_c$, the longitudinal magnetisation

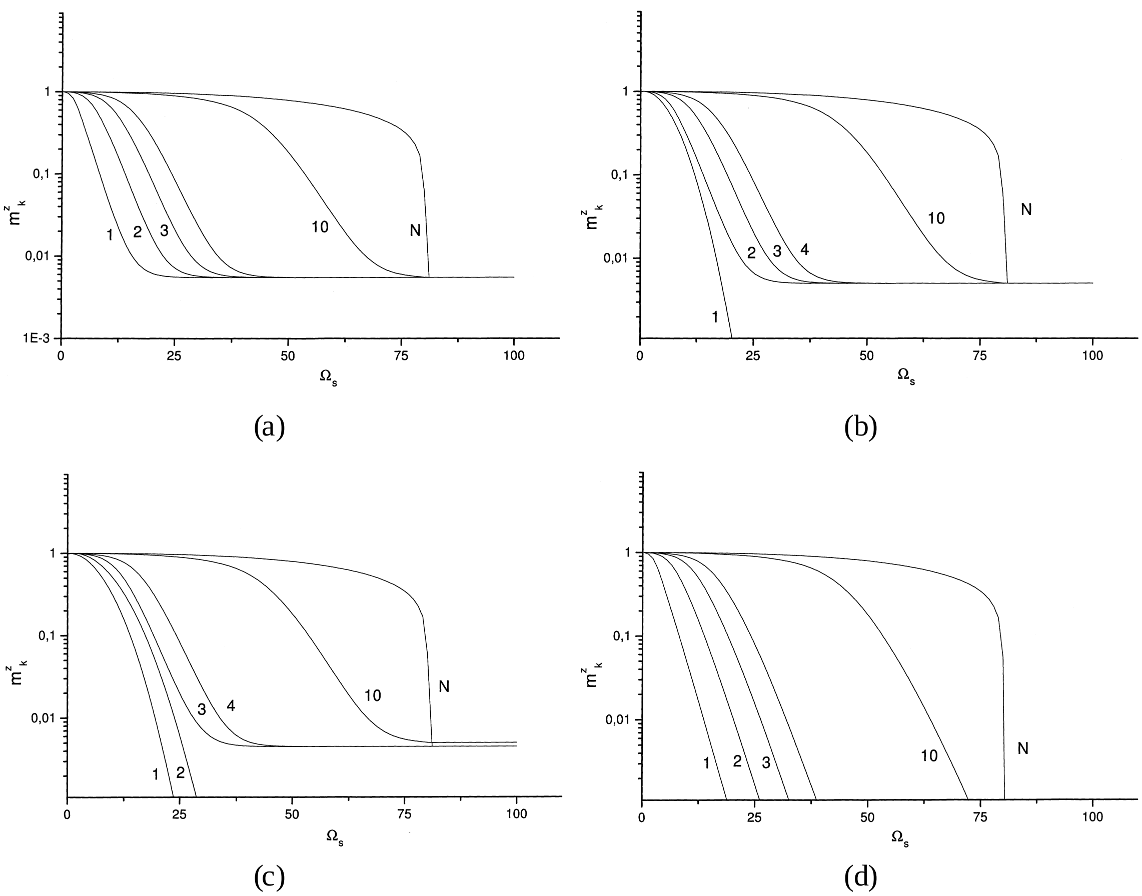

FIG. 3. The behaviour of the longitudinal magnetisation m_k^z as a function of the surface transverse magnetic field for $\alpha = 1.0$ and a very low temperature $T = 0.05$. Different values of the probability are chosen: $p(= 0.9945) < p_c(= 0.9949)$ (a), $p_c < p \quad p_c(k = 1) = 0.9950$ (b), $p_c(k = 1) < p \quad p_c(k = 2) = 0.9955$ (c) and $p = 1.0$ (d). The number accompanying each curve denotes the layer number.

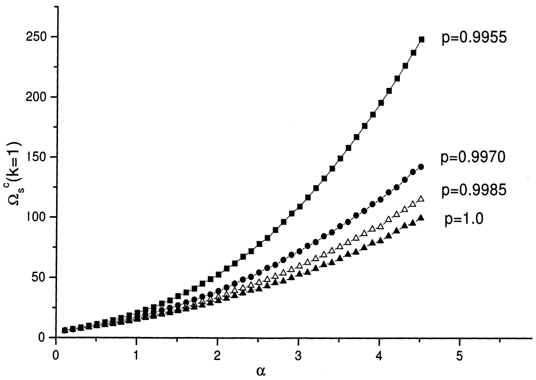

FIG. 4. The dependence of the critical surface transverse magnetic field $^c_s(k = 1)$ as a function of the parameter α for a fixed temperature $T = 0.05$ and different probability values: $p = 0.9955 < p_c = 0.9949$, $p = 0.9970$, $p = 0.9985$ and $p = 1.0$.

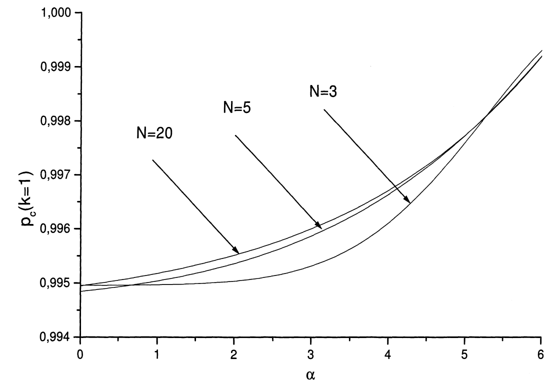

FIG. 5. The dependence of the critical probability p_c as a function of the parameter α for a fixed temperature $T = 0.05$ and different thicknesses of the film $N = 3$, $N = 4$, $N = 5$ and $N = 20$ layers.

of each layer is non null at low temperatures, even for large values of $_s$ (Fig. 3a). When $p_c < p \quad p_c(k = 1)$, the longitudinal magnetisations are: $m_1^z = 0$ and $m_k^z \neq 0$ for each layer $k > 1$, (Fig. 3b). For $p_c(k = 1) < p \quad p_c(k = 2)$ (Fig. 3c) $m_1^z = 0$, $m_2^z = 0$ and $m_k^z \neq 0$ for all layers $k > 2$, and so on. The totally ordered film case, seen for $p = 1.0$, where each layer becomes disordered at a finite surface transverse field value is illustrated in Fig. 3d. The scenario in Fig. 2 is exactly reproduced here, when the longitudinal magnetisation behaviour is analyzed.

In the following we will focus on the order-disordering of the surface (layer $k = 1$). Therefore $^c_s(k = 1)$ and $p_c(k = 1)$ will be used to denote the critical surface transverse magnetic field and the critical probability corresponding to this layer, respectively. To illustrate how the critical surface transverse magnetic field varies with the parameter α we present in Fig. 4 the results found for several values of the probability $p > p_c(k = 1)$. It is found that $^c_s(k = 1)$ increases when the parameter α increases and decreases when p increases for a fixed value of α. The former finding is due to the effect of the factor k^α on the layers $k \geq 2$, since the surface transverse magnetic field ($k = 1$) is not affected by increasing α values. While the applied transverse magnetic field in the other layers is reduced by the factors 2^α, 3^α,... and so on. The later result is due to the fact that, for a fixed exponent α, with increasing probability ($p \to 1.0$), the applied surface transverse magnetic field acts on all the sites of the surface, so this layer needs less surface transverse magnetic field to become disordered (Fig. 4).

On the other hand, the effect of increasing α on the critical probability $p_c(k = 1)$ is illustrated for several film thickness values in Fig. 5. The critical probability increases when the film thickness and/or the exponent α increases. Indeed, for a fixed parameter α, the thick film rate of spin that is subject to the transverse magnetic field must be higher to overcome the influence of the other layers. The effect of increasing α as mentioned above is still valid here.

To show the effect of the film thickness on these critical parameters, we present, in Figs. 6 and 7, our results for several values of the exponent α. These two figures show that $^c_s(k = 1)$,

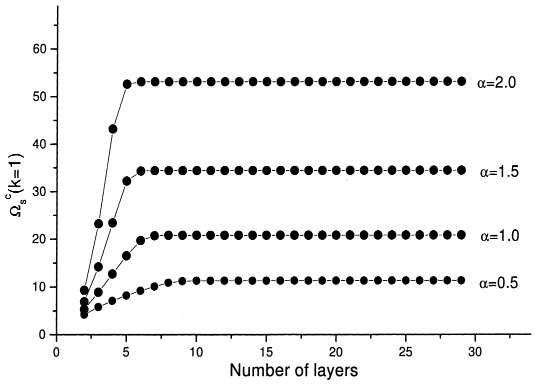

FIG. 6. The dependence of the critical surface transverse magnetic field $^c_s(k = 1)$ as a function of the number of layers for $T = 0.05$ and different values of the exponent $\alpha = 0.5$, $\alpha = 1.0$, $\alpha = 1.5$ and $\alpha = 2.0$.

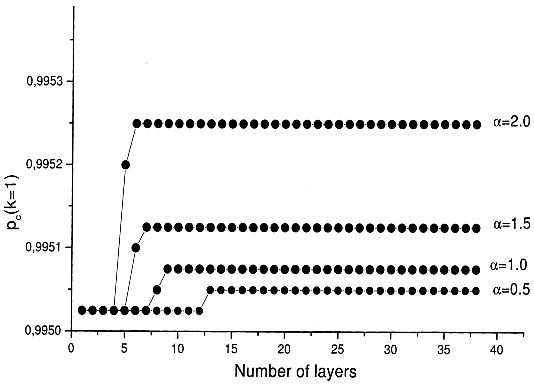

FIG. 7. The dependence of the critical probability p_c as a function of the number of layers for $T = 0.05$ and different values of the exponent $\alpha = 0.5$, $\alpha = 1.0$, $\alpha = 1.5$ and $\alpha = 2.0$.

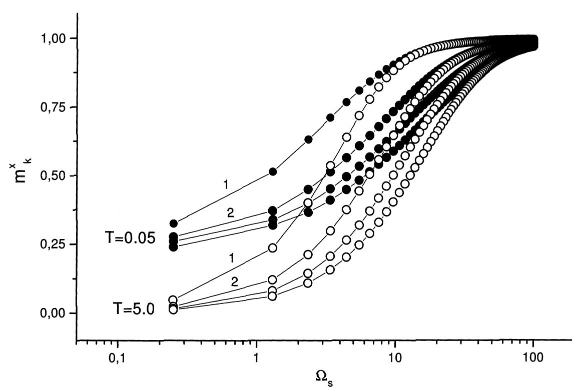

FIG. 8. The behaviour of the transverse magnetisation m_k^x as a function of the surface transverse magnetic field $_s$ for $\alpha = 1.0$ and two temperatures $T = 0.05$ and $T = 5.0$. The number accompanying each curve denotes the layer number.

(resp. $p_c(k = 1)$) undergoes a jump, but stabilises at a certain value not affected by the film thickness increase. From these figures one can also conclude that $^c_s(k = 1)$ (resp. $p_c(k = 1)$) increases when the exponent α increases, as has already been shown in Figs. 4 and 5, respectively. From Fig. 7 we see that for a thin film and sufficiently large values of the exponent α, $p_c(k = 1)$ depends strongly on the size of the film. While for small values of α and/or a large film thickness, $p_c(k = 1)$ is independent of the thickness of the film. This finding is in good agreement with previous results established for a uniform transverse magnetic field ($\alpha = 0$) acting on each layer. The behaviour of the transverse magnetisations is presented in Fig. 8 for two temperatures, $T = 0.05$, $T = 5.0$, and $\alpha = 1.0$. Indeed, for a fixed low value of the transverse magnetic field,

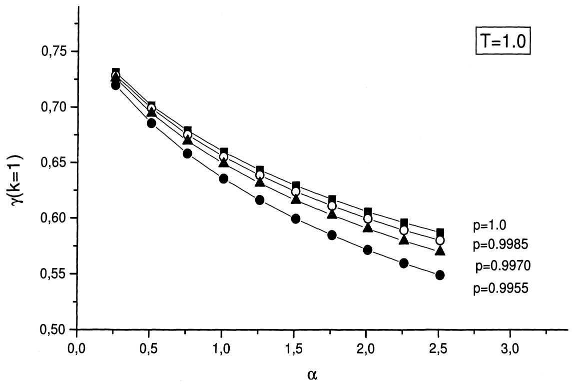

FIG. 9. The dependence of the surface critical exponent $\gamma(k=1)$ on the parameter α for a fixed temperature $T=1.0$ and different values of the probability p.

the effect of the increasing temperature is to decrease the transverse magnetisation amplitudes for small values of the surface transverse field, as is illustrated by Fig. 8. This figure shows also that the effect of increasing the surface transverse magnetic field is to increase the transverse layer magnetisation amplitudes and to overcome the temperature effect.

In order to complete this study, we investigate the behaviour of the critical exponent $\gamma(k)$ for a fixed layer k, defined as the behaviour of the longitudinal magnetisation m_k^z:

$$m_k^z = [(\ _k - \ _s^c(k))/\ _s^c(k)]^{\gamma(k)}. \tag{10}$$

We deduce the critical exponent to be $\gamma(k) = Log(m_k^z)/Log(\omega_k^r)$, where the reduced transverse magnetic field is defined by $\omega_k^r = [\ _k - \ _s^c(k)]/\ _s^c(k)$. The numerical results for the surface critical exponent $\gamma(k=1)$ are given in Fig. 9. The critical exponents corresponding to the other layers, $\gamma(k)$, $k \geq 2$, exhibit the same behaviour as $\gamma(k=1)$. Indeed, Fig. 9 shows that the critical exponent $\gamma(k=1)$ decreases for increasing α values at a fixed probability $p > p_c(k=1)$. It is also found that, for a fixed value of the exponent α, the critical exponent increases when the probability increases ($p \to 1.0$). These considerations are in good agreement with the results found in the literature.

IV. Conclusion

Using the finite cluster (FC) method, we have studied the order-disorder layering transitions under the effect of a variable surface transverse magnetic field, according to the law $\ _k = \ _s/k^{\alpha}$, $(k = 1, ..., N)$. The surface transverse magnetic field $\ _s$ is distributed following the probability law Eq. 3. We show the existence of a critical probability p_c below which the film is always ordered, at very low temperatures, even for large values of the surface transverse magnetic field. Above the critical probability we found a sequence of critical probabilities $p_c(k)$ at which the first k layers become disordered at a sequence of critical transverse magnetic field values $\ _s^c(k)$. It arises that, when comparing the pure case ($p = 1.0$) with the presence of a probability, the dilution effect is to increase the surface transverse field values needed to disorder each layer of the system.

Indeed, a sequence of order-disorder layering transitions occurs when the probability decreases from the value $p = 1.0$, corresponding to a totally ordered film at very low temperatures.

Moreover, it is found that the critical transverse magnetic field, ${}^{c}_{s}(k)$ and the critical probability $p_c(k)$ are functions of the exponent α and the thickness of the film. The behaviour of the longitudinal layer and the transverse magnetisations were illustrated for several values of the film thickness and the exponent α. Finally, in order to complete this study, a numerical study of the surface critical exponent $\gamma(k = 1)$ was investigated.

Appendix

The coefficients $A_k, (k = 0, 1, ..., 6)$ were calculated to be

$$
\begin{aligned}
A_0 &= (1/64)g_1 + (3/32)g_2 + (15/64)g_3 + (5/16)g_4 + (15/64)g_5 + (3/32)g_6 + (1/64)g_7 \\
A_1 &= (1/64)g_1 + (1/16)g_2 + (5/64)g_3 - (5/64)g_5 - (1/32)g_6 - (1/64)g_7 \\
A_2 &= (1/64)g_1 + (1/32)g_2 - (1/64)g_3 - (1/16)g_4 - (1/64)g_5 + (1/32)g_6 + (1/64)g_7 \\
A_3 &= (1/64)g_1 - (3/64)g_3 + (3/64)g_5 - (1/64)g_7 \\
A_4 &= (1/64)g_1 - (1/32)g_2 - (1/64)g_3 + (1/16)g_4 - (1/64)g_5 - (1/32)g_6 + (1/64)g_7 \\
A_5 &= (1/64)g_1 - (1/16)g_2 + (5/64)g_3 - (5/64)g_5 + (1/16)g_6 - (1/64)g_7 \\
A_6 &= (1/64)g_1 - (3/32)g_2 + (15/64)g_3 - (5/16)g_4 + (15/64)g_5 - (3/32)g_6
\end{aligned}
\tag{11}
$$

with

$$
\begin{aligned}
g_1 &= [(6 + \sqrt{36 + {}^{2}_{s}} - {}^{2}_{s})/(6 + \sqrt{36 + {}^{2}_{s}} + {}^{2}_{s})] \tanh(\beta\sqrt{36 + {}^{2}_{s}}), \\
g_2 &= [(4 + \sqrt{16 + {}^{2}_{s}} - {}^{2}_{s})/(4 + \sqrt{16 + {}^{2}_{s}} + {}^{2}_{s})] \tanh(\beta\sqrt{16 + {}^{2}_{s}}), \\
g_3 &= [(2 + \sqrt{4 + {}^{2}_{s}} - {}^{2}_{s})/(2 + \sqrt{4 + {}^{2}_{s}} + {}^{2}_{s})] \tanh(\beta\sqrt{4 + {}^{2}_{s}}), \\
g_4 &= [({}_{s} - {}^{2}_{s})/({}_{s} + {}^{2}_{s})] \tanh(\beta {}_{s}), \\
g_5 &= [(-2 + \sqrt{4 + {}^{2}_{s}} - {}^{2}_{s})/(-2 + \sqrt{4 + {}^{2}_{s}} + {}^{2}_{s})] \tanh(\beta\sqrt{4 + {}^{2}_{s}}), \\
g_6 &= [(-4 + \sqrt{16 + {}^{2}_{s}} - {}^{2}_{s})/(-4 + \sqrt{16 + {}^{2}_{s}} + {}^{2}_{s})] \tanh(\beta\sqrt{16 + {}^{2}_{s}}), \\
g_7 &= [(-6 + \sqrt{36 + {}^{2}_{s}} - {}^{2}_{s})/(-6 + \sqrt{36 + {}^{2}_{s}} + {}^{2}_{s})] \tanh(\beta\sqrt{36 + {}^{2}_{s}}).
\end{aligned}
\tag{12}
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