

## Wetting of an Ising system with perfect and corrugated surfaces in a transverse field

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Using the mean field theory, a comparative study of the wetting and layering transitions of a spin-1/2 Ising model with perfect and corrugated surfaces, is established. The phase diagrams are investigated and compared in the presence of both a longitudinal and surface fields. The effect of both the temperature and the transverse field on the wetting and layering transitions are established

### I. INTRODUCTION

Recently, the wetting and layering transitions of magnetic Ising systems have been subject of great interest. Experimental studies have motivated much theoretical works in order to understand and explain the growth of thin layers from only single atoms. A simple lattice-gas model with layering transitions has been introduced and studied in the mean field approximation by de Oliveira and Griffiths [1].

Multilayer films adsorbed on attractive substrates may exhibit a variety of possible phase transitions, as has been reviewed by Pandit *et al.* [2], Nightingale *et al.* [3], Patrykiewicz *et al.* [4] and Ebner *et al.* [5-8]. One type of transitions is the layering transitions, in which the thickness of a solid film increases discontinuously by one layer as the pressure is increased. Such transitions have been observed in a variety of systems including for example  $^4\text{He}$  [9,10] and ethylene [11,12] adsorbed on graphite. Ebner and Saam [13] carried out Monte Carlo simulations of such a lattice gas model. Huse [14] applied renormalization group technique to this model. It allowed the study of the effects on an atomic scale in the adsorbed layers. The lattice gas models applied to the wetting phenomena was reviewed by Dietrich [15]. The effect of finite size on such transitions has been studied, in a thin film confined between parallel planes or walls, by Nakanishi and Fisher [16] using mean field theory.

The model of transverse field was originally introduced by de Gennes [17] for hydrogen-bonded ferroelectrics such as  $\text{KH}_2\text{PO}_4$ . Since then, this model has been applied to several physical systems, like  $\text{DyVO}_2$ , and studied by a variety of sophisticated techniques [18-21].

In order to study the amorphization of a crystalline Ising ferromagnet with a transverse field, Kaneyoshi [22] introduced the differential operator technique as a generalised but approximate Callen relation derived by Sa Barreto and Fittipaldi [23]. The system has a finite transition temperature, which can be decreased by increasing the transverse field to a critical value  $\Omega_c$ . The effect of a transverse field on the critical behaviour and the

magnetisation curves was studied [18-21] and by Kaneyoshi *et al.* [24,25]. Using the perturbative theory, Harris *et al.* [26] have studied the layering transitions at  $T=0$  in the presence of a transverse field.

Benyoussef and Ez-Zahraouy have studied the layering transitions of Ising model thin films using a real space renormalization group [27], and transfer matrix [28] methods. In a previous work [29] we have established the effect of temperature and transverse field, for a fixed surface field values, on the wetting and layering transitions of an Ising system with perfect surfaces.

The purpose of this work is to study the effect of a corrugated surface on the wetting and layering transitions, of an Ising system spin-1/2, using the mean field theory. The outline of this work is as follows. In Section 2, the model and method are presented. Section 3 is devoted to study the ground state for the perfect and corrugated surface cases. The results and the phase diagrams obtained are discussed in Section 4.

### II. MODEL AND METHOD

We consider a film with finite thickness of a three dimensional spin-1/2 model, with  $N$  layers, limited by two surfaces. Figure 1 represents the geometry of this system for :

- a) two perfect surfaces,
- b) presence of a corrugated surface.

The Hamiltonian describing this system can be written as

$$H = - \sum_{\langle i,j \rangle} J_{ij} S_i^z S_j^z - \sum_i (H_i S_i^z + \Omega S_i^x) \quad (1)$$

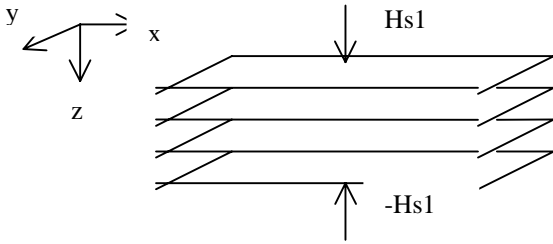
where the first summation is carried out over nearest-neighbour pairs of spins.  $S_i^\alpha = \pm 1$ ,  $\alpha = z, x$  are the Pauli matrices for a spin  $i$ . The exchange interaction  $J_{ij} = J$  is assumed to be constant, and  $\Omega$  is the transverse field.

The total longitudinal field  $H_i$ , applied on a site  $i$ , is distributed according to the nature of the top surface as it is discussed below.

For a system with perfect surfaces, Fig. 1a,  $H_i$  is assumed to be uniform in a layer  $k$ , and defined by:

$$H_k = \begin{cases} H + H_{s1} & \text{for } k=1 \\ H & \text{for } 1 < k < N \\ H + H_{sN} & \text{for } k=N \end{cases} \quad (2)$$

where the surface fields  $H_{s1}$  and  $H_{sN} = -H_{s1}$  are applied on the first layer  $k=1$  and the last layer  $k=N$ , respectively.  $H$  is the external field applied on the whole system.

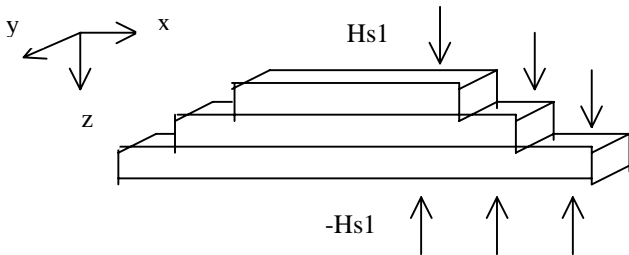


**FIG. 1a.** Geometry of the model of perfect surface case with  $N$  layers in the  $z$  direction. The system is infinite in the  $x$  and  $y$  directions.

For a corrugated surface film with  $n$  steps, each step containing  $L$  spins in the  $x$  direction,  $H_i$  is given by:

$$H_k = \begin{cases} H + H_{s1} & \text{for } i \in S_1 \\ H & \text{for } i \in S_k : 1 < k < N \\ H + H_{sN} & \text{for } i \in S_N \end{cases} \quad (3)$$

where the surface field  $H_{s1}$  acts on the corrugated surface  $S_1$ , and  $H_{sN} = -H_{s1}$  is applied on the bottom surface  $S_N$ , Fig. 1b.



**FIG. 1b.** Geometry of the model of corrugated surface case with  $n$  steps, each step contains  $L$  spins in the ' $x$ ' direction.

The configurations  $S_k$  ( $0 \leq k \leq N$ ) are defined in Section 3 for both the perfect and corrugated surfaces.  $H$  is the external field applied on the whole system. The part of the Hamiltonian describing a site  $i$ , for the perfect and corrugated surfaces, is given by :

$$H_i = -(\sum_{j \neq i} J_{ij} S_i^z + H_i) + \Omega S_i^x \quad (4)$$

the summation runs over nearest neighbour sites  $j$  of  $i$ . The diagonalization of the operator  $H_i$  leads to the eigen values

$$\lambda_i^\pm = \pm \sqrt{x_i^2 + H_i^2}, \text{ where } x_i = \sum_{j \neq i} J_{ij} S_j^z$$

The magnetisation per site can be written as

$$m_i = \frac{\text{Tr} S_i^z \exp(-\beta H_i)}{\text{Tr} \exp(-\beta H_i)} = \left[ \frac{(k_i + \lambda_i^+)^2 - \Omega^2}{(k_i + \lambda_i^+)^2 + \Omega^2} \right] \tanh(\beta \sqrt{x_i^2 + \Omega^2}). \quad (5)$$

Using the mean field theory, the free energy of the system can be written as follows :

$$F = -\frac{1}{\beta} \sum_i \log(2 \cosh(\beta \lambda_i^+)) + \frac{1}{2} \sum_i \sum_j J_{ij} m_i m_j \quad (6)$$

For a simple cubic lattice, the magnetisation and the free energy for each plane  $k$  are given, respectively, by the following expressions:

$$m_k = \frac{1}{\lambda} [4m_k + m_{k+1} + m_{k-1} + H'] \tanh(\beta') \quad (7)$$

and

$$F_k = -\frac{1}{\beta} \log(2 \cosh(\beta \lambda_k)) + \frac{1}{2} (4m_k + m_{k+1} + m_{k-1}) \quad (8)$$

with

$$\lambda_k = \sqrt{(4m_k + m_{k+1} + m_{k-1} + H')^2 + \Omega'^2}, \quad (9)$$

assuming that  $J_{ij} = J$ , the reduced parameters are defined by:

$$\beta' = \beta J, H' = \frac{H}{J},$$

and:

$$\Omega' = \frac{\Omega}{J}.$$

### III. GROUND STATE

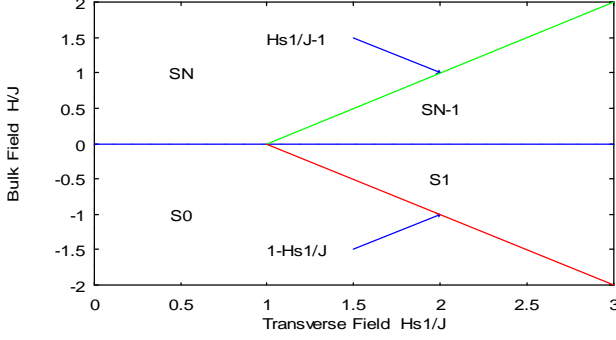
#### A. PERFECT SURFACE

The ground state of this model is established in Fig. 2a. The start point is a situation where all spins are down: configuration  $S_0$ .

For  $H_{s1}/J \leq 1$ , we have only one transition,  $S_0 \leftrightarrow S_N$ . By contrast, for  $H_{s1}/J > 1$ , we have three transitions namely; the first transition,  $S_0 \leftrightarrow S_1$ , arises for  $H/J = 1 - H_{s1}/J$ , the second transition,  $S_1 \leftrightarrow S_{N-1}$ , occurs for  $H/J = 0$ , while the last transition  $S_{N-1} \leftrightarrow S_N$ , is seen for  $H/J = 1 + H_{s1}/J$ . The

notation  $S_k (k=0,1,\dots,N)$  is a situation where, starting from the top surface,  $k$  layers are spin-up and the remainder  $N-k$  layers are spin-down.

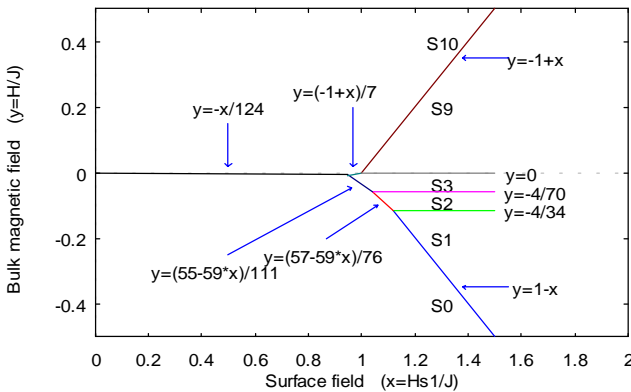
The Fig. 2a shows that the transitions arise for values of  $H_{s1}/J$  above a critical value,  $H_{s1}^c/J=1$ .



**FIG 2a.** Ground state phase diagrams in the  $(H/J, H_{s1}/J)$  plane for the perfect surface case ( $N=20$  layers).

### B. CORRUGATED SURFACE

The model is described in section 2, the corresponding ground state is illustrated in Fig. 2b for a system formed with  $N=10$  layers,  $n=2$  steps and  $L=10$  spins, for each step, in the  $x$  direction. The start point is a situation, called  $S_0$ , where all the spins are down. Under the effect of increasing the surface field  $H_{s1}/J$ , and for a bulk field value  $H/J$  close to  $1-H_{s1}/J$ , the spins of the top external surface, called  $S_1$ , will flip and become up. Increasing the bulk field, the spins of the layer 2 will flip, this situation is noted  $S_2$ .



**FIG 2b.** Ground state phase diagrams in the  $(H/J, H_{s1}/J)$  plane for the the corrugated surface case with  $N=10$  layers,  $n=2$  steps and  $L=10$  spins for each step.

Increasing the bulk field more and more, the spins of the layer 3 will flip, this configuration is noted  $S_3$ , and so on. As it is shown Fig. 2b, the transition  $S_0 \leftrightarrow S_1$ , which appears for  $H/J=1-H_{s1}/J$  and the transition  $S_{N-1} \leftrightarrow S_N$ , arising for  $H/J=-1+H_{s1}/J$ , are fixed only by the surface

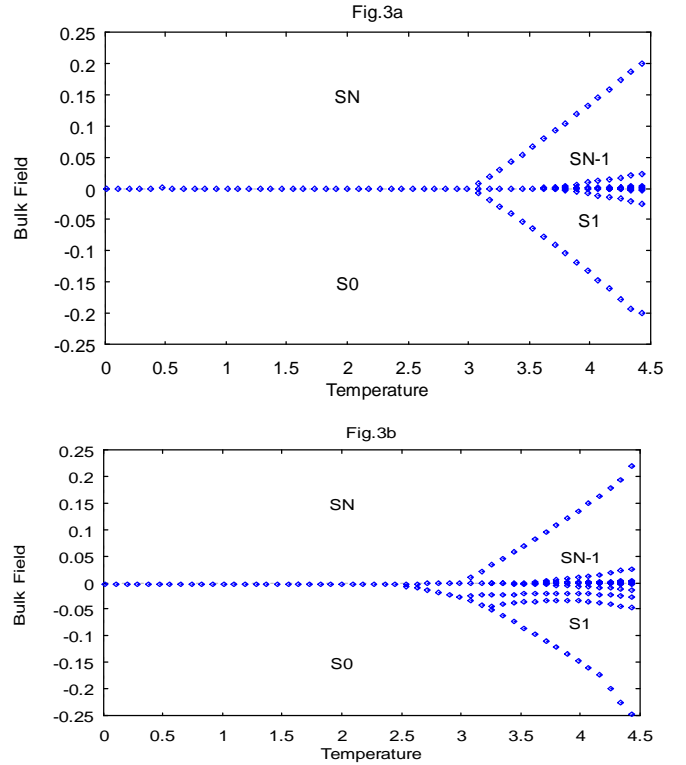
field  $H_{s1}/J$  value, and do not depend on the parameters  $n$  and  $L$ .

By contrast, the number of transitions parallel to the line  $H/J=0$  is close to the number of corrugated surfaces  $n$ , and the corresponding value of  $H/J$  is fixed by the number of spins per step  $L$ .

A generalisation of the ground state energy  $E(S_k, n, L, N)$ , of this system, is given in Appendix , as a function of arbitrary values of the parameters:  $n, L$  and  $N$ .

### IV. RESULTS AND DISCUSSION

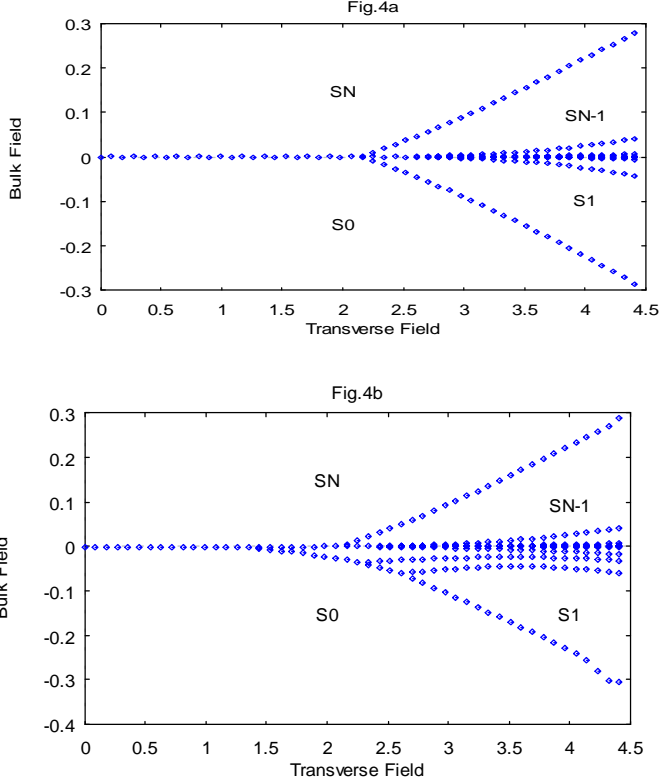
Numerical results are giving for a system formed with  $N=20$  ferromagnetic layers of a spin-1/2 Ising model with free bound conditions. In order to examine the temperature effect, in absence of transverse magnetic field,  $\Omega/J=0$ , on the wetting and layering transitions, we plot in Fig. 3 the corresponding phase diagrams.



**FIG 3.** Phase diagrams in  $(H/J, T/J)$  plane for  $H_{s1}/J=0.9$  and  $\Omega/J=0$ : a) perfect surface case, b) presence of a corrugated surface.

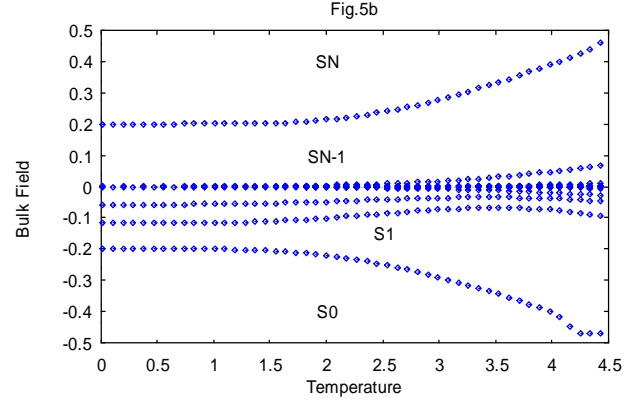
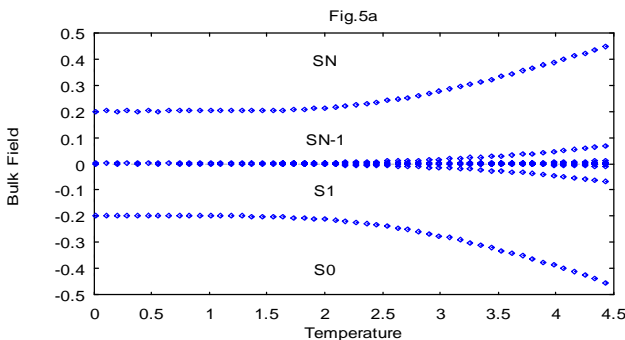
By increasing the temperature we show the existence of a critical value,  $T_w/J$ , above which a sequence of layering transitions occurs this means that the temperature effect is sufficient to produce layering transitions. This temperature,  $T_w/J$ , is called the "wetting temperature", which depends on the transverse field and surface magnetic field values. The first and last layer transitions occur in the absence of the transverse magnetic field, but only under the increasing bulk magnetic field for a temperature  $T/J > T_w/J$ , the other layering transitions arise for increasing temperatures. On the other hand, the corrugation effect is to accelerate the layering transitions phenomenon since the transitions

$S_0 \leftrightarrow S_2$  and  $S_0 \leftrightarrow S_3$  are present in the corrugated surface case: Fig. 3b and are absent in the perfect surface situation: Fig. 3a. The same behaviour is found when inverting the temperature and the transverse field roles, as it is summarised in Fig. 4. The phase diagrams show that the layer transitions are found for  $\Omega/J > \Omega_w/J$  with increasing transverse magnetic field at fixed temperature.  $\Omega_w/J$  is called the "wetting" transverse field. The same transitions, found in Fig. 3, are still present for the corrugated surface case, Fig. 4b, and disappear for the perfect surface situation, Fig. 4a. Figs. 3 and 4 are plotted for a surface field value  $H_{s1}/J=0.9$ , less than the critical value 1.

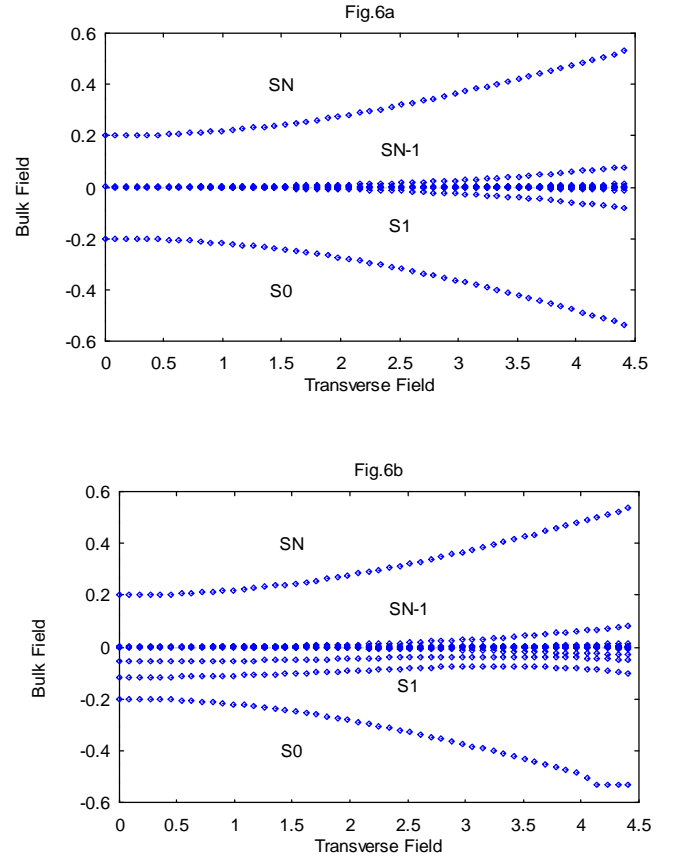


**FIG 4.** Phase diagrams in  $(H/J, \Omega/J)$  plane for  $H_{s1}/J=0.9$  and  $T/J=0.5$ : a) perfect surface case, b) corrugated surface case.

It is worth to note that the "wetting" parameters,  $T_w/J$  and  $\Omega_w/J$ , disappear since the layering transitions are present even for a very low temperature: Figs 5a and 5b, and a very low transverse field: Figs 6a and 6b.



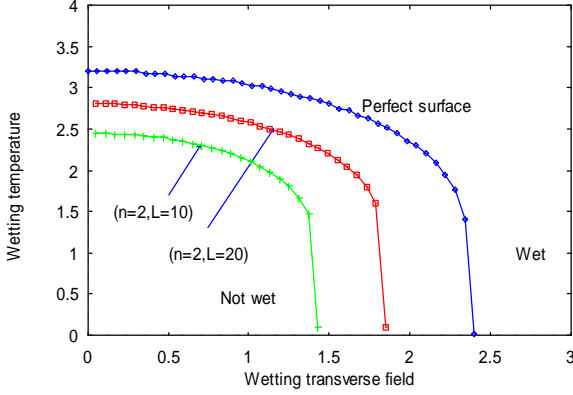
**FIG 5.** Phase diagrams in  $(H/J, T/J)$  plane for  $H_{s1}/J=1.2$  and  $\Omega/J=0$ : a) perfect surfaces case, b) presence of a corrugated surface.



**FIG 6.** Phase diagrams in  $(H/J, \Omega/J)$  plane for  $H_{s1}/J=1.2$  and  $T/J=0.5$ : a) perfect surface case, b) presence of a corrugated surface

The effect of increasing the surface field above the critical value is summarised in Figs. 5 and 6 for  $H_{s1}/J=1.2$ . Furthermore, the transitions  $S_1 \leftrightarrow S_2$  and  $S_2 \leftrightarrow S_3$  are present in Figs. 5b and 6b for  $T/J \rightarrow 0$  and  $\Omega/J \rightarrow 0$ , respectively, in good agreement with the ground state illustrated in Fig. 2b, for the corrugated surface case.

On the other hand, the dependency of the wetting temperature  $T_W/J$  on the wetting transverse field  $\Omega_W/J$ , is illustrated in Fig. 7, corresponding to the surface field value  $H_{S1}/J=0.9$ , for the both cases: perfect and corrugated surfaces.



**FIG 7.** The wetting temperature  $T_W/J$  dependency on the wetting transverse field  $\Omega_W/J$ , with fixed surface field  $H_{S1}/J=0.9$ , for the both cases: perfect and corrugated surface ( $N=20$  layers). For the corrugated surface model, two cases are presented:  $(n=2, L=10)$  and  $(n=2, L=20)$ .

As it has been outlined above, the corrugation effect is to accelerate the wetting phenomenon since the wetting region, of the phase diagram in Fig. 7, occurs first for the corrugated surface before that one corresponding to the perfect surface. Furthermore, when the number of spins  $L$  increases ( $L=10$  and  $L=20$  in Fig. 7), the corrugated surface model become similar the perfect surface model

## V. CONCLUSION

Within the mean field theory, we have studied the wetting and layer transitions of a 3-D spin-1/2 Ising model. For a surface field less than the critical value 1, the system exhibits a sequence of layering transitions only above a wetting temperature (wetting transverse field) for fixed transverse field (temperature). For surface fields higher than the critical value, the layering transitions under only

under the effect of increasing the bulk field even for  $\Omega/J=0$  or  $T/J \rightarrow 0$ . Furthermore the corrugation effect is accelerate the layering transitions and wetting phenomena compared to perfect surfaces.

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## APPENDIX : THE GROUND STATE ENERGY

The ground state energy  $E_j$  of a given configuration  $S_j$  is calculated exactly from the Hamiltonian (1). The transition from a configuration  $S_j$  to an other configuration  $S_k$  is obtained by the equality of their energies  $E_j$  and  $E_k$ . It is found that the ground state transitions ( $S_j \leftrightarrow S_k$ ) illustrated by Fig. 2, occur according to linear forms:

$$H/J = a + b(H_{S1}/J).$$

As examples we give, hereafter, the constants  $a$  and  $b$  for some transitions:

- The surface transitions  $S_0 \leftrightarrow S_1$  and  $S_{N-1} \leftrightarrow S_N$  are located, respectively, at  $H/J=1-H_{S1}/J$  and  $H/J=-1+H_{S1}/J$ .
- The bulk layering transitions  $S_j \leftrightarrow S_{j+1}$  ( $j=1, \dots, n$ ), occur at  $H/J=(-2)/(2j(L-1)-1)$ .
- The prewetting transitions  $S_0 \leftrightarrow S_j$  ( $j=2, \dots, n+1$ ) are localised at  $H/J=a+b(H_{S1}/J)$  with:  

$$a=(4(n+1)[L(2M-1)-n(L-1)+M]-2n(2M-1)-M+2j)/(2L(n+1)+j^2(L-1)-jL),$$

$$b=(1-2L(n+1))/(2L(n+1)+j^2(L-1)-jL).$$

It is worth to note that the transitions:  $S_0 \leftrightarrow S_1$  and  $S_{N-1} \leftrightarrow S_N$  depend only the surface field  $H_{S1}$  value. The number of transitions  $S_j \leftrightarrow S_{j+1}$  is close to the corrugation number  $n$ . On the other hand for large values of number of spins in each layer,  $L \rightarrow \infty$ , the transitions  $S_j \leftrightarrow S_{j+1}$  are shifted to  $H/J=0$ .

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