Spontaneous breaking of layer symmetry in an Ising film and universality (Physica A 237 (1997) 320-330) ⋆

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Abstract

Within the correlation length equality approach, introduced in previous papers, it is shown a spontaneous symmetry breaking phenomenon among the identical planes of a two-layer ferromagnetic Ising film, according to which the divergence of the correlation length at the critical point is essentially due to a single plane developing strong correlations, the other plane acting as a "spectator", which profits by these correlations. The phenomenon is responsible for the fact that the thermal critical exponent ν does not depend on the coupling between the two planes and coincides with its value in the $2D$ Ising model.

1 Introduction

Recently, we have investigated some critical properties of a two-layer film made of two identical isotropic planes of Ising spins coupled ferromagnetically by nearest-neighbor interactions also along the vertical direction [1]. Denoting by $s_{\mathbf{r}}$ and $u_{\mathbf{r}}$ the spin variables on each plane ($s_{\mathbf{r}}, u_{\mathbf{r}} = \pm 1$), the Hamiltonian H of the model is given by

$$-\beta H \equiv K \sum_{\langle \mathbf{r},\mathbf{r}' \rangle} (s_{\mathbf{r}} s_{\mathbf{r}'} + u_{\mathbf{r}} u_{\mathbf{r}'}) + \rho K \sum_{\mathbf{r}} s_{\mathbf{r}} u_{\mathbf{r}} \qquad (K, \rho > 0) \tag{1}$$

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where $\langle \mathbf{r}, \mathbf{r}' \rangle$ denotes a nearest-neighbor pair on the same plane.

This model is not exactly soluble and has been analysed through several approximate methods (see references in [1]). In [1], by making use of the correlation length equality (CLE) approach, we have obtained quite reliable estimates of the correlation length of the model in the whole paramagnetic region and then of the critical line $K_c(\rho)$ for any positive value of the vertical coupling parameter ρ. Some previous partial results, based on the same approach, were reported in [2].

The two-layer film is exactly soluble in the two cases $\rho = 0$ and $\rho = +\infty$, where it is related to the $2D$ square Ising model. So we know, for $\rho = 0$ and $\rho = +\infty$, that the critical exponent ν associated to the correlation length, is given by $\nu = 1$. Universality arguments then lead to the prediction

$$\nu(\rho) = 1 \qquad , \tag{2}$$

also for $0 < \rho < +\infty$. This equation has been conformed by explicit calculations in [1].

Universality is usually explained on the basis of the general features of the renormalization group transformations (RGT), such as the notion of fixed point [3]. If the RGT's are applied to the model (1), it is expected that, for any ρ, one finally obtains an effective vertical coupling which is infinite (or zero).

In this paper we show, at least for the model (1) and eqn. (2), that universality can also be produced by a subtle dynamical mechanism related to a symmetry breaking phenomenon involving the two identical planes. This feature of universality is obtained in the framework of the CLE approach through some unexpected properties of the reduced probability distributions (RPD) associated to our model. The mechanism, which is described in sect. 3, can also be relevant in connection with the crossover phenomenon which appears when one goes to the $3D$ Ising model. The results given in sect. 3 are based on some preliminary considerations about the CLE method, which are developed in sect. 2.

2 The CLE and CVM methods

It is useful to start from the $2D$ square Ising model and to recall briefly the role of the CLE in this case [4]. For simplicity we consider the isotropic case, with Hamiltonian H

$$-\beta H = K \sum_{\langle \mathbf{r},\mathbf{r}' \rangle} s_{\mathbf{r}} s_{\mathbf{r}'} \qquad (K > 0) \tag{3}$$

The square is made of m rows and n columns and we are interested in the limit $m, n \to \infty$. We assume in the following that $T > T_{\mathrm{c}}$.

Let us consider the RPD along a column, i.e., the probability $p_1(\sigma)$ for a column to have the configuration $\sigma \equiv (s_1, s_2, \ldots, s_m)$. It is obtained by thermal–averaging over the configuration of all the other columns. In the limit $n \to \infty$, we have

$$p_1(\sigma) = \frac{\phi^2(\sigma)}{z_1} \tag{4}$$

where z_1 is a normalization factor, fixed by Tr $p_1 = 1$, and $\phi(\sigma)$ is the σ-component of the eigenvector of the transfer matrix of the model (3),

$$L(\sigma|\sigma') = \exp\left[\frac{K}{2}\sum_{i=1}^{m} s_i s_{i+1} + K \sum_{i=1}^{m} s_i s_i' + \frac{K}{2}\sum_{i=1}^{m} s_i' s_{i+1}'\right] \tag{5}$$

associated to its largest eigenvalue.

Let us consider also the RPD $p_2(\sigma, \sigma')$ for two adjacent columns. It is given by

$$p_2(\sigma, \sigma') = \frac{\phi(\sigma) L(\sigma|\sigma') \phi(\sigma')}{z_2} \tag{6}$$

where z_2 is fixed by Tr $p_2 = 1$.

Now, we introduce a trial function $\widetilde{\phi}(\sigma)$, describing in an approximate manner the exact $\phi(\sigma)$, thus obtaining the trial RPD's

$$\begin{aligned} \widetilde{p}_1(\sigma) &= \frac{\widetilde{\phi}^2(\sigma)}{\widetilde{z}_1} \\ \widetilde{p}_2(\sigma, \sigma') &= \frac{\widetilde{\phi}(\sigma) L(\sigma|\sigma') \widetilde{\phi}(\sigma')}{\widetilde{z}_2} \end{aligned} \tag{7}$$

The CLE consists in requiring $\widetilde{p}_1$ and $\widetilde{p}_2$ to have the same correlation length (in the limit $m \to \infty$).

The simplest possible ansatz for ϕ is given by

$$\widetilde{\phi}_0(\sigma) = \exp\left(A \sum_{i=1}^{m} s_i s_{i+1}\right) \qquad (A > 0) \tag{8}$$

containing a single parameter in the form of an effective coupling among the nearest-neighbor spins of the column. For large T, $\widetilde{\phi}_0(\sigma)$ is surely appropriate, with $A = K/2$; large correlations are taken into account by changing only this dependence of A on K.

Let us consider the trial RPD's (7) defined through $\widetilde{\phi}_0(\sigma)$. The calculation of the correlation length associated to $\widetilde{p}_i$ ($i = 1, 2$) can be achieved by using the transfer matrix formalism: to $\widetilde{p}_i$ there corresponds a suitable transfer matrix and its correlation length is given by

$$\frac{1}{\xi_i} = \ln \frac{\lambda_1^{(i)}}{\lambda_2^{(i)}} \quad , \quad (i = 1, 2) \quad , \tag{9}$$

where $\lambda_1^{(i)}$ and $\lambda_2^{(i)}$ are the largest and next-to-largest eigenvalues of the transfer matrix. The CLE condition determines the parameter A as a function of K, and then $\xi(K) = \xi_1(K) = \xi_2(K)$. It turns out that $\xi(K)$ is coincident with the exact correlation length in the whole paramagnetic region, diverging at the exact critical point $K_\mathrm{c} = \frac{1}{2}\ln(1+\sqrt{2})$ [4]; as a matter of fact we have $\lim_{K\to K_\mathrm{c}} A(K) = +\infty$.

It is relevant for what follows to illustrate the mathematical mechanism by which the CLE, through the ansatz (8), allows to obtain the exact critical exponent $\nu = 1$. In proximity of K_c, where A is large and $x \equiv \exp(-2A)$ is small, we can perform perturbation expansions in powers of x. We have

$$\begin{aligned} \frac{\lambda_1^{(1)}}{\lambda_2^{(1)}} &= 1 + 2x^2 + 2x^4 + \mathrm{O}(x^6) \\ \frac{\lambda_1^{(2)}}{\lambda_2^{(2)}} &= 1 + \alpha(K)\, x^2 + \beta(K)\, x^4 + \mathrm{O}(x^6) \end{aligned} \tag{10}$$

with

$$\begin{aligned} \alpha(K) &= \frac{2\, e^{-2K}\,(1+e^{-2K})}{1-e^{-2K}} \\ \beta(K) &= \frac{2\, e^{-4K}\,(1+e^{-2K})\,(1-4e^{-2K}-e^{-4K})}{(1-e^{-2K})^3} \end{aligned} \tag{11}$$

Then, in proximity of the critical point, the CLE amounts to

$$x^2 \,\Big[\, \alpha(K) - 2 + \Big(\beta(K) - 2\Big)\, x^2 \,\Big] \; = 0 \tag{12}$$

Discarding the trivial solution $x = 0$, one obtains A in terms of K from

$$x^2 = \frac{\alpha(K) - 2}{2 - \beta(K)} \tag{13}$$

We have then that x^2 approaches zero linearly at $K = K_\mathrm{c}$, (the region where (13) makes sense, that is, positive x^2, corresponds to $K < K_\mathrm{c}$), and $\frac{1}{\xi}$ has the same behavior, being proportional to x^2, in proximity of K_c.

Now, we go back to the two-layer film (1). We extend [1,2] in an obvious way the above procedure for the $2D$ Ising model. The analogue of a column in this case is a vertical section, made of two columns, one in each plane. Let us denote by $\mu \equiv (s_1, \dots, s_m; u_1, \dots, u_m)$ a configuration of the spins on a section. Considering also two, three, ..., sections, we are led to the RPD's

$$\begin{aligned} P_1(\mu) &= \frac{\Phi^2(\mu)}{Z_1} \\ P_2(\mu, \mu') &= \frac{\Phi(\mu)L(\mu|\mu')\Phi(\mu')}{Z_2} \\ P_3(\mu, \mu', \mu'') &= \frac{\Phi(\mu)L(\mu|\mu')L(\mu'|\mu'')\Phi(\mu'')}{Z_3} \\ &\cdots\cdots\cdots \end{aligned} \tag{14}$$

where L is the symmetrized transfer matrix of our model. We have also given P_3 for future use.

Now, as in the previous case, we introduce an ansatz for $\Phi(\mu)$. On the basis of the structure and symmetry of the Hamiltonian (1), the most immediate generalization of (8) is the ansatz [1,2]

$$\widetilde{\Phi}_0(\mu) = \exp\left\{\sum_{i=1}^{m}\Big[A(s_i s_{i+1} + u_i u_{i+1}) + B s_i u_i\Big]\right\} \qquad (A, B > 0) \quad , \tag{15}$$

containing an effective horizontal coupling A, the same for the two planes, and an effective vertical interaction B. We consider then the RPD's

$$\begin{aligned} \widetilde{P}_1(\mu) &= \frac{\widetilde{\Phi}_0^2(\mu)}{\widetilde{Z}_1} \\ \widetilde{P}_2(\mu, \mu') &= \frac{\widetilde{\Phi}_0(\mu)L(\mu|\mu')\widetilde{\Phi}_0(\mu')}{\widetilde{Z}_2} \\ \widetilde{P}_3(\mu, \mu', \mu'') &= \frac{\widetilde{\Phi}_0(\mu)L(\mu|\mu')L(\mu'|\mu'')\widetilde{\Phi}_0(\mu'')}{\widetilde{Z}_3} \\ &\cdots\cdots\cdots \end{aligned} \tag{16}$$

In order to estimate the correlation length $\xi(K, \rho)$ of the model along a vertical section, we impose the CLE for $\widetilde{P}_1$ and $\widetilde{P}_2$, in the limit $m \to \infty$. But, in this case, we have two parameters. Suppose that the CLE has been solved with respect to A, giving a function $A(K, \rho, B)$. Then, having satisfied a basic consistency condition at large distances, the residual parameter B can be fixed by requiring to obtain the lowest value for the free energy, that is by considering

$$\sup_{B \geq 0} \frac{\widetilde{Z}_2}{\widetilde{Z}_1}\Big(A(K, \rho, B), B, K, \rho\Big) \tag{17}$$

This is the content of the constrained variational method (CVM) [1,2].

Let us call $\widetilde{\xi}(K,\rho)$ the estimate of $\xi(K,\rho)$ obtained through $\widetilde{P}_1$, $\widetilde{P}_2$ and the CVM. For any $\rho > 0$, there is a value $\widetilde{K}_c(\rho)$ at which $\widetilde{\xi}(K,\rho)$ diverges. This again happens through the divergence of the effective parameter A at $\widetilde{K}_c(\rho)$. On the other hand, at $\widetilde{K}_c(\rho)$, the effective vertical coupling B is strictly positive and finite, for any $\rho > 0$. The behavior of $\widetilde{\xi}(K,\rho)$ in the whole paramagnetic region has been determined in [1]. Here we point out the most relevant feature for what follows: for every fixed ρ (see figure 1), there is always a significant interval $K_1(\rho) < K < K_2(\rho)$, near $\widetilde{K}_c(\rho)$, where $1/\widetilde{\xi}(K,\rho)$ is practically linear. This trend essentially confirms eqn. (2). However, between $K_2(\rho)$ and $\widetilde{K}_c(\rho)$, there is a crossover phenomenon, from $\nu(\rho) = 1$ to $\nu(\rho) = 2$. We have then a signal that $\widetilde{\Phi}_0(\mu)$, the most obvious generalization of the ansatz (8), is not fully reliable when we are very near the critical point.

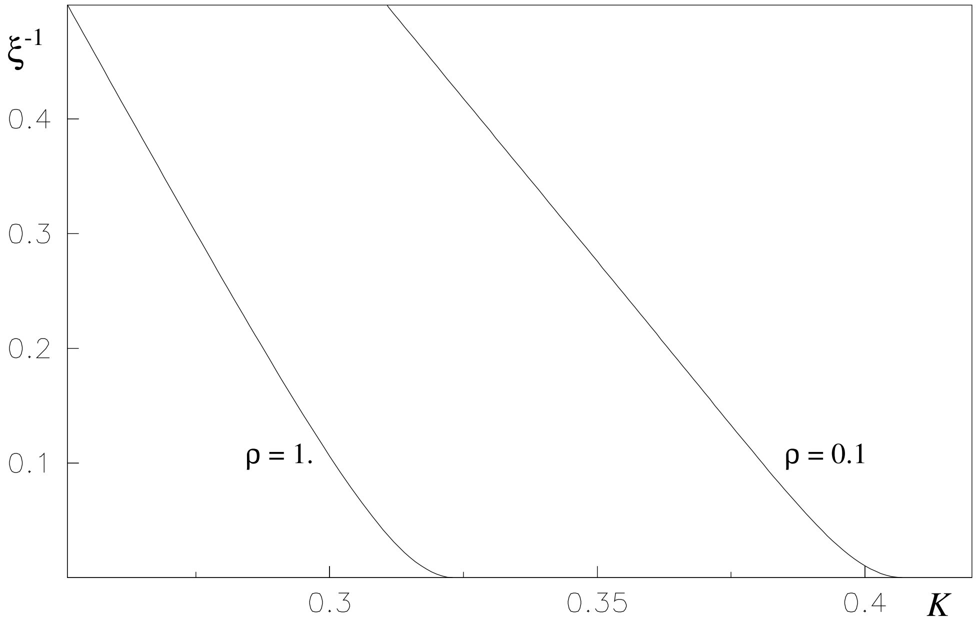

Fig. 1. The behavior of the correlation length in proximity of the critical point as determined by the CVM applied to the trial function (15).

It is useful to see the mathematical origin of this behavior. Let us introduce also in this case the variable $x = \exp(-2A)$ and consider expansions around $x = 0$. The ratio of the relevant eigenvalues of the transfer matrix associated to $\widetilde{P}_1$ is given by

$$1 + a(B)x^4 + \mathrm{O}(x^8) \quad , \quad (B > 0) \quad , \tag{18}$$

while for $\widetilde{P}_2$ we obtain

$$1 + a'(K,\rho,B)\; x^4 + b(K,\rho,B)\; x^6 + \mathrm{O}(x^8) \quad , \quad (\rho > 0, B \geq 0) \tag{19}$$

This analytic structure, which differs from the previous one eqn. (10), is responsible, as it can easily be verified, for $\nu = 2$ at $\widetilde{K}_c(\rho)$.

The origin of the analytic structures (18) and (19) lies in the fact that in $\widetilde{\Phi}_0(\mu)$ we have not one, but two lines of spins where the action of the "critical" parameter A develops. We would have expansions of type (10), for every ρ, and therefore no crossover phenomenon, if it happened that only the spins on a single line were coupled through an effective critical parameter like A. In fact this condition can be authomatically satisfied through the ansatz [1]

$$\widetilde{\Phi}_1(\mu) = \sum_{\{\tau_i=\pm 1\}} \exp\left[A\sum_{i=1}^{M} \tau_i \tau_{i+1} + B\sum_{i=1}^{M} \tau_i(s_i + u_i)\right] \tag{20}$$

The CVM applied to $\widetilde{\Phi}_1(\mu)$ gives quite reliable results as far as the critical point, and fully confirms eqn. (2).

However there remains the problem of the dynamical origin of the analytic structure of the type (10), for any ρ, and of the unreliability of the "obvious" ansatz $\widetilde{\Phi}_0(\mu)$ very near the critical point. In the next section it is shown that this origin is provided by a spontaneous symmetry breaking mechanism.

3 Spontaneous breaking of the layer symmetry within the CLE method and universality

Having two identical planes with the same horizontal coupling, the model (1) is invariant under the exchange of the spins $s_{\mathbf{r}}$ with the spins $u_{\mathbf{r}}$. Unexpectedly, as we will see, the CLE equations admit solutions which do not have this invariance property, thus giving a spontaneous breaking of the layer symmetry of our Hamiltonian (1).

Let us modify the most immediate ansatz (15), by allowing for the possibility to have two different horizontal effective couplings. Instead of (15), let us consider now the three parameter ansatz

$$\widetilde{\Phi}'_0(\mu) = \exp\left\{\sum_{i=1}^{m} \left[(A_1 s_i s_{i+1} + A_2 u_i u_{i+1}) + B s_i u_i\right]\right\} \quad , \tag{21}$$

and try again to calculate the correlation length of the model (1), along a vertical section, by making use of the CLE approach outlined in the previous section.

We start, as we did above, from the trial RPD's

$$
\begin{aligned}
\widetilde{P}'_1(\mu) &= \frac{[\widetilde{\Phi}'_0(\mu)]^2}{\widetilde{Z}'_1} \\
\widetilde{P}'_2(\mu,\mu') &= \frac{\widetilde{\Phi}'_0(\mu)L(\mu|\mu')\widetilde{\Phi}'_0(\mu')}{\widetilde{Z}'_2}
\end{aligned}
\tag{22}
$$

At fixed ρ and K, the CLE for $\widetilde{P}'_1(\mu)$ and $\widetilde{P}'_2(\mu,\mu')$ gives an equation for the three parameters of (21),

$$
F(A_1, A_2, B) = 0 \quad , \tag{23}
$$

with $F(A_1, A_2, B) = F(A_2, A_1, B)$ as a consequence of the layer symmetry. It turns out that, besides the solution $A_1 = A_2 = A(K, \rho, B)$ found in the previous section, eqn. (23) admits solutions such that $A_1 \neq A_2$. For such solutions, in addition to B, another parameter, A_1 or A_2, remains free.

Now, let us see how, from the point of view of the quantity which we are interested into, that is, the correlation length ξ, the solutions of (23) with $A_1 \neq A_2$, can be more appropriate. Firstly we note that the exact ξ is the same for all the RPD's $P_n(\mu_1, \mu_2, \ldots, \mu_n)$. Then, let us consider also the trial RPD

$$
\widetilde{P}'_3(\mu,\mu',\mu'') = \frac{\widetilde{\Phi}'_0(\mu)L(\mu|\mu')L(\mu'|\mu'')\widetilde{\Phi}'_0(\mu'')}{\widetilde{Z}'_3} \tag{24}
$$

and impose a more complete consistency condition at large distances, by requiring $\widetilde{P}'_3$ to have the same correlation length as $\widetilde{P}'_1$ and $\widetilde{P}'_2$. Thus we obtain the further equation

$$
G(A_1, A_2, B) = 0 \quad , \tag{25}
$$

with $G(A_1, A_2, B) = G(A_2, A_1, B)$.

It turns out that, if we impose $A_1 = A_2 = A$, it is impossible to satisfy simultaneously the two equations (23) and (25), notwithstanding the two parameters A and B at our disposal. This is an intrinsic signal of the unreliability of the ansatz $\widetilde{\Phi}_0(\mu)$. On the contrary, if we take in general $A_1 \neq A_2$, the two equations (23) and (25) can be solved with respect to A_1 and A_2, for any B belonging to a some interval I which depends on K and ρ. Then, on the basis of this property, and by exploiting again the variational bounds to the free energy provided by $\widetilde{Z}'_2/\widetilde{Z}'_1$, that is by considering

$$
\sup_{B\geq 0} \frac{\widetilde{Z}'_2}{\widetilde{Z}'_1}\Big(A_1(K,\rho,B), A_2(K,\rho,B), B, K, \rho\Big) \quad , \tag{26}
$$

we determine completely the three effective parameters of the ansatz (21). As a consequence of the layer symmetry, we obtain a unique set of three functions

$A_1(K,\rho)$, $A_2(K,\rho)$, $B(K,\rho)$ such that

$$A_1 = A_1(K,\rho) \quad , \quad A_2 = A_2(K,\rho) \quad , \quad B = B(K,\rho) \tag{27}$$

and

$$\bar{A}_1 = A_2(K,\rho) \quad , \quad \bar{A}_2 = A_1(K,\rho) \quad , \quad B = B(K,\rho) \tag{28}$$

provide all the solutions of (23), (25) and (26).

It turns out that, of these three functions, only one, which we denote by $A_1(K,\rho)$, diverges at a point $\widetilde{K}'_c(\rho)$. At this point also the estimated correlation length $\tilde{\xi}'(K,\rho)$ diverges, while the other two functions $A_1(K,\rho)$ and $B(K,\rho)$ are bounded and finite. The estimates of the critical point given by $\widetilde{K}'_c(\rho)$ are quite good, if compared with previous results [1].

In figures 2 and 3, we plot in K the functions

$$x_1 \equiv \exp[-2A_1(K,\rho)] \quad , \quad x_2 \equiv \exp[-2A_2(K,\rho)] \quad , \quad y \equiv \exp[-B(K,\rho)] \tag{29}$$

for $\rho = 1$ and 0.1, respectively. In figure 4, we give for these values of ρ the estimated correlation length $\tilde{\xi}'(K,\rho)$ compared with the calculations of the previous section.

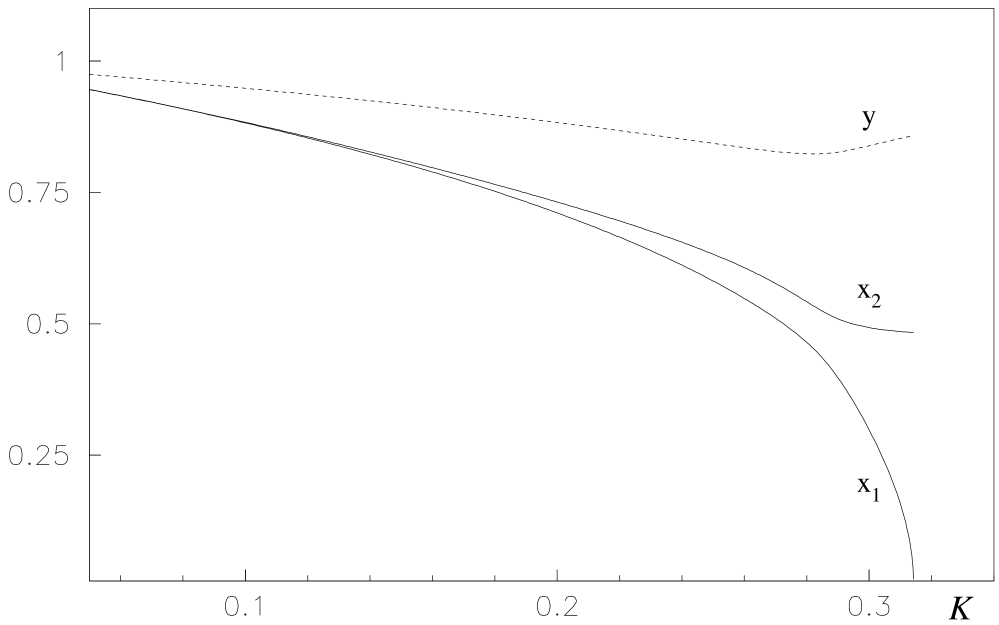

Fig. 2. The solution of (23), (25) and (26) in terms of the variables defined by (29), for $\rho = 1$.

We see from figures 2 and 3 that the reliability of the "natural" ansatz $\widetilde{\Phi}_0(\mu)$ given by (15) is really recovered only far from the critical point, while the spontaneous breaking of the layer symmetry attains its maximum at the estimated critical point. Thus we obtain a physical picture, in which the two layers as a

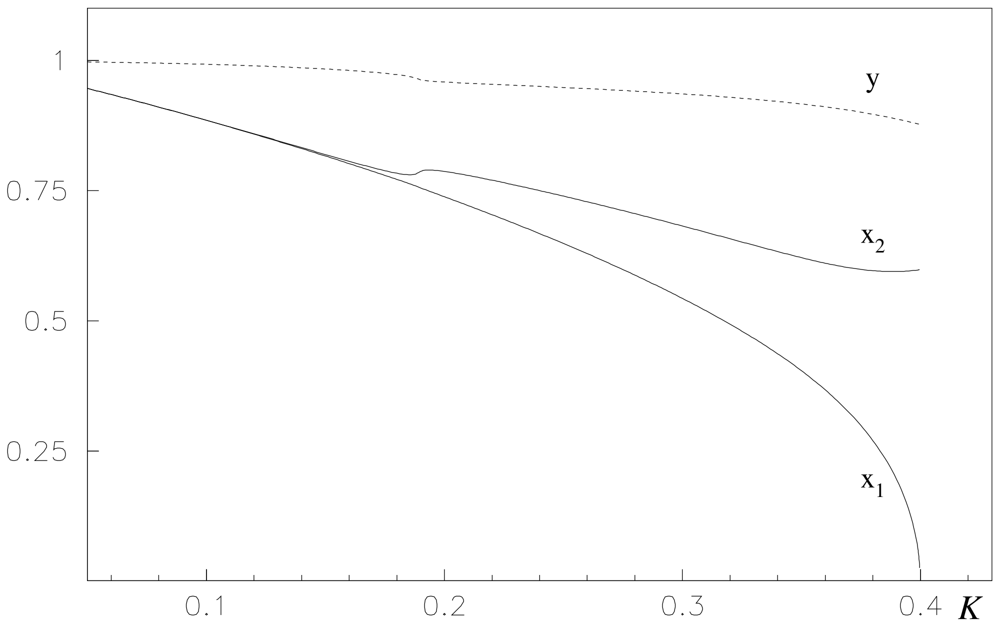

Fig. 3. The solution of (23), (25) and (26) in terms of the variables defined by (29), for $\rho = 0.1$.

whole do have a critical behavior, but showing some differences at an internal level: one is effectively critical, developing strong correlations among its spins through a strong effective coupling, the other acts as a "spectator", keeping a finite effective interaction among its spins and adsorbing the correlations which are significant for criticality from the other plane's ones, thanks to the

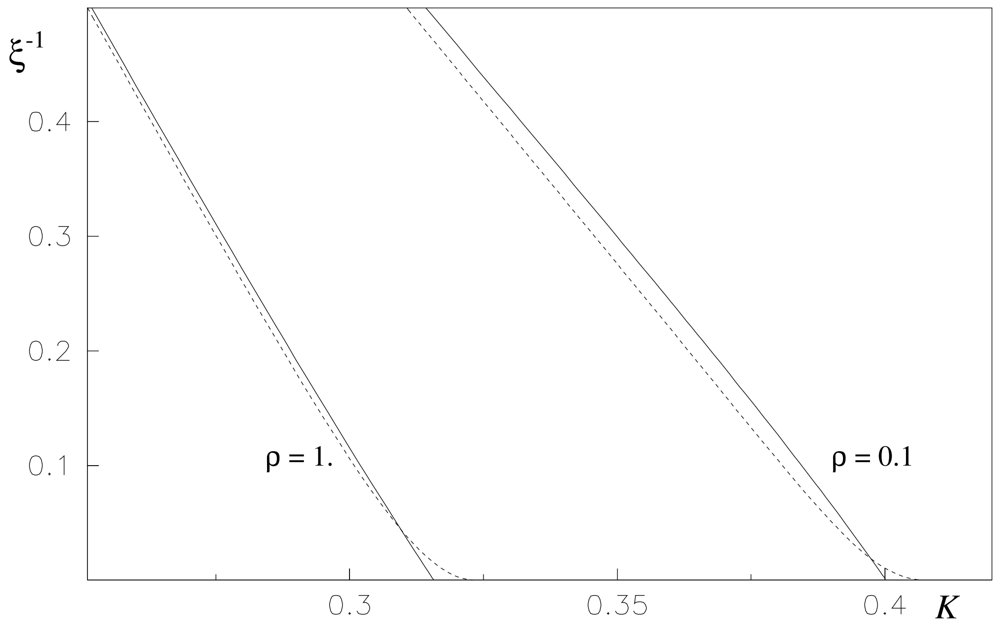

Fig. 4. The behavior of the correlation length in proximity of the critical point as obtained through the ansatz (21). The results of sect. 2, already given in figure 1, are reported here (dotted lines) for comparison.

vertical coupling ρK between the two layers. Which of the layers is effectively critical or spectator is a-priori unknown, due to the original symmetry of the Hamiltonian (1).

Criticality being due to the divergence of an effective coupling involving a single line of spins, eqn. (2) is now fully established, as shown in figure 4 for two typical values of ρ. The mathematical mechanism for this is a consequence of the fact that the inverse correlation length behaves near the critical point as $(x_1 x_2)^2$, but now *only one* of these parameters vanishes at the critical point, thus causing the inverse correlation length to approach zero linearly at the critical point.

4 Conclusions

The spontaneous breaking phenomenon described in the previous section has been detected in terms of some variational parameters. It would be interesting to complete the analysis of this paper, by singling out some physical quantity directly related to the actual symmetry breaking, having a role analogous to the order parameter in the usual phase transitions.

Usually, the degeneracy of the principal eigenvector of the transfer matrix in the thermodynamic limit manifests itself through a strong dependence on the boundary conditions. This fact suggests, in our case, to consider an Ising film made of two non-identical planes, i.e. with different horizontal couplings $K_s \neq K_u$ and to see how the degeneracy is removed. An interesting study of the case $K_s \neq K_u$ has already been done in the literature [5].

The results of sect. 3 are expected to hold also in the case of an $L-$layer Ising film, made of $L > 2$ identical planes. The spontaneous symmetry breaking phenomenon would cause a single plane among them to develop a strong effective horizontal coupling and then strong correlations, the other planes playing the role of spectators which profit by such a situation. In this way one can understand why the critical behavior of this system is really characteristic of the $2D$ Ising model, made of only one plane. However, in the limit $L \to \infty$, we have a symmetry breaking involving infinite elements and this can give rise to additional singularities. This additional singularities can explain the crossover to a different universality class, when we pass from the $2D$ to the $3D$ Ising model [6].

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