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Scaling relationship between effective critical exponents throughout the crossover region in thin Ising films

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Abstract. The Monte Carlo (MC) approach is used to check the validity of the scaling relationship $\gamma = \beta(\delta - 1)$ for the effective critical exponents in thin Ising films. We investigate this relationship not just in the critical region but throughout the crossover to the expected two-dimensional behavior. Our results indicate that this scaling relationship is very well-fulfilled throughout the entire crossover temperature region, as predicted by a previous renormalization group analysis. The two-dimensional universality class of Ising films is confirmed by means of data collapsing plots for $L \times L \times D$ plates with increasing L, up to $L = 100$. The evolution of the maximum value of the effective critical exponents with film thickness is discussed.

PACS. 75.10.Hk Classical spin models – 64.60.Fr Equilibrium properties near critical points, critical exponents – 75.70.-i Magnetic films and multilayers

1 Introduction

Ising films with geometry $L \times L \times D$ ($L \gg D$) have been extensively studied for some years using the MC approach [1–3]. More recently the crossover to two-dimensional behavior in thin films has been also investigated. The main idea is that, as the temperature on the system grows from 0 K, the correlation length takes note eventually that the Ising film is in fact a two-dimensional system. Then the crossover to two dimensional critical behavior begins.

This crossover was considered a long time ago using series expansions techniques [4]. More recently this dimensional crossover has been investigated by means of MC calculations in Ising systems [5], as well as in XY-models [6].

On the other hand, the possibility to produce experimentally thin magnetic films made it possible to carry out comparison with the crossover observed in ferromagnets with a few monolayers in thickness [7,8].

From the theoretical point of view O'Connor and coworkers [9] have calculated analytical expressions for effective critical exponents in systems with film geometry using an "environment friendly" renormalization group analysis. They predict that scaling relations hold for the D dependent effective critical exponents over the entire crossover region.

Up to now, as far as we know, no MC numerical simulation at the crossover region for thin Ising films has been performed in order to check the scaling prediction by O'Connor *et al.* [9]. The problem appears to be that the explicit calculation of the effective critical exponent $\alpha_{\rm eff}(T)$ is non trivial, while $\beta_{\rm eff}(T)$ and $\gamma_{\rm eff}(T)$ can be easily calculated from $M(T)$ and $\chi(T)$, respectively.

We take advantage of the fact that another scaling relation at the crossover region can be alternatively checked, looking at another exponent, $\delta_{\rm eff}(T)$, for which only data for $M(H)$ at $T = T_{\rm c}$ (critical isotherm) are needed.

In the present work we perform MC calculations of $\beta_{\rm eff}$, $\gamma_{\rm eff}$ and $\delta_{\rm eff}$, for Ising films of various thicknesses (D) through the crossover region, and we show that, by an appropriate re-scaling between the variables (H) and $t = (T_{\rm c} - T)$, the relationship $\gamma_{\rm eff} = \beta_{\rm eff}(\delta_{\rm eff} - 1)$ is well fulfilled over the entire crossover region. We also present data collapsing at a constant value of D for different values of L, showing, for the first time with MC data, that the scaling is excellent with the two-dimensional critical exponents approaching the critical point, but that it is spoiled at the crossover region, where the effective exponents become clearly different from the two-dimensional ones.

One difference between our calculation and those in previous work is that, in order to get rid of surface effects [4], we introduce *periodic boundary* conditions in all directions. So our system may be considered as one with anisotropic geometry [10–12], due to the marked difference between D and L. Our MC calculation shows that no specific surface effects are needed in order to observe crossover to the two-dimensional regime, in contrast with systems

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previously investigated using *free surfaces* perpendicular to the films.

2 Numerical results

Determination of $M(T)$, $\chi(T)$ and $M(H)$ were performed by Monte Carlo calculations using a length for the Monte Carlo runs of about 50 000 MCS. We have used a mixed Metropolis/Wolff single cluster algorithm [13] in order to decrease critical slowing down effects near the critical point. The L values considered were 10, 20, 40 and 100, and the D values 3, 5 and 7. The effective exponent numerical values were directly obtained from the raw MC data using the definitions:

$$\beta_{\mathrm{eff}} \equiv \partial \log M / \partial \log t, \quad 1/\delta_{\mathrm{eff}} \equiv \partial \log M / \partial \log H, \quad \text{and} \quad \gamma_{\mathrm{eff}} \equiv \partial \log \chi / \partial \log t.$$

In order to have enough accuracy, we need to calculate in very small steps (for field and temperature) near the critical point. Small steps imply that the derivatives, calculated numerically, contain relatively large errors. To avoid this problem, we just smooth out our data calculating the derivatives with larger steps (±5 data points). In fact, we have used small (±1 data points), intermediate (±3 data points) and relative large steps (±5 data points), and we have checked that with (±5 data points) the errors are minimized, without averaging too much. With this procedure we still have many experimental points at very closely spaced temperatures (fields) near the critical point for the derivatives giving β_{eff}, γ_{eff}, and $1/\delta_{\mathrm{eff}}$. We have checked that this procedure is meaningful for β and $1/\delta$ in the pure two-dimensional and three-dimensional cases. To improve our accuracy we use "early thermalization". This means that we start at $T \approx 0$, $M \approx 1$. At this point, the system is obviously in equilibrium. Proceeding by small steps we expect that, without spending too much calculation time, the system is kept close to equilibrium all the way to the critical point.

The critical temperatures for the different film thicknesses were determined in the usual way, by means of the Binder cumulant method U_L [14,15], using different lateral film sizes. In all cases the Binder cumulant value at the critical temperature comes out very close to the two-dimensional Ising value, which is consistent with the idea that thin films must be in the same university class that two-dimensional Ising systems [5].

Figure 1 presents the calculated values of β_{eff} *vs.* $\log(T_{\mathrm{c}}-T)$ and δ_{eff} *vs.* $\log(H)$ for different values of D and $L = 100$. There are clearly three different zones. A first zone corresponds to the interval of temperatures where the correlation length is not large enough to detect the finite thickness of the film. In this zone the correlation length increases and the effective critical exponents grow towards the three-dimensional value. The second zone starts at a temperature (field) where the correlation length is large enough to note that the system is really a thin film. The effective critical exponents cannot grow anymore, and the crossover to the two-dimensional values begins. Note that the maximum value of β_{eff} depends on D. This may be understood taking into account that for larger D values the system must rise to higher values of ξ (correlation length) in order to initiate the crossover. For all the values of D considered in this work the effective critical exponents do not rise up to the three-dimensional values, due to the small (D) values used [4]. Finally we arrive to the third zone. This is the zone where finite size effects begin to dominate. For larger values of L this zone will begin at higher temperatures (or lower fields). As far as we known this is the first time crossover effects in $(1/\delta)$ have been numerically determined.

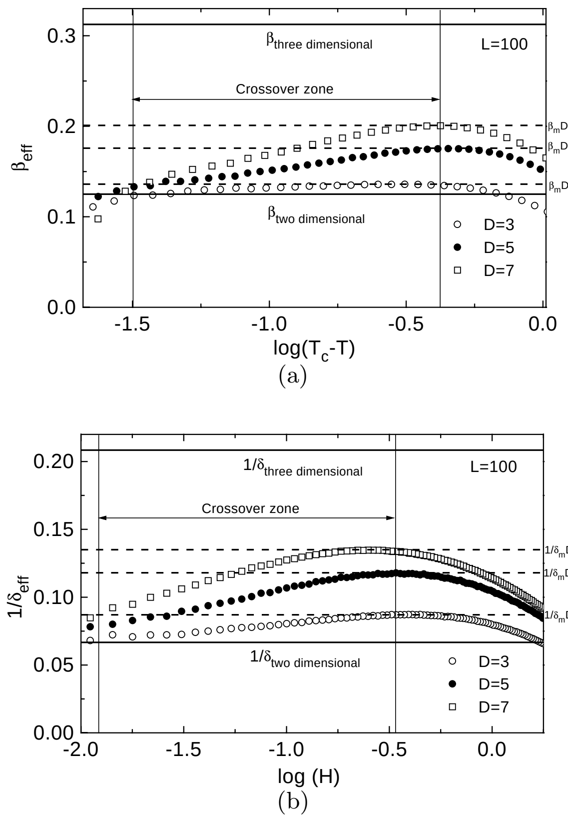

Fig. 1. (a) β_{eff} *vs.* $\log(T_{\mathrm{c}}-T)$ and (b) $1/\delta_{\mathrm{eff}}$ *vs.* $\log(H)$ for $L \times L \times D$ Ising films with $L = 100$ and $D = 3, 5, 7$. Straight lines correspond to the three- and two-dimensional critical exponent values. Doted lines indicate the maximum value of the effective critical exponent for the Ising films.

The finite size dependence on L is checked in Figure 2, where β_{eff} *vs.* $\log(T_{\mathrm{c}}-T)$ is represented for different values of L and for a constant value of $D = 5$. Note how the crossover zone starts always at the same place, due to the constant value of D, but finite size effects start at different temperatures depending on the value of L.

The (more complete) data in Figure 2 show clearly the region where finite size effects become too important, and spoil the numerical value of β, as indicated by the fact that the effective exponent drops clearly below the β (two-dimensional) value as we approach the critical point. This behavior becomes even clearer for $L = 100$.

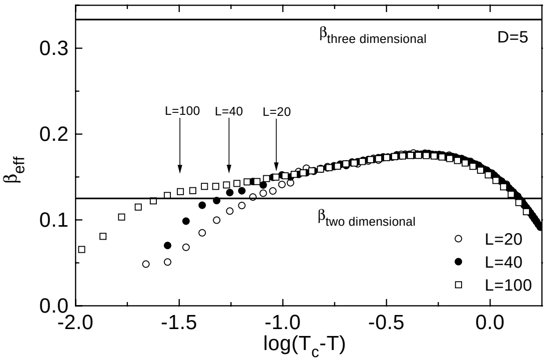

Fig. 2. $\beta_{\rm eff}$ *vs.* $\log(T_{\rm c}-T)$ for $L\times L\times D$ Ising films with $D=5$ and $L=20,40,100$. Straight lines corresponds to the three- and two-dimensional critical exponent values. Arrows indicate the points at which finite size effects start for each L value.

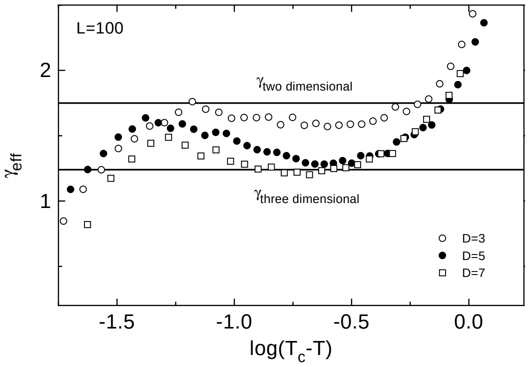

Fig. 3. $\gamma_{\rm eff}$ *vs.* $\log(T_{\rm c}-T)$ for $L\times L\times D$ Ising films with $L=100$ and $D=3,5,7$. Straight lines corresponds to the three- and two-dimensional γ values.

The same analysis can be done for the susceptibility. Figure 3 represents $\gamma_{\rm eff}$ *vs.* $\log(T_{\rm c}-T)$ for $L=100$ and $D=3,5,7$. Again, we find three zones, for the same reasons as above. The behavior is not exactly the same as in the previous case. We can see that the three-dimensional critical exponent value is reached even with the small value $D=5$. Of course this continues to happen with higher D values, but, in contrast to what was seen in Figure 3a of reference [5], no decrease of $\gamma_{\rm eff}$ at the beginning of the crossover region is observed. This decrease in $\gamma_{\rm eff}$ is presumably due to surface effects [4]. Since we are taking full periodic boundary conditions in every direction, it is normal that the decrease in $\gamma_{\rm eff}$ is smoothed.

Once we know $\beta_{\rm eff}(T)$ and $\gamma_{\rm eff}(T)$ for a constant value of D, (for example $D=5$), we are able to calculate $\delta_{\rm eff}$ using the scaling relation $\delta=(\gamma/\beta)+1$ over the entire crossover region. Reference [9] predicts, using renormalization group arguments, that this scaling relation should hold over the whole crossover region. In order to check this prediction we use numerical MC simulations of $\delta_{\rm eff}(H)$ in this zone, and we compare the results so obtained with the ones determined from the scaling relationship.

The independent variable is in one case the magnetic field, $\delta_{\rm eff}(H)$, and the temperature in the other, $\delta_{\rm eff}(T)$. So

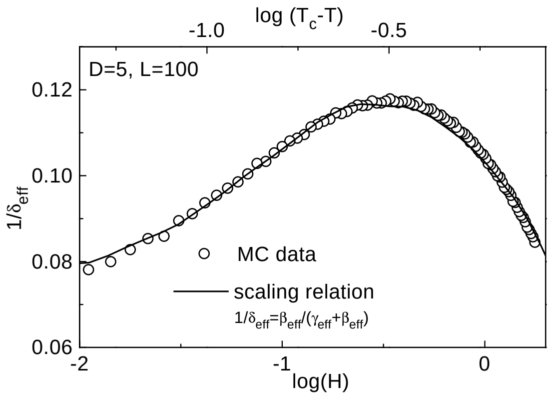

Fig. 4. $1/\delta_{\rm eff}$ *vs.* $\log(H)$ obtained by MC data (open circles) and $1/\delta_{\rm eff}$ *vs.* $\log(T_{\rm c}-T)$ obtained by means of the pertinent scaling relation (full line) for $L=100$ and $D=5$.

the effective critical exponent is not expressed in terms of the same variable in both cases. However both variables can be easily re-scaled visually as shown below.

Figure 4 represents $1/\delta_{\rm eff}$ (obtained from the scaling relation) *vs.* $\log(T_{\rm c}-T)$ and $1/\delta_{\rm eff}$ (obtained directly by MC calculations) *vs.* $\log(H)$, both for the case of $D=5$ and $L=100$. We choose $L=100$ in order to have a large enough crossover zone to check the scaling relationship. Note that the coincidence between both results is excellent. An important point to observe is that the scaling relationship holds not only at the crossover region, but also well before it. That is, at lower temperatures or higher fields. To check hyperscaling ($\nu=\beta(\delta+1)/d$, with d the system dimension) and other scaling relations (*e.g.* $\alpha=2-2\beta-\gamma$) the correlation length and the specific heat are needed.

Since the crossover of the effective critical exponents to the two-dimensional values is clearly seen in Figures 1, 2, 3 and 4, one would expect to find data collapsing near the critical point when plotting $\mathrm{M}L^{\beta/\nu}$ *vs.* $|\varepsilon|L^{1/\nu}$, $\varepsilon=(T_{\rm c}-T)/T_{\rm c}$ for a fixed value of $D=5$, with different values of L, using the two-dimensional Ising critical exponents. This data collapsing are shown in Figure 5a. This result clearly indicates that Ising films belong to the two-dimensional Ising university class as expected. It is well known that scaling only holds well relatively close to the critical point. In addition the scaling region becomes shorter for Ising films ($D=5$ in the case of Fig. 5a), a fact directly related to the occurrence of crossover in the exponents from effective toward pure two-dimensional ($d=2$) exponents. In Figure 5b we have plotted also the same data using three-dimensional critical exponents, in this case scaling is completely spoiled.

Figures 5a and 5b clearly prove that thin Ising films show the same critical behavior than the pure two-dimensional Ising system. However, the behavior of the effective exponents is not two-dimensional. The pure two- and three-dimensional systems do not show, of course, local maxima of $\beta_{\rm eff}$ and $1/\delta_{\rm eff}$ at a certain temperature (field) below the critical point. In other words, they always increase monotonously towards their asymptotic values.

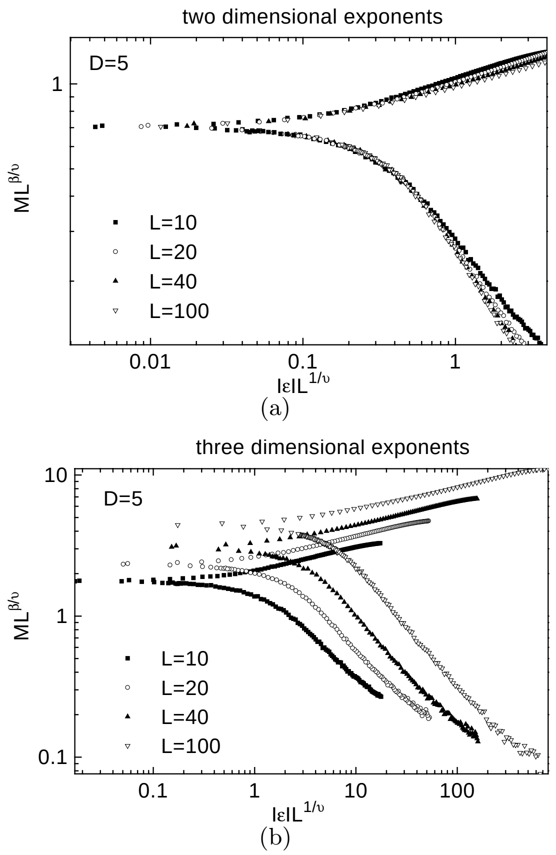

Fig. 5. Data collapsing plot for Ising films with $D = 5$ and $L = 10, 20, 40, 100$ with (a) two-dimensional critical exponents, and (b) three-dimensional critical exponents.

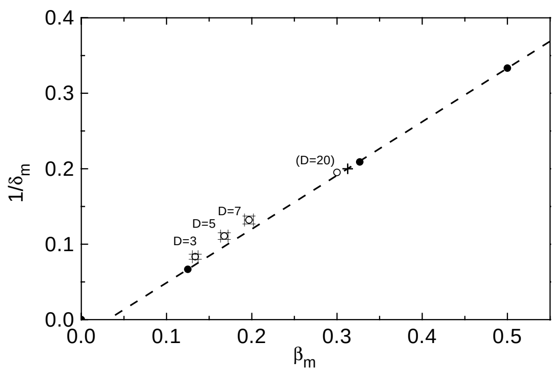

Fig. 6. $1/\delta_{\mathrm{m}}$ *vs.* β_{m} for the pure *one*-, *two*-, *three*- and *four*-dimensional Ising systems (black circles) and for Ising films $L \times L \times D$ with $L = 100$ and $D = 3, 5, 7, 20$, the last from reference [5], (open circles). The cross indicates the point interpolated between $d = 2$ and $d = 4$, with coordinates $(5/16, 1/5)$.

Systems with film geometry, however, present maxima of the effective critical exponents (β_{m} and $1/\delta_{\mathrm{m}}$) which lay between the values corresponding to the two-dimensional and three-dimensional Ising systems. This is seen for β_{eff} and $1/\delta_{\mathrm{eff}}$ in Figure 1. In order to show the evolution of the maximum value for the effective critical exponents we present in Figure 6 $(1/\delta)_{\mathrm{m}}$ *vs.* β_{m} for the pure one-, two-, three-, and four-dimensional Ising systems, together with the effective values obtained with Ising thin films of $D = 3, 5, 7, 20$ (the last value is estimated from Ref. [5]).

In order to avoid problems coming from a possible wrong interpretation of a single local absolute maximum of the effective critical exponent $1/\delta_{\mathrm{eff}}$ we have developed statistics of 40 points around the maximum. With this provision we get values with errors that are somewhat smaller than 5%. The same analysis has been performed for β_{eff}. In this case, however, the number of available points is smaller and the statistics perhaps less representative.

Note that the evolution of the pure systems is linear. For Ising films the points depart somewhat from perfect linearily. The overall behavior is unmistakably consistent, indicating that the maximum effective critical exponents (for plates with $D = 3, 5, 7, 20$) while meaningful only over a limited range of temperature away from the critical point, approach gradually the straight line defined by the pure exponents.

As noted $(1/\delta)$ *vs.* (β) values for the three-dimensional $(d = 3)$ Ising systems fall perfectly in line with the exactly known points for $d = 2$ and $d = 4$. In addition, a cross marks the $(1/\delta)$ and (β) point corresponding to $\{[1/\delta(d = 2)] + [1/\delta(d = 4)]\}/2$ and $\{\beta(d = 2) + \beta(d = 4)\}/2$ which gives exactly $1/\delta = 1/5$ and $\beta = 5/16$, very close to the best estimates of $1/\delta(d = 3) = 0.208\,9$ and $\beta(d = 3) = 0.326\,7$ [16]. Recent studies have gone to much higher values of D ($D = 48$) for systems in the same universality class as the Ising model [17].

3 Conclusions

To conclude, we presented MC simulations for the evolution of the effective critical exponents β_{eff}, γ_{eff} and δ_{eff} in thin Ising films with different thicknesses D. We clearly recognize three zones: a first one corresponding to low temperatures where the finite thickness of the system is not yet felt, a second one corresponding to the crossover towards the two-dimensional values, and a final third zone where finite size effects take over. We also show that the scaling relation $\gamma = \beta(\delta - 1)$ holds well, not just in the critical region, but also over the whole crossover zone and before it. We presented data collapsing plots for Ising films using two-dimensional values of the critical exponents. Our data neatly show that the asymptotic behavior is clearly governed by the two-dimensional fixed point for Ising films. Finally, we depicted the evolution of the maximum effective critical exponents $1/\delta_{\mathrm{m}}$ *vs.* β_{m} for different thicknesses. This evolution approaches a linear behavior towards the line going from $d = 2$ to $d = 4$ using our data and other data in the literature.

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