Critical behavior of magnetic thin films as a function of thickness

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During the last 30 years, physics of surfaces and objects of nanometric size have attracted an immense interest. This is due to important applications in industry\textsuperscript{12}. An example is the so-called giant magneto-resistance (GMR) used in data storage devices, magnetic sensors, etc. In parallel to these experimental developments, much theoretical effort\textsuperscript{7} has also been devoted to the search of simple magnetic systems lying behind new properties found in nanoscale objects such as ultrathin films, ultrafine particles, quantum dots, spintronic devices etc. This effort aimed not only at providing explanations for experimental observations but also at predicting new effects for future experiments.

The physics of two-dimensional (2D) systems is very exciting. Some of those 2D systems can be exactly solved: one famous example is the Ising model on the square lattice which has been solved by Onsager.\textsuperscript{2} This model shows a phase transition at a finite temperature $T_c$ given by $\sinh^2(2J/k_BT_c) = 1$ where $J$ is the nearest-neighbor (NN) interaction. Another interesting result is the absence of long-range ordering at finite temperatures for the continuous spin models (XY and Heisenberg models) in 2D\textsuperscript{12}. In general, three-dimensional (3D) systems for any spin models cannot be exactly solved. However, several methods in the theory of phase transitions and critical phenomena can be used to calculate the critical behaviors of these systems.\textsuperscript{11}

This paper deals with systems between 2D and 3D. Many theoretical studies have been devoted to thermodynamic properties of thin films, magnetic multilayers,...\textsuperscript{7,8,12,13,14} In spite of this, several points are still not yet understood. It is known a long time ago that the presence of a surface in magnetic materials can give rise to surface spin-waves which are localized in the vicinity of the surface.\textsuperscript{16} These localized modes may be acoustic with a low-lying energy or optical with a high energy, in the spin-wave spectrum. Low-lying energy modes contribute to reduce in general surface magnetization at finite temperatures. One of the consequences is the surface disordering which may occur at a temperature lower than that for interior magnetization.\textsuperscript{16} The existence of low-lying surface modes depends on the lattice structure, the surface orientation, the surface parameters, surface conditions (impurities, roughness, ...) etc. There are two interesting cases: in the first case a surface transition occurs at a temperature distinct from that of the interior spins and in the second case the surface transition coincides with the interior one, i.e. existence of a single transition. Theory of critical phenomena at surfaces\textsuperscript{7,8} and Monte Carlo (MC) simulations\textsuperscript{17,18} of critical behavior of the surface-layer magnetization at the extraordinary transition in the three-dimensional Ising model have been carried out. These works suggested several scenarios in which the nature of the surface transition and the transition in thin films depends on many factors in particular on the symmetry of the Hamiltonian and on surface parameters.

We confine ourselves here in the case of a simple cubic film with Ising model. For our purpose, we suppose all interactions are the same everywhere even at the surface. This case is the simplest case where there is no surface-localized spin-wave modes and there is only a single phase transition at a temperature for the whole system (no separate surface phase transition).\textsuperscript{15,16} Other complicated cases will be left for future investigations. However, some preliminary discussions on this point for complicated surfaces have been reported in some of our previous papers.\textsuperscript{19,20} In the case of a simple cubic film with Ising model, Capehart and Fisher have studied the critical behavior of the susceptibility using a finite-size

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scaling analysis. They showed that there is a crossover from 2D to 3D behavior as the film thickness increases. The so-called "effective" exponent $\gamma$ has been shown to vary according to a scaling function depending both on the film thickness and the distance to the transition temperature. As will be seen below the scaling suggested by Capehart and Fisher is in agreement with what we find here using extensive MC simulation.

The aim of this paper is to investigate the effect of the thickness on the critical exponents of the film. To carry out these purposes, we shall use MC simulations with highly accurate multiple histogram technique. The paper is organized as follows. Section II is devoted to a description of the model and method. Results are shown and discussed in section III. Concluding remarks are given in section IV.

II. MODEL AND METHOD

A. Model

Let us consider the Ising spin model on a film made from a ferromagnetic simple cubic lattice. The size of the film is $L \times L \times N_z$. We apply the periodic boundary conditions (PBC) in the $xy$ planes to simulate an infinite $xy$ dimension. The $z$ direction is limited by the film thickness $N_z$. If $N_z = 1$ then one has a 2D square lattice.

The Hamiltonian is given by

$$\mathcal{H} = -\sum_{\langle i,j \rangle} J_{i,j} \sigma_i \cdot \sigma_j$$  \hspace{1cm} (1)

where $\sigma_i$ is the Ising spin of magnitude 1 occupying the lattice site $i$, $\sum_{\langle i,j \rangle}$ indicates the sum over the NN spin pairs $\sigma_i$ and $\sigma_j$.

In the following, the interaction between two NN surface spins is denoted by $J_s$, while all other interactions are supposed to be ferromagnetic and all equal to $J = 1$ for simplicity. Let us note in passing that in the semi-infinite crystal the surface phase transition occurs at the bulk transition temperature when $J_s \simeq 1.52J$. This point is called "extraordinary phase transition" which is characterized by some particular critical exponents. In the case of thin films, i.e. $N_z$ finite, it has been theoretically shown that when $J_s = 1$ the bulk behavior is observed when the thickness becomes larger than a few dozens of atomic layers. Surface effects are insignificant on thermodynamic properties such as the value of the critical temperature, the mean value of magnetization at a given $T$, ... When $J_s$ is smaller than $J$, surface magnetization is destroyed at a temperature lower than that for bulk spins. The criticality of a film with uniform interaction, i.e. $J_s = J$, has been studied by Capehart and Fisher as a function of the film thickness using a scaling analysis and by MC simulations. The results by Capehart and Fisher indicated that as long as the film thickness is finite the phase transition is strictly that of the 2D Ising universality class. However, they showed that at a temperature away from the transition temperature $T_c(N_z)$, the system can behave as a 3D one when the spin-spin correlation length $\xi(T)$ is much smaller than the film thickness, i.e. $\xi(T)/N_z \ll 1$. As $T$ gets very close to $T_c(N_z)$, $\xi(T)/N_z \rightarrow 1$, the system undergoes a crossover to 2D criticality. We will return to this work for comparison with our results shown below.

B. Multiple histogram technique

The multiple histogram technique is known to reproduce with very high accuracy the critical exponents of second order phase transitions.

The overall probability distribution at temperature $T$ obtained from $n$ independent simulations, each with $N_j$ configurations, is given by

$$P(E, T) = \frac{\sum_{i=1}^{n} H_i(E) \exp[\frac{E}{k_B T}(T_j - f_j)]}{\sum_{j=1}^{n} N_j \exp[\frac{E}{k_B T_j}]}.$$  \hspace{1cm} (2)

where

$$\exp[f_i] = \sum_E P(E, T_i).$$  \hspace{1cm} (3)

The thermal average of a physical quantity $A$ is then calculated by

$$\langle A(T) \rangle = \sum_E A \cdot P(E, T)/z(T),$$  \hspace{1cm} (4)

in which

$$z(T) = \sum_E P(E, T).$$  \hspace{1cm} (5)

Thermal averages of physical quantities are thus calculated as continuous functions of $T$, now the results should be valid over a much wider range of temperature than for any single histogram.

In MC simulations, one calculates the averaged order parameter $\langle M \rangle$ ($M$: magnetization of the system), averaged total energy $\langle E \rangle$, specific heat $C_v$, susceptibility $\chi$, first order cumulant of the energy $C_U$, and $n^{th}$ order cumulant of the order parameter $V_n$ for $n = 1$ and 2. These quantities are defined as

$$\langle E \rangle = \langle \mathcal{H} \rangle,$$  \hspace{1cm} (6)

$$C_v = \frac{1}{k_B T^2} \langle (E^2) - \langle E \rangle^2 \rangle,$$  \hspace{1cm} (7)

$$\chi = \frac{1}{k_B T} \langle (M^2) - \langle M \rangle^2 \rangle,$$  \hspace{1cm} (8)

$$C_U = 1 - \frac{\langle E^4 \rangle}{3 \langle E^2 \rangle^2},$$  \hspace{1cm} (9)

$$V_n = \frac{\partial \ln M^n}{\partial (1/k_B T)} = \langle E \rangle - \frac{\langle M^n E \rangle}{\langle M^n \rangle}.$$  \hspace{1cm} (10)
Let us discuss the case where all dimensions can go to infinity. For example, consider a system of size $L^d$ where $d$ is the space dimension. For a finite $L$, the pseudo "transition" temperatures can be identified by the maxima of $C_v$ and $\chi$, .... These maxima do not in general take place at the same temperature. Only at infinite $L$ that the pseudo "transition" temperatures of these respective quantities coincide at the real transition temperature $T_c(\infty)$. So when we work at the maxima of $V_n$, $C_v$ and $\chi$, we are in fact working at temperatures away from $T_c(\infty)$. Let us define the reduced temperature which measures the "distance" from $T_c(\infty)$ by

$$t = \frac{T - T_c(\infty)}{T_c(\infty)}$$ (11)

This distance tends to zero when all dimensions go to infinity. For large values of $L$, the following scaling relations are expected (see details in Ref. [24]):

$$V_1^{\text{max}} \propto L^{1/\nu}, \quad V_2^{\text{max}} \propto L^{1/\nu},$$ (12)

$$C_v^{\text{max}} = C_0 + C_1 L^{\alpha/\nu},$$ (13)

and

$$\chi^{\text{max}} \propto L^{\gamma/\nu}$$ (14)

at their respective 'transition' temperatures $T_c(L)$, and

$$C_U = C_U[T_c(\infty)] + A L^{-\alpha/\nu},$$ (15)

$$M_{T_c(\infty)} \propto L^{-\beta/\nu}$$ (16)

and

$$T_c(L) = T_c(\infty) + C_A L^{-1/\nu},$$ (17)

where $A, C_0, C_1$ and $C_A$ are constants. We estimate $\nu$ independently from $V_1^{\text{max}}$ and $V_2^{\text{max}}$. With this value we calculate $\gamma$ from $\chi^{\text{max}}$ and $\alpha$ from $C_v^{\text{max}}$. Note that we can estimate $T_c(\infty)$ using the last expression. Then, using $T_c(\infty)$, we can calculate $\beta$ from $M_{T_c(\infty)}$. The Rushbrooke scaling law $\alpha + 2\beta + \gamma = 2$ is then in principle verified.

Let us emphasize that the expressions Eqs. (12)-(17) are valid for large $L$. To be sure that $L$ is large enough, one has to allow for corrections to scaling of the form, for example,

$$\chi^{\text{max}} = B_1 L^{\gamma/\nu}(1 + B_2 L^{-\omega})$$ (18)

$$V_n^{\text{max}} = D_1 L^{1/\nu}(1 + D_2 L^{-\omega})$$ (19)

where $B_1, B_2, D_1$ and $D_2$ are constants and $\omega$ is a correction exponent. Similar forms exist also for the other exponents. Usually, these corrections are extremely small if $L$ is large enough as is the case with today’s large-memory computers. So, in general they do not therefore alter the results using Eqs. (12)-(17).

C. The case of films with finite thickness

In the case of a thin film of size $L \times L \times N_z$, Capehart and Fisher [2] have showed that as long as the film thickness $N_z$ is not allowed to go to infinity, there is a 2D-3D crossover if one does not work at the real transition temperature $T_c(L = \infty, N_z)$. Following Capehart and Fisher, let us define

$$i = \frac{T - T_c(L = \infty, N_z)}{T_c(3D)}$$ (20)

$$x = N_z^{1/\nu_3D} i$$ (21)

where $\nu_3D$ is the 3D $\nu$ exponent and $T_c(3D)$ the 3D critical temperature. When $x$ is larger than a value $x_0$, i.e. at a temperature away from $T_c(L = \infty, N_z)$, the system behaves as a 3D one. While when $x < x_0$, it should behave as a 2D one. This crossover was argued from a comparison of the correlation length in the $z$ direction to the film thickness. As a consequence, if we work exactly at $T_c(L = \infty, N_z)$ we should observe the 2D critical exponents for finite $N_z$. Otherwise, we should observe the so-called "effective critical exponents" whose values are found between those of 2D and 3D cases. This point is fundamentally very important. There have been some attempts to verify it by MC simulations [23] but these results were not convincing due to their poor MC quality. In the following we show with high-precision MC technique that the prediction of Capehart and Fisher is really verified.

III. RESULTS

The $xy$ linear sizes $L = 20, 24, 30, ..., 80$ have been used in our simulations. For $N_z = 3$, sizes up to 160 have been used to evaluate corrections to scaling.

In practice, we use first the standard MC simulations to localize for each size the transition temperatures $T_j^{E}(L)$ for specific heat and $T_j^{m}(L)$ for susceptibility. The equilibrating time is from 200000 to 400000 MC steps/spin and the averaging time is from 500000 to 1000000 MC steps/spin. Next, we make histograms at 8 different temperatures $T_j(L)$ around the transition temperatures $T_j^{E,m}(L)$ with 2 millions MC steps/spin, after discarding 1 millions MC steps/spin for equilibrating. Finally, we make again histograms at 8 different temperatures around the new transition temperatures $T_j^{E,m}(L)$ with $2 \times 10^6$ and $4 \times 10^6$ MC steps/spin for equilibrating and averaging time, respectively. Such an iteration procedure gives extremely good results for systems studied so far. Errors shown in the following have been estimated using statistical errors, which are very small thanks to our multiple histogram procedure, and fitting errors given by fitting software.

We note that only $\nu$ is directly calculated from MC data. Exponent $\gamma$ obtained from $\chi^{\text{max}}$ and $\nu$ suffers little
TABLE I: Maxima and temperatures at the maxima of $V_n$ ($n = 1, 2$), $C_v$ and $\chi$ for various $L$ with $N_z = 7$.

| $L$ | $C_v^{\text{max}}$ | $\chi^{\text{max}}$ | $V_1^{\text{max}}$ | $V_2^{\text{max}}$ | $T_c(C_v^{\text{max}})$ | $T_c(\chi^{\text{max}})$ | $T_c(V_1^{\text{max}})$ | $T_c(V_2^{\text{max}})$ |
|------|--------------------|----------------------|--------------------|--------------------|------------------------|------------------------|------------------------|------------------------|
| 30   | 2.21115658         | 25.29532589          | 164.05948154       | 275.71581036       | 4.19027500             | 4.22755000             | 4.24277500             | 4.24000000             |
| 40   | 2.36517434         | 41.20958927          | 219.30094769       | 368.72462473       | 4.19305000             | 4.21895000             | 4.23025000             | 4.23500000             |
| 50   | 2.50496719         | 60.82008190          | 275.66203381       | 463.17327477       | 4.19275000             | 4.21340000             | 4.22210000             | 4.22600000             |
| 60   | 2.59177903         | 82.96529587          | 329.65562622       | 554.47606570       | 4.19270000             | 4.20940000             | 4.21710000             | 4.22045000             |
| 70   | 2.70129995         | 109.00528127         | 387.47245040       | 651.24905512       | 4.19250000             | 4.20640000             | 4.21260000             | 4.21530000             |
| 80   | 2.76931676         | 138.78113065         | 443.00488386       | 743.61068938       | 4.19220000             | 4.20410000             | 4.20965000             | 4.21205000             |

errors (systematic errors and errors from $\nu$). Other exponents are obtained by MC data and several-step fitting. For example, to obtain $\alpha$ we have to fit $C_v^{\text{max}}$ of Eq. 13 by choosing $C_0$, $C_1$ and by using the value of $\nu$. So, in practice, in most cases, one calculates $\alpha$ or $\beta$ from MC data and uses the Rushbrooke scaling law to calculate the remaining exponent.

Now, similar to the discussion given in subsection II B if we work at a distance away from $T_c(L = \infty, N_z)$ we should observe "effective critical exponents". This is the case because in the finite size analysis using the multiple histogram technique, we measure the maxima of $V_n$, $C_V$ and $\chi$ which occur at different temperatures for a finite $L$. These temperatures, though close to, are not $T_c(L = \infty, N_z)$. To give a precision on this point, we show the values of these maxima and the corresponding temperatures for $N_z = 7$ in Table I For the value of $T_c(L = \infty, N_z = 7)$, see Table I

FIG. 1: Layer magnetizations (a) and layer susceptibilities (b) versus $T$ with $N_z = 5$ and $L = 24$.

A. Finite size scaling

Let us show some results obtained from multiple histograms described above. Figure 3 shows the susceptibility and the first derivative $V_1$ versus $T$ around their maxima for several sizes.

We show in Fig. 4 the maximum of the first derivative of $\ln M$ with respect to $\beta = (k_BT)^{-1}$ versus $L$ in the $\ln - \ln$ scale for several film thicknesses up to $N_z = 13$. If we use Eq. 12 to fit these lines, i.e. without correction to scaling, we obtain $1/\nu$ from the slopes of the remarkably straight lines. These values are indicated on
FIG. 2: Total magnetization (a) and total susceptibility (b) versus $T$ with $N_z = 5$ and $L = 24$.

FIG. 3: (a) Susceptibility and (b) $V_1$, as functions of $T$ for several $L$ with $N_z = 11$, obtained by multiple histogram technique.

FIG. 4: Maximum of the first derivative of $\ln M$ versus $L$ in the $\ln - \ln$ scale. The slopes are indicated on the figure.

FIG. 5: Effective exponent $\nu$ versus $N_z$.

$\gamma_{2D} = 1.75$. The very high precision of our method is thus verified in the rather modest range of the system sizes $L = 20 - 80$ used in the present work. Note that the result of Ref. 25 gave $\nu = 0.96 \pm 0.05$ for $N_z = 1$ which is very far from the exact value.

The deviation of $\nu$ from the 2D value when $N_z$ increases is due, as discussed earlier, to the crossover to 3D ($\dot{t}$ is not zero). Other exponents will suffer the same deviations as seen below.

We show in Fig. 6 the maximum of the susceptibility versus $L$ in the $\ln - \ln$ scale for film thicknesses up to $N_z = 13$. We have used only results of $L \geq 30$. Including $L = 20$ and 24 will result, unlike the case of $\nu$, in a decrease of $\gamma$ of about one percent for $N_z \geq 7$. From the slopes of these straight lines, we obtain the values of effective $\gamma/\nu$. Using the values of $\nu$ obtained above, we deduce the values of $\gamma$ which are plotted in Fig. 7 as a function of thickness $N_z$. Unlike the case of $\nu$, we observe here a stronger deviation of $\gamma$ from its 2D value (1.75) with increasing thickness. This finding is somewhat interesting: the magnitude of the deviation from the 2D value may be different from one critical exponent to another: $\approx 3\%$ for $\nu$ and $\approx 8\%$ for $\gamma$ when $N_z$ goes from 1 to 13. We will see below that $\beta$ varies even more strongly.

We show now in Fig. 8 the maximum of $C_v^{\max}$ versus the figure. In order to see the deviation from the 2D exponent, we plot in Fig. 6 $\nu$ as a function of thickness $N_z$. We observe here a small but systematic deviation of $\nu$ from its 2D value ($\nu_{2D} = 1$) with increasing thickness. To show the precision of our method, we give here the results of $N_z = 1$. For $N_z = 1$, we have $1/\nu = 1.0010 \pm 0.0028$ which yields $\nu = 0.9990 \pm 0.0031$ and $\gamma/\nu = 1.7537 \pm 0.0034$ (see Figs. 6 and 7 below) yielding $\gamma = 1.7520 \pm 0.0062$. These results are in excellent agreement with the exact results $\nu_{2D} = 1$ and $\gamma_{2D} = 1.75$. The very high precision of our method is thus verified in the rather modest range of the system sizes $L = 20 - 80$ used in the present work. Note that the result of Ref. 25 gave $\nu = 0.96 \pm 0.05$ for $N_z = 1$ which is very far from the exact value.

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idea that the finite correlation in the $z$ direction may show an example of this, let us plot in Fig. 10 the transition temperature at $L = \infty$ for several $N_z$, using Eq. (17) for each given $N_z$. As seen, $T_c(N_z) \approx 4.379$ at $N_z = 13$ while its value at 3D is 4.51. A rough extrapolation shows that the 3D values is attained for $N_z \approx 25$ while the critical exponents at this thickness are far away from the 3D ones.

Let us show the prediction of Capehart and Fisher on the critical temperature as a function of $N_z$. Defining the critical-point shift as

$$\varepsilon(N_z) = \left[ T_c(L = \infty, N_z) - T_c(3D) \right] / T_c(3D)$$

(22)

they showed that

$$\varepsilon(N_z) \approx \frac{b}{N_z^{1/\nu}} \left[ 1 + a/N_z \right]$$

(23)

where $\nu = 0.6289$ (3D value). Using $T_c(3D) = 4.51$, we fit the above formula with $T_c(L = \infty, N_z)$ taken from Table III. We obtain $a = -1.37572$ and $b = -1.92629$. The MC results and the fitted curve are shown in Fig. 11. Note that if we do not use the correction factor $[1 + a/N_z]$, the fit is not good for small $N_z$. The prediction of Capehart and Fisher is thus very well verified.

We give here the precise values of $T_c(L = \infty, N_z)$ for each thickness. For $N_z = 1$, we have $T_c(L = \infty, N_z = 1)$...
versus the film thickness. The agreement is excellent.

FIG. 10: Critical temperature at infinite \( L \) as a function of the film thickness. Points are MC results, continuous line is the prediction of Capehart and Fisher, Eq. (23). The agreement is excellent.

![Graph showing critical temperature at infinite L as a function of film thickness.](image)

**FIG. 11:** Effective exponent \( \beta \), obtained by using Eq. (16) versus the film thickness.

![Graph showing effective exponent \( \beta \) versus film thickness.](image)

**B. Larger sizes and correction to scaling**

We consider here the effects of larger \( L \) and of the correction to scaling. For the effect of larger \( L \), we will extend our size up to \( L = 160 \), for just the case \( N_z = 3 \).

The results indicate that larger \( L \) does not change the results shown above. Figure (12(a)) displays the maximum of \( V_1 \) as a function of \( L \) up to 160. Using Eq. (12), i.e. without correction to scaling, we obtain \( 1/\nu = 1.009 \pm 0.001 \) which is to be compared to \( 1/\nu = 1.008 \pm 0.002 \) using \( L \) up to 80. The change is therefore insignificant because it is at the third decimal i.e. at the error level. The same is observed for \( \gamma/\nu \) as shown in Fig. (12(b)): \( \gamma/\nu = 1.752 \pm 0.002 \) using \( L \) up to 160 instead of \( \gamma/\nu = 1.751 \pm 0.002 \) using \( L \) up to 80.

Now, let us allow for correction to scaling, i.e. we use Eq. (15) instead of Eq. (14) for fitting. We obtain the following values: \( \gamma/\nu = 1.751 \pm 0.002 \), \( B_1 = 0.05676 \), \( B_2 = 1.57554 \), \( \omega = 3.26618 \) if we use \( L = 70 \) to 160 (see Fig. 13). The value of \( \gamma/\nu \) in the case of no scaling correction is 1.752 \pm 0.002. Therefore, we can conclude that this correction is insignificant. The large value of \( \omega \) explains the smallness of the correction.

Finally, for convenience, let us summarize our results in Table II for \( N_z = 1, 3, \ldots, 13 \). Except for \( N_z = 1 \), all other cases are effective exponents discussed above. Due to the smallness of \( \alpha \), its value is shown with 5 decimals without rounding.

**C. Role of boundary condition**

To close this section, let us touch upon the question: does the absence of PBC in the \( z \) direction cause the deviation of the critical exponents? The answer is no: we have calculated \( \nu \) and \( \gamma \) for \( N_z = 5 \) in both cases, with and without PBC in the \( z \) direction. The results show no significant difference between the two cases as seen in Figs. 14 and 15. We have found the same thing with \( N_z = 11 \) shown in Figs. 16 and 17. So, we conclude that the fixed thickness will result in the deviation of the critical exponents, not from the absence of the PBC. This is somewhat surprising since we may think, incorrectly, that the PBC should mimic the infinite dimension so that we should obtain the 3D behavior when applying the PBC. As will be seen below, the 3D behavior is recovered only when the finite size scaling is applied in the \( z \) direction at the same time in the \( xy \) plane. To show this, we plot in Figs. 18 and 19 the results for the 3D case.

Calculating now \( M(L) \) at these values of \( T_c(L = \infty, N_z) \) and using Eq. (16) we obtain \( \beta/\nu \) for each \( N_z \). For \( N_z = 1 \), we have \( \beta/\nu = 0.1268 \pm 0.0022 \) which yields \( \beta = 0.1266 \pm 0.0049 \) which is in excellent agreement with the exact result 0.125. Note that if we calculate \( \beta \) from \( \alpha + 2\beta + \gamma = 2 \), then \( \beta = (2 - 1.75198 - 0.00199)/2 = 0.12302 \pm 0.0035 \) which is in good agreement with the direct calculation within errors. We show in Fig. 11 the values of \( \beta \) obtained by direct calculation using Eq. (16). Note that the deviation of \( \beta \) from the 2D value when \( N_z \) varies from 1 to 13 is due to the crossover effect discussed in subsection (1C). It represents about 60%. Remember that the 3D value of \( \beta \) is 0.3258 \pm 0.0044.22
TABLE II: Critical exponents, effective dimension and critical temperature at infinite $xy$ limit as obtained in this paper.

| $N_z$ | $\nu$ | $\gamma$ | $\alpha$ | $\beta$ | $d_{eff}$ | $T_c(L = \infty, N_z)$ |
|-------|-------|-------|-------|-------|-------|---------------------|
| 1     | 0.9990 ± 0.0028 | 1.7520 ± 0.0062 | 0.00199 ± 0.00279 | 0.1266 ± 0.0049 | 2.0000 ± 0.0028 | 2.2699 ± 0.0005 |
| 3     | 0.9922 ± 0.0019 | 1.7377 ± 0.0035 | 0.00222 ± 0.00192 | 0.1452 ± 0.0040 | 2.0135 ± 0.0019 | 3.6365 ± 0.0024 |
| 5     | 0.9876 ± 0.0023 | 1.7220 ± 0.0069 | 0.00222 ± 0.00234 | 0.1639 ± 0.0051 | 2.0230 ± 0.0023 | 4.0234 ± 0.0028 |
| 7     | 0.9828 ± 0.0024 | 1.7042 ± 0.0087 | 0.00223 ± 0.00238 | 0.1798 ± 0.0069 | 2.0328 ± 0.0024 | 4.1939 ± 0.0032 |
| 9     | 0.9780 ± 0.0016 | 1.6736 ± 0.0084 | 0.00224 ± 0.00161 | 0.1904 ± 0.0071 | 2.0426 ± 0.0016 | 4.2859 ± 0.0022 |
| 11    | 0.9733 ± 0.0025 | 1.6354 ± 0.0083 | 0.00224 ± 0.00256 | 0.1995 ± 0.0088 | 2.0526 ± 0.0026 | 4.3418 ± 0.0032 |
| 13    | 0.9692 ± 0.0026 | 1.6122 ± 0.0102 | 0.00226 ± 0.00268 | 0.2059 ± 0.0092 | 2.0613 ± 0.0027 | 4.3792 ± 0.0034 |

Even with our modest sizes (up to $L = N_z = 21$, since it is not our purpose to treat the 3D case here), we obtain $\nu = 0.613 ± 0.005$ and $\gamma = 1.250 ± 0.005$ very close to their 3D best known values $\nu_{3D} = 0.6302 ± 0.0001$ from Ref. 28 and $\nu_{3D} = 0.6289 ± 0.0008$ and $\gamma_{3D} = 1.2390 ± 0.0025$ obtained by using $24 \leq L \leq 96$ given in Ref. 27.

IV. CONCLUDING REMARKS

We have considered a simple system, namely the Ising model on a simple cubic thin film, in order to clarify the point whether or not there is a continuous deviation of the 2D exponents with varying film thickness. From results obtained by the highly accurate multiple histogram technique shown above, we conclude that the critical exponents in thin films show a continuous deviation from their 2D values as soon as the thickness departs from

FIG. 12: (a) $V_1^{\max}$ and (b) $\chi^{\max}$ vs $L$ up to 160 with $N_z = 3$.

FIG. 13: $\chi^{\max}$ vs $L$ (a) from 20 up to 160 (b) from 70 up to 160, for $N_z = 3$.

FIG. 14: Maximum of the first derivative of ln $M$ versus $L$ in the ln – ln scale for $N_z = 5$ (a) without PBC in $z$ direction (b) with PBC in $z$ direction. The slopes are indicated on the figure. See text for comments.
1. This deviation stems from a deep physical mechanism: Capehart and Fisher have argued that if one works exactly at the critical temperature $T_c(L = \infty, N_z)$ then the critical exponents should be those of 2D universality class as long as the film thickness is finite. At $T_c(L = \infty, N_z)$, the correlation in the $z$ direction $\xi$ remains finite while those in the $xy$ planes become infinite. Hence $\xi$ is irrelevant to the criticality. This yields therefore the 2D behavior. However, when the system is away from $T_c(L = \infty, N_z)$, as is the case in numerical simulations using finite sizes, the system may have a 3D behavior as long as $\xi << N_z$. This should yield a deviation of 2D critical exponents. The results we obtained in this paper verify this picture. In addition, the prediction of Capehart and Fisher for the shift of the critical temperature with the film thickness is in a perfect agreement with our simulations. Note furthermore that (i) the deviations of the exponents from their 2D values are very different in magnitude: while $\nu$ and $\alpha$ vary very little over the studied range of thickness, $\gamma$ and specially $\beta$ suffer stronger deviations, (ii) with a fixed thickness $N_z \neq 1$, the same “effective” exponents are observed, within errors, in simulations with and without periodic boundary condition in the $z$ direction, (iii) to obtain the 3D behavior, the finite size scaling should be applied si-
multaneously in the three directions, i.e. all dimensions should be allowed to go to infinity. If we do not apply the scaling in the $z$ direction, we will not obtain 3D behavior even with a very large, but fixed, thickness and even with periodic boundary condition in the $z$ direction, (iv) with regard to the critical behavior, thin films behave as systems with effective critical exponents whose values are those between 2D and 3D.

To conclude, we hope that the numerical results shown in this paper will help experimentalists to interpret their data which are usually obtained at a finite distance from the critical point. It should be also desirable to study more cases to clarify the role of thickness on the behavior of very thin films, in particular the effect of the film thickness on the bulk first-order transition.

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