BULK CRITICAL EXPONENTS IN A PRESENCE OF THE CAPILLARY CONDENSATION

Andrzej Drzewiński[1] and Katarzyna Szota[2]

[1] *Institute of Physics, University of Zielona Góra, Poland*
[2] *Institute of Mathematics, Czestochowa University of Technology, Poland*

Abstract. The properties of a simple fluid or magnet with strong one-axis anisotropy can be studied by means of the Ising model. Such a model, but in an confined geometry with identical boundary fields, is studied along various thermodynamic paths using the density-matrix renormalization group technique. It has been found that also in the presence of the capillary condensation the critical exponent β of the bulk system can be found.

Introduction

In the thermodynamic limit of the two-dimensional system the correlation length and some other quantities diverge at the critical point ($T = T_c$, $H = 0$) [1]. One of them is magnetization that vanishes above T_c in zero bulk field (the paramagnetic regime). Phase coexistence occurs for temperatures $T < T_c$ (the thick line at Fig. 1) separating two regimes with opposite magnetizations. When one dimension is finite (an $L\times\infty$ geometry) all those values instead of singularities exhibit more or less pronounces maxima at different temperatures [2]. In a case of magnetization a jump is replaced by very steep slope.

In this paper the Ising model is built on a strip with identical boundary fields. It is known that the combined effect of identical boundary fields and confinement shifts phase coexistence to a finite value of the bulk magnetic field $h = h_0(L) \neq 0$. For large L it is governed by, so-called, the Kelvin equation

$$h_0(L) = \frac{\sigma_0 \cos\theta}{m_b} \frac{1}{L}$$

where σ_0, m_b, and θ are the surface tension, bulk spontaneous magnetization, and contact angle, respectively. This phenomenon is analogous to the capillary condensation for a fluid confined between parallel surfaces, where the gas-liquid transition occurs at a lower pressure than in the bulk.

For the two-dimensional system there is a discontinuity of the first derivative of the free energy f upon changing the sign of the bulk magnetic field at T = const ($T_c > T$). It results in a jump of the magnetization $m = -\partial f/\partial H$ at $H = 0$, whereas the limit value $m_b = m$ (T = const, $H \to 0$) is finite and named the spontaneous magnetization. In the other words, when the thermodynamic path for fixed but very small H (the dashed arrow at Fig. 1) is closer and closer to the $H = 0$ axis, then the magnetization resembles more and more the spontaneous magnetization (full dots in Fig. 2).

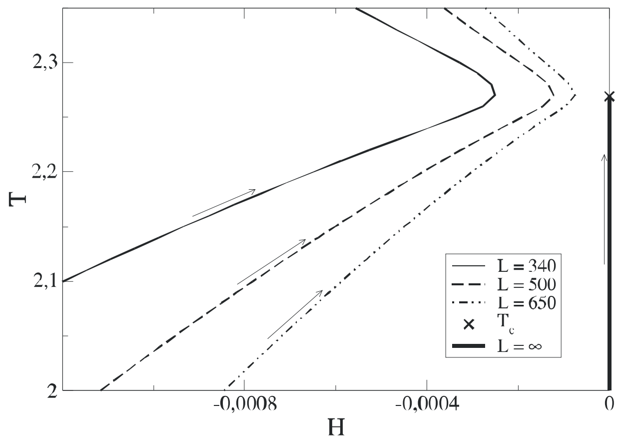

Fig. 1. Numerically determined coexistence curves for finite systems in the (T, H) phase diagram. The thick solid line indicates the bulk coexistence line. The dashed arrow denotes the thermodynamic path for the infinite systems but others for finite systems

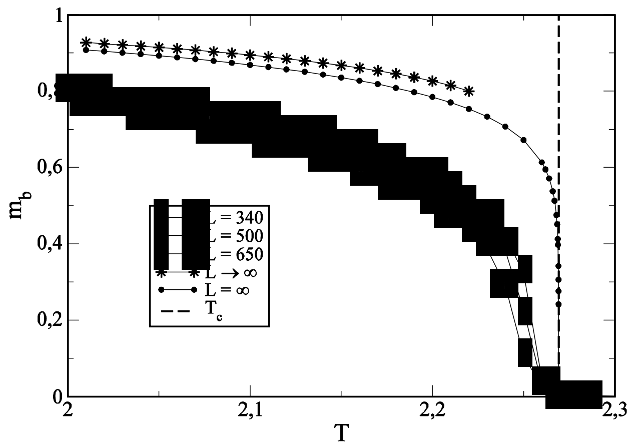

Fig. 2. Spontaneous magnetization m_b as a function of temperature along the thermodynamic paths presented in the Fig. 1 with a constant shift -10^{-5} away from the coexistence lines

There is an interesting question. What happens when the system is confined in the presence of the boundary fields. Is it possible to apply the same procedure and, exploiting the magnetizations along the (curvilinear) coexistence lines, reconstruct the behaviour of the spontaneous magnetization?

1. The model and the method

Our model Hamiltonian for the infinitely long strip has the form:

$$H = -J\left(\sum \sigma_{k,l}\sigma_{k',l'} - h_1\sum_k \sigma_{k,1} + h_1\sum_k \sigma_{k,L} + H\sum_{k,l}\sigma_{k,l}\right)$$

where the first sum is over all nearest-neighbour pairs and we have measured the surface field h_1 and the bulk field H in units of J.

In order to find out the free energy f and the longitudinal correlation length $\xi_{\|}$ we have used the density-matrix renormalization group (DMRG) [3]. It was originally proposed by White as a new tool for diagonalization of quantum spin chains [4] and was later adapted to classical two-dimensional equilibrium statistical mechanics by Nishino [5]. The DMRG allows one to study much larger systems (up to L = 650 in the present paper) than is possible with standard exact diagonalization methods (typically L ~50) and provides data with remarkable accuracy. We estimate that the errors in the plots are smaller than the symbol size.

2. Results

We recall that although there is no longer any true phase transition for finite L, in two-dimensional Ising strips with large L there is still a line of extremely weakly rounded first-order transitions. These pseudo-lines have been identified as those positions (T, H) in the phase diagram where the total magnetization of the strip vanishes. It turns out that those positions correspond to the maximum of the free energy of the strip. The present results are calculated along those lines with the bulk field shifted -10^{-5} at fixed temperature and collected in Figure 2.

As one can see all curves look like the spontaneous magnetization curve for the infinite system until T ~2.22. It seems to be related to the correlation length behaviour. The Figure 3 shows that the longitudinal correlation length grows when one goes to higher temperatures and around T = 2.22 is comparable with the system size L. Nevertheless we can extrapolate the results to the two-dimensional system for T < 2.22. The result is a bit over-estimated what seems to stem from the fact that we have done the extrapolation using only three values of L.

In order to infer a possible power law governing the behaviour of the magnetization along different paths we have calculated local exponents z of the magnetization as a function of the reduced temperature $\tau = (T_c - T)/T_c$.

$$z_i = \frac{\ln m_{i+1} - \ln m_i}{\ln \tau_{i+1} - \ln \tau_i}$$

which is the discrete derivative of m as a function of τ in the log-log plot. Such a quantity probes the local slope at a given value of τ_i at the point i along the path considered. It provides a better estimate of the leading exponent than a log-log plot itself. The high quality of the DMRG data allows us to reliably carry out this numerical differentiation.

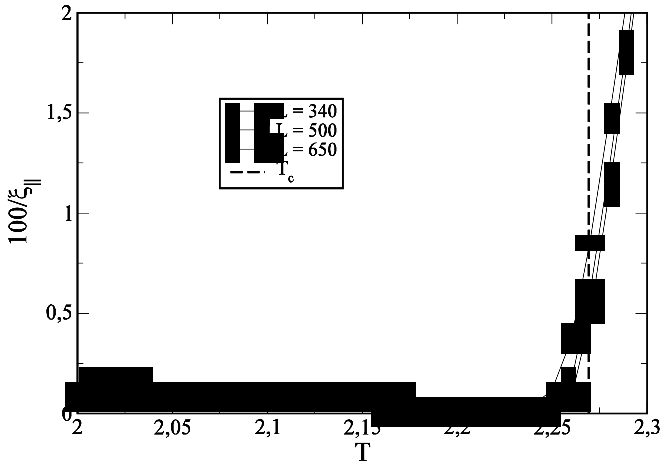

Fig. 3. The inverse of the longitudinal correlation lengths (along an Ising strip) for the same values as in Fig. 2

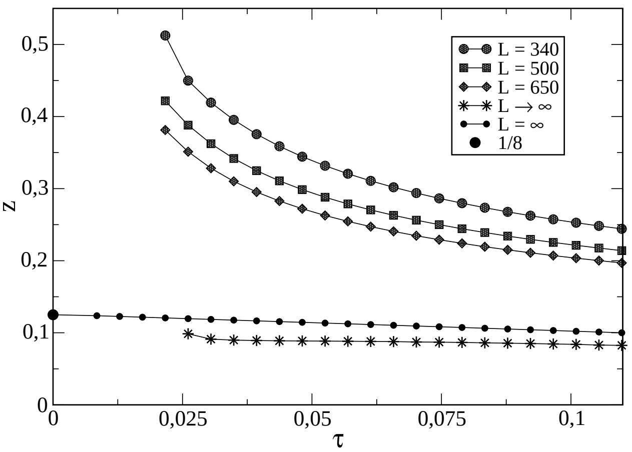

Fig. 4. The local exponents of the spontaneous magnetization for different system sizes. Stars correspond to the values of m(T = const, L) extrapolated to the infinite system

The power law of the spontaneous magnetization has the form

$$m_b \sim \tau^{\beta}$$

where β is 1/8 for the two-dimensional Ising model [6]. The local exponents for different L have been presented in Figure 4 and the conclusion is clear. The larger system the closer the local exponents to the bulk value.

3. Discussion

Continuous phase transitions and associated strict powers laws can be observed only in the thermodynamic limit of the infinite system. Nevertheless, they should be also seen in an approximate form for finite systems and allow to estimate the critical exponents [6]. We have confirmed it for the Ising model in the strip geometry with parallel boundary fields, where the bulk coexistence line is shifted to non-zero bulk fields.

References

[1] Yeomans J.M., Statistical Mechanics of Phase Transitions, Clarendon Press, Oxford 1992.

[2] Binder K., in Phase Transitions and Critical Phenomena, ed. C. Domb and J.L. Lebowitz, Academic, London 1983, vol. 8, p. 1; S. Dietrich, in Phase Transitions and Critical Phenomena, ed. by C. Domb and J.L. Lebowitz, Academic, London 1988, vol. 12, p. 1.

[3] Schollwoeck U., Rev. Mod. Phys. 2005, 77, 259.

[4] White S.R., Phys. Rev. Lett. 1992, 69, 2863; White S.R., Phys. Rev. B 48, 1993, 10345.

[5] Nishino T., J. Phys. Soc. Japan 1995, 64, 3598.

[6] Fisher M.E., Barber M.N., Phys. Rev. Lett. 1972, 28, 1516.