



ELSEVIER

Available online at www.sciencedirect.com

SCIENCE @ DIRECT®

Computer Physics Communications 169 (2005) 230–233

Computer Physics
Communications

www.elsevier.com/locate/cpc

Multicanonical simulations of the tails of the order-parameter distribution of the two-dimensional Ising model

Rudolf Hilfer^{a,b}, Bibudhananda Biswal^{a,c}, Hans-Georg Mattutis^d, Wolfhard Janke^{e,*}

^a ICA-I, Universität Stuttgart, Pfaffenwaldring 27, 70569 Stuttgart, Germany

^b Institut für Physik, Universität Mainz, 55099 Mainz, Germany

^c Department of Physics, Sri Venkateswara College, University of Delhi, New Delhi-110 021, India

^d Tokyo University of Electro-communications, Department of Mechanical Engineering and Intelligent Systems, Chofu, Tokyo 182-8585, Japan

^e Institut für Theoretische Physik, Universität Leipzig, Augustusplatz 10/11, 04109 Leipzig, Germany

Available online 9 April 2005

Abstract

We report multicanonical Monte Carlo simulations of the tails of the order-parameter distribution of the two-dimensional Ising model for fixed boundary conditions. Clear numerical evidence for “fat” stretched exponential tails is found below the critical temperature, indicating the possible presence of fat tails at the critical temperature.

© 2005 Elsevier B.V. All rights reserved.

PACS: 05.50.+q; 64.60.Cn; 64.60.Fr; 05.70.Ln

Keywords: Order-parameter distribution; 2D Ising model; Multicanonical simulations

1. Introduction

A quantity of central importance for finite-size scaling (FSS) analyses of critical phenomena is the order-parameter distribution $p(m)$ [1]. Most properties of $p(m)$ at criticality are known from computer simulations [2]. Analytical information comes from field theoretic renormalization group calculations [3], con-

formal field theory [4], and also a generalized classification theory of phase transitions [5,6]. While some of the analytical predictions seem to have been corroborated by numerical simulations [6,7], the predictions for the tails of the critical order-parameter distribution could not be confirmed. Recording of the very small probabilities in the tails requires special techniques such as multicanonical simulations [8]. Many recent studies [7,9] have attempted this, but failed in establishing the true behavior of the tails of $p(m)$.

In the present paper we report results of high precision multicanonical Monte Carlo simulations for the two-dimensional (2D) Ising model on square lat-

* Corresponding author.

E-mail addresses: biswal@ica1.uni-stuttgart.de (B. Biswal), hg@mce.uec.ac.jp (H.-G. Mattutis), wolfhard.janke@itp.uni-leipzig.de (W. Janke).

tices with fixed (i.e. all boundary spins fixed to +1) boundary conditions. One of the objectives is to study whether the order-parameter distribution obtained from the simulation can be considered to be asymptotic with respect to system size. A secondary objective is to study fixed (symmetry breaking) boundary conditions because the asymmetry should give rise to an asymmetry in the far tail behavior.

2. Analysis methods

We consider the 2D Ising model on a square lattice with $N = L^2$ spins $\sigma_i = \pm 1$ interacting according to the usual Hamiltonian

$$H = -J \sum_{\langle ij \rangle} \sigma_i \sigma_j, \tag{1}$$

where $J > 0$ is the ferromagnetic coupling strength and the summation $\sum_{\langle ij \rangle}$ runs over all nearest neighbor pairs on the lattice. The order parameter is the magnetization per spin, $-1 \leq m = (1/N) \sum_{i=1}^N \sigma_i \leq 1$. In the following we set $J = 1$, the Boltzmann constant to unity and denote the temperature by T .

The probability density $p(m)$ of the order parameter depends parametrically on temperature and system size, $p(m) = p(m; T, L)$. At criticality, traditional FSS predicts the scaling form [1]

$$p(m; T = T_c, L) = L^{\beta/\nu} \tilde{p}(mL^{\beta/\nu}), \tag{2}$$

where $\tilde{p}(\tilde{m})$ with $\tilde{m} = mL^{\beta/\nu}$ is a universal scaling function. Since for the 2D Ising model $\nu = 1$ and $\beta = 1/8$, the scaling variable is thus $\tilde{m} = mL^{1/8}$. For the analysis of the tails of $p(m)$ we first determine constants A, B, C such that $p_0(x) = Ap(B(m - C))$ has mean zero, unit norm and unit variance. Then we split the peak into its left and right tails by defining the functions

$$p_{0l}(x) = p_0(x_{\text{peak}} - x) \quad \text{for } x < x_{\text{peak}}, \tag{3}$$

$$p_{0r}(x) = p_0(x - x_{\text{peak}}) \quad \text{for } x > x_{\text{peak}}, \tag{4}$$

where x_{peak} is the position of the maximum. To exhibit stretched exponential tails we finally calculate the logarithmic derivatives

$$q(y) = \frac{d \log_{10}(-\log_{10} p_{0i})}{d \log_{10} x}, \tag{5}$$

where $i = l, r$, and plot them against $y = \log_{10} x$. In this representation, tails of the form $p_0(x) \sim B(x + c)^\beta \exp[-A(x + c)^\alpha]$ lead to a plateau at the value α for large x . A standard Gaussian distribution $(1/\sqrt{2\pi}) \exp(-x^2/2)$ thus approaches asymptotically the value 2.

3. Results

We performed multicanonical simulations [8] by flattening the probability distribution of the magnetization for system sizes up to $L = 64$ at three characteristic temperatures. The right tails in the high-temperature phase at $T = 3.5$ are shown in the upper left plot of Fig. 1. With increasing system size the distribution approaches Gaussian behavior as is expected from the central limit theorem for a finite correlation length $\xi = 1/[-\ln \tanh(1/T) - 2/T] = 1.41235 \dots$. In fact, assuming heuristically that there are effectively L_{eff}^2 uncorrelated spins with $L_{\text{eff}} = L/2\xi$ ($= 6, 12, 23$ for $L = 16, 32, 64$), we obtain the very similar looking curves in the upper right plot of Fig. 1, explaining the finite-size effects.

At the critical temperature $T_c = 2/\text{arcsinh}(1) = 2.2691 \dots$, theory predicts a right tail of the form $x^{(\delta-1)/2} \exp(-x^{\delta+1})$, where $\delta = 15$ is the equation of state exponent, leading to a plateau at 16 [7]. Our data shown in the lower left plot of Fig. 1 reveal a shoulder developing with increasing L . The convergence, however, is extremely slow [10]. The solid line is a fit using this theoretical prediction,

$$p_0(x) = a((x + c)/b)^7 \exp(-((x + c)/b)^{16}), \tag{6}$$

with $a = 1.31, b = 8.59$, and $c = 7.79$.

For low temperatures the magnetization is close to unity. At $T = 1.5$ a true peak starts developing only for system sizes $L > 16$, and even for $L = 32$ only five data points exist to the right of the peak, cf. Fig. 2. We therefore found only weak evidence for Gaussian behavior with increasing L for the right tails [10]. Here the left tails shown in the lower right plot of Fig. 1 are more interesting. Near the peak (i.e. for small x) we see a narrow regime over which the curves approach Gaussian behavior as one would expect again from the central limit theorem. In the intermediate range of x , the curves show a plateau at 0.5, corresponding to a fat stretched exponential $\sim \exp(-\sqrt{x})$. This

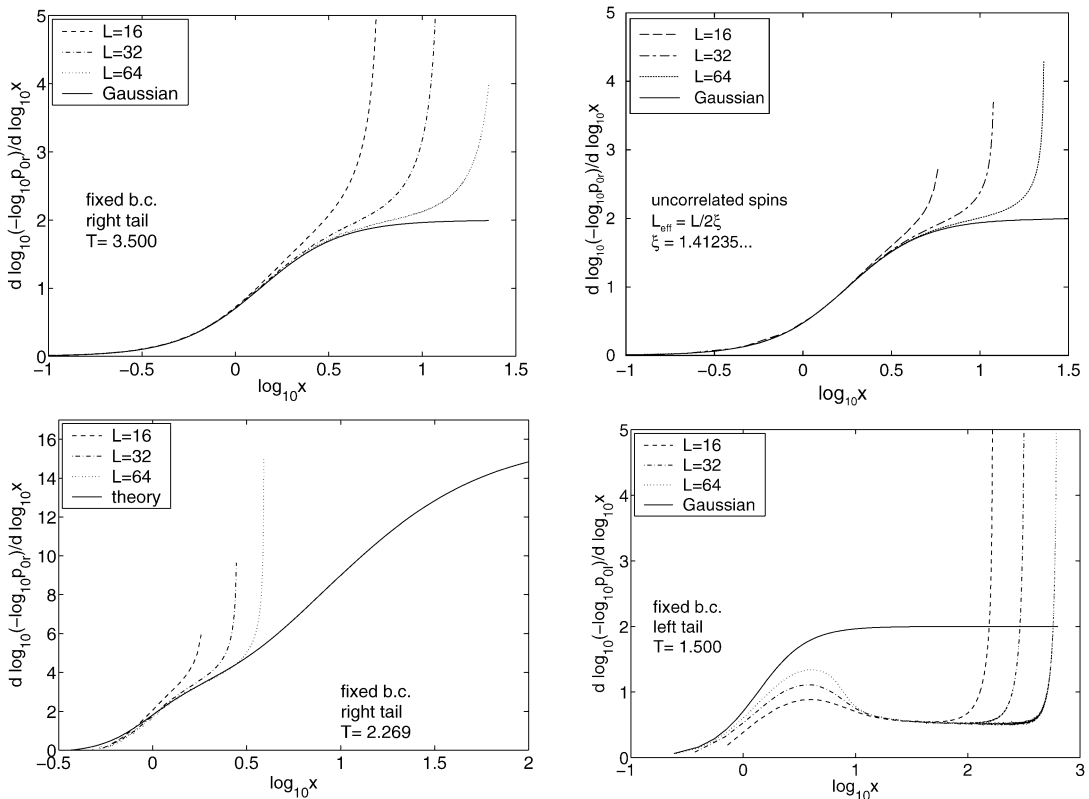


Fig. 1. Tail analyses for the 2D Ising model with fixed boundary conditions.

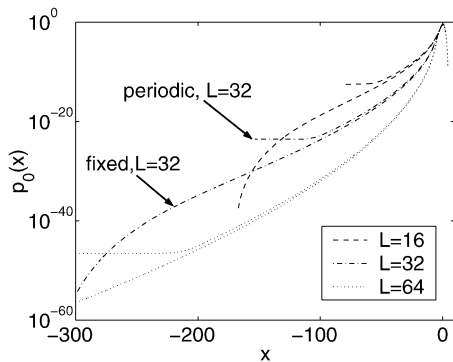


Fig. 2. Rescaled order parameter distributions $p_0(x)$ on a logarithmic scale for $T = 1.5$ and $L = 16, 32, 64$ for fixed and periodic boundary conditions. For periodic boundary conditions only the right half of the distribution is shown.

represents the well known droplet regime predicted analytically [11]. We observed this stretched exponential tail in the distributions for low temperatures all the

way up to T_c . For periodic boundary conditions the stretched exponential tails eventually cross over into a flat bottom, reflecting phase coexistence on finite lattices governed by strip-like spin configurations. For fixed boundary conditions the same stretched exponential tail is terminated by a cutoff function. Visually the three different regimes can also easily be identified in the logarithmic plot of $p_0(x)$ shown in Fig. 2.

4. Summary

To summarize, the order-parameter distribution at the critical point is found to approach its asymptotic universal scaling function extremely slowly. This is also true for periodic boundary conditions in two dimensions [10] as well as for the 3D Ising model, where a similar multi-overlap simulation study [12] has recently focused on the distributions of the overlap parameter instead of the magnetization considered here.

Our extrapolations discussed in detail in Ref. [10] indicate that the required system sizes ($L \gtrsim 10^5$) are beyond present day numerical resources even for the 2D Ising model.

References

- [1] J. Cardy (Ed.), *Finite-Size Scaling*, North-Holland, Amsterdam, 1988;
- V. Privman (Ed.), *Finite-Size Scaling and Numerical Simulation of Statistical Systems*, World Scientific, Singapore, 1990.
- [2] K. Binder, *Z. Phys. B* 43 (1981) 119;
- A. Bruce, *J. Phys. C* 14 (1981) 3667;
- J. Kim, A. Souza, D.P. Landau, *Phys. Rev. E* 54 (1996) 2291;
- H. Blöte, J. Heringa, M. Tsy-pin, *Phys. Rev. E* 62 (2000) 77.
- [3] E. Brezin, J. Zinn-Justin, *Nucl. Phys. B* 257 (1985) 867;
- A. Esser, V. Dohm, M. Hermes, J. Wang, *Z. Phys. B* 97 (1995) 205;
- X. Chen, V. Dohm, A. Talapov, *Physica A* 232 (1996) 375.
- [4] T. Burkhardt, B. Derrida, *Phys. Rev. B* 32 (1985) 7273.
- [5] R. Hilfer, *Phys. Scripta* 44 (1991) 321;
- R. Hilfer, *Phys. Rev. Lett.* 68 (1992) 190;
- R. Hilfer, *Mod. Phys. Lett. B* 6 (1992) 773;
- R. Hilfer, *Int. J. Mod. Phys. B* 7 (1993) 4371;
- R. Hilfer, *Phys. Rev. E* 48 (1993) 2466.
- [6] R. Hilfer, *Z. Phys. B* 96 (1994) 63.
- [7] R. Hilfer, N.B. Wilding, *J. Phys. A: Math. Gen.* 28 (1995) L281.
- [8] B.A. Berg, T. Neuhaus, *Phys. Lett. B* 267 (1991) 249;
- B.A. Berg, T. Neuhaus, *Phys. Rev. Lett.* 68 (1992) 9;
- W. Janke, *Int. J. Mod. Phys. C* 3 (1992) 1137;
- W. Janke, *Physica A* 254 (1998) 164.
- [9] G. Smith, A. Bruce, *J. Phys. A: Math. Gen.* 28 (1995) 6623;
- D. Stauffer, *Int. J. Mod. Phys. C* 9 (1998) 625;
- M. Tsy-pin, H. Blöte, *Phys. Rev. E* 62 (2000) 73.
- [10] R. Hilfer, B. Biswal, H.G. Mattutis, W. Janke, *Phys. Rev. E* 68 (2003) 046123.
- [11] S.B. Shlosman, *Comm. Math. Phys.* 125 (1989) 81.
- [12] B.A. Berg, A. Billoire, W. Janke, *Phys. Rev. E* 66 (2002) 046122.