Cumulant ratios and their scaling functions for Ising systems in a strip geometry

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We calculate the fourth-order cumulant ratio (proposed by Binder) for the two-dimensional Ising model in the strip geometry $L\times\infty$. The density-matrix renormalization-group method enables us to consider typical open boundary conditions up to $L=200$. Universal scaling functions of the cumulant ratio are determined for strips with parallel as well as opposing surface fields. Their asymptotic properties are also examined.

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I. INTRODUCTION

An universality principle is a cornerstone of contemporary theory of phase transitions. According to this principle, the following sorts of quantities are universal: critical exponents, certain amplitude ratios, and scaling functions [1]. They differ each from other in their status. The (bulk) critical exponents are independent on boundary conditions, whereas two other groups are dependent.

The critical exponents are known for many models (both exactly and approximately). The collection of results available for amplitude ratios is also rich, but significantly smaller than for exponents; see Ref. [1] for exhaustive information.

Among amplitude ratios, so called cumulant ratios are of great importance. In physical terms, they measure deviation of magnetization fluctuations at criticality from a Gaussian distribution. Cumulant ratios have also been used to locate the critical points and critical lines in many models [2–5]. Last, cumulants give subsequent approximations of the scaling function for free energy (as they are expressible by derivatives of the free energy with respect to the magnetic field, i.e., higher susceptibilities). This way, cumulants enter such important and experimentally measurable quantities such as, for instance, the scaling equation of state—and thus play very important role at criticality.

Cumulant ratios are dependent on boundary conditions. They were calculated mainly for periodic boundary conditions or for infinite systems [2,5–13]. However, from an experimental point of view, the systems in finite ''open'' geometries are most frequently investigated. It correspond to boundary conditions of ''open'' type: ''free'' (no surface fields), ''wall'' (infinite surface fields). We are aware of only very few results of calculations with the above boundary conditions [2,4]. Motivated by this situation, we state the aim of this paper: Calculation of universal cumulant ratios for the two-dimensional Ising model in strip geometry under boundary conditions of ''free'' and ''wall'' types, including the intermediate regime.

We have calculated cumulant ratios using method called the density-matrix renormalization-group (DMRG). Since the DMRG is most powerful for open boundary conditions, it is particularly suited for our goals.

II. DEFINITION OF CUMULANTS

We consider the two-dimensional Ising system on a square lattice in strip geometry (L is width of the strip and N is its length) with the Hamiltonian

$$\mathcal{H}=-J\left[\sum_{\langle i,j\rangle} s_i s_j - H\sum_i s_i - H_1\sum_i^{(1)} s_i - H_L\sum_i^{(L)} s_i\right], \quad (1)$$

where the first sum runs over all nearest-neighbor pairs of sites while the last two sums run over the first and the Lth column, respectively. H is the bulk magnetic field, whereas H_1 and H_L are the surface fields (all of them are dimensionless quantities measured in units of J). In the course of calculations of the cumulant in the termodynamic limit, two limiting processes are taken: $T\to T_c$ and $L\to\infty$. In general, a value of the cumulant does depend on ordering of these limits [12]. In our paper we analyze so-called ''massless'' case (analogously as in Ref. [12]): $T=T_c=2/\ln(1+\sqrt{2})\simeq 2.269185$ followed by $L\to\infty$. Therefore, we do not notice the temperature dependence below. We also drop (as unnecessary) explicit dependence on surface fields until the discussion of scaling functions.

We consider the ratio of moments of magnetization proposed by Binder [2], with a modification for a system in strip geometry [2,5,8,11]. Let us first define

$$U_L=\lim_{N\to\infty}[N(\langle M^4\rangle\langle M^2\rangle^{-2}-3)]/3, \quad (2)$$

where $M=\Sigma_i s_i$ is the total (extensive) magnetization. Then, the cumulant ratio r in question is

$$r=\lim_{L\to\infty} L^{-1}U_L. \quad (3)$$

The r quantity defined above is equal to *minus* Binder cumulant. We use this sign convention in order to compare it with some theoretical estimates, see below.

An equivalent (but more convenient for us) formula for the above cumulant is as follows: Let $\lambda(L;H)$ be the largest eigenvalue of transfer matrix for the strip of width L [so the quantity $-T\ln\lambda(L;H)$ is the free energy for one column of spins]. We define

$$m_k(L)=\frac{d^k}{dH^k}\ln\lambda(L;H)|_{H=0}. \quad (4)$$

Then our cumulant is equal to [5]

$$r = \lim_{L\to\infty} r(L) \equiv \lim_{L\to\infty} m_4(L)/3Lm_2^2(L). \quad (5)$$

Our method of calculation is based directly on the definition (5). We first find logarithms of the largest eigenvalue $\lambda(L;H)$ for some values of H (at fixed L). Next, we numerically calculate derivatives (4) for $k=2$ and 4, then the ratio $r(L)$, and finally perform the extrapolation $L\to\infty$.

III. SOME TECHNICAL DETAILS OF CALCULATIONS

We use the DMRG method for calculations of $\ln \lambda(L;H)$. Originally, this method was proposed by White [14] for finding accurate approximations to the ground state and the low-lying excited states of quantum chains. Its heart is the recursive construction of the effective Hamiltonian of a very large system using a truncated basis set, starting from an exact solution for small systems. Later, the DMRG was adapted by Nishino [15] for two-dimensional classical systems, where the effective transfer matrix is constructed. We use this version of DMRG. The DMRG has been applied successfully to many different problems and now it can be treated as a standard method, which is very flexible, relatively easy to implement and very precise. For a comprehensive review see Ref. [16].

A factor crucial for precision of DMRG is the so-called number of states kept m, describing the dimensionality of effective transfer matrix [14,16]; the larger number of states kept, the more accurate the value of the free energy. Using $m=50$ we can calculate the free energy with accuracy of the order 10^{-12} for strips of width of the order $L=200$. This is an one order more than the size of systems available by exact diagonalization of the transfer matrix. This fact is crucial for us, because of using the extrapolation procedures. In our calculations we apply the finite system algorithm, developed by White for studying finite systems [14]. An additional factor determining the accuracy of the method is the number of sweeps, i.e., the number of iterations made in order to obtain self-consistency of results. Our numerical experience shows that in most cases, it is sufficient to apply only one sweep (although in the ''wall$+-$'' case two sweeps are necessary—see below).

In our calculations also another factor limiting the accuracy is involved (independently of the DMRG method): it is an error originated from a numerical differentiation. In the procedure of numerical differentiation, a suitable choice of increment ΔH of an argument is of crucial importance. It is clear that ΔH should be taken as small as possible; on the other hand, due to the finite accuracy of the calculation of λ, an error of the difference quotient increases with decreasing ΔH. The increments used in our calculations have been determined as a compromise between the above two tendencies. Additional factor determining the accuracy of numerical differentiation, is a number of points used to calculate the derivative. We use formulas where a derivative is determined from the second-order Taylor expansion [i.e., we need $n+3$ values of function for nth derivative; this way, an accuracy is of the order $\mathcal{O}((\Delta H)^3)$]. Therefore, the m_2 was determined from five points [three points in symmetrical case, i.e., $f(H)=f(-H)$] and from seven points for m_4 (four points when the symmetry was present).

TABLE I. Values of cumulant ratios for some values of L.

L	$r(L)$, free	$r(L)$, wall$++$	$r(L)$, wall$+-$
160	-1.098525	0.462556	-0.304831
170	-1.098234	0.462225	-0.304859
180	-1.097964	0.461859	-0.304883
190	-1.097723	0.461525	-0.304902
200	-1.097481	0.461133	-0.304915
∞	-1.0932(3)	0.455(2)	-0.3050(1)

We have tested correctness of our calculations in several ways. One of them was the L dependence of derivatives m_2 and m_4. Finite-size scaling (FSS) theory [1,8] predicts the following behavior:

$$\left.\frac{d^n f}{dH^n}(L)\right|_{H=0} \sim L^{-\tilde{d}+n\Delta/\nu}, \quad (6)$$

where we have $\Delta=15/8$ and $\nu=1$ for the two-dimensional Ising model. $\tilde{d}$ is a dimension of system in the ''finite-size direction,'' i.e., it is a number of linearly independent directions along which a size of the system is finite. For our case (the strip) we have to take $\tilde{d}=1$ that gives the following predictions for derivatives:

$$m_2 \sim L^{\rho_2}, \quad m_4 \sim L^{\rho_4}, \quad (7)$$

where $\rho_2=11/4$ and $\rho_4=13/2$. An extrapolation procedure has been performed with use of the powerful Bulirsch-Stoer (BS) method [17].

IV. RESULTS: THE ''FREE'' CASE

The ''free'' case corresponds to zero surface fields $H_1=H_L=0$ in the formula (1). We have performed calculations for L in the range $160\leq L\leq 200$ with step 10; these values of L were taken in all situations. We took an increment of ''bulk'' magnetic field $\Delta H=5\times 10^{-6}$, $m=50$ and one sweep. The results are listed in Table I.

As a byproduct we have tested the FSS predictions for the L dependence of derivatives m_2 and m_4. Values of corresponding exponents [see Eq. (7)] are $\rho_2=2.7495(3)$ and $\rho_4=6.50(3)$, so predictions of FSS are confirmed in excellent manner. The same conclusion is true in next two situations.

As another test of correctness (and quality) of DMRG results, we have calculated ratios by the immediate numerical diagonalization of transfer matrix for $10\leq L\leq 18$ (L even; these values of L are also used in the next cases). We proceeded as above, i.e., by calculation of logarithm of the largest eigenvalue for some values of bulk field H, followed by numerical differentiation of $f(H)$ and computation of ratio and extrapolation, without any ''renormalization.'' We took the increment $\Delta H=10^{-4}$. We have obtained $r=-1.094(1)$; $\rho_2=2.746(1)$; $\rho_4=6.46(1)$. It is seen that the results are fully consistent with the DMRG calculations but less precise; we have the same situation for two other boundary conditions.

V. RESULTS: THE ''WALL++'' CASE

The ''wall++'' boundary condition corresponds to the assumption that all boundary spins have the same value and sign. It is equivalent to putting $H_1 = H_L = \infty$ in Eq. (1). Numerical experience suggests that it is sufficient to take $H_1 = 10$ – for larger values of H_1 the changes of the free energy are negligible [18].

The ''wall++'' system is more intricate, from numerical point of view, than the ''free'' one. The complication is due to the fact that, for parallel surface fields, the maximum of the free energy $f(H)$ does not appear for $H=0$ but it is shifted to a certain nonzero value $H_0(L)$. This phenomenon is called the capillary condensation [18,19]. In order to calculate derivatives and ratios at zero magnetization (i.e., at the maximum of the free energy), we first have to find its position $H_0(L)$. FSS predicts [19] the following dependence: $H_0(L) \sim L^{-\Delta/\nu}$. From our DMRG calculations, we have obtained the value $\Delta/\nu = 1.8749(2)$.

For the ''wall++'' configuration the free energy is not longer a symmetric function of the bulk field H, so we have been forced to calculate m_2 from 5 points and m_4 from 7 points. We have taken the increment $\Delta H = 5\times10^{-6}$, $m=50$ and one sweep. The results are presented in Table I. For exponents of m_2 and m_4, we have obtained: $\rho_2 = 2.7504(3)$ and $\rho_4 = 6.5024(3)$. The precision of these results is a little bit less than in the ''free'' case, although still very satisfactory (three significant digits). However, it should be stressed that here we must do much more numerical computations than in the ''free'' case, so some lack of precision is inevitable. Exact diagonalization of transfer matrix gave the following values: $r=0.45(4)$; $\rho_2 = 2.75(1)$; $\rho_4 = 6.5(2)$.

VI. RESULTS: THE ''WALL+−'' CASE

One of the important physical implications of the ''+−'' boundary condition is the presence of an *interface* between ''+'' and ''−'' phases in the system. It causes large fluctuations, which have an implication in numerical practice, namely, *two sweeps* are necessary to ensure self-consistency of results. In our calculations, the value of surface field $H_1 = 100$ the increment $\Delta H = 2\times10^{-5}$, and $m=40$ were taken. The results are listed in Table I. The values of exponents are $\rho_2 = 2.7502(2)$, $\rho_4 = 6.502(2)$.

The procedure of exact diagonalization of transfer matrix gave the following values: $r=-0.305(2)$; $\rho_2 = 2.755(1)$; $\rho_4 = 6.50(2)$. As a matter of some interest, let us remark that for the ''wall+−'' boundary condition the L dependence is much weaker than for the ''free'' and ''wall++'' situations.

VII. SCALING FUNCTIONS FOR RATIOS

The ''wall++/+−''-type conditions can be treated as limiting cases of the systems with equal *finite* parallel/antiparallel (++/+−) surface fields. Another limiting case is the ''free'' boundary condition (BC), where the values of surface fields are set to zero. One can expect that for intermediate situations, i.e., finite values of boundary field H_1, cumulants would be smooth functions of H_1. Particularly interesting are scaling properties of these functions. The scaling theory predicts that at criticality, the system depends on the surface field H_1 and strip width L only through dimensionless combination $\zeta = LH_1^2$ [20]. We have calculated r for both ''++'' and ''+−'' boundary conditions for $L = 40,80,120$ using $m=40$, and at full range of scaling variable. The results are presented in Figs. 1(a), 1(b). It is seen that scaling properties are confirmed in excellent manner.

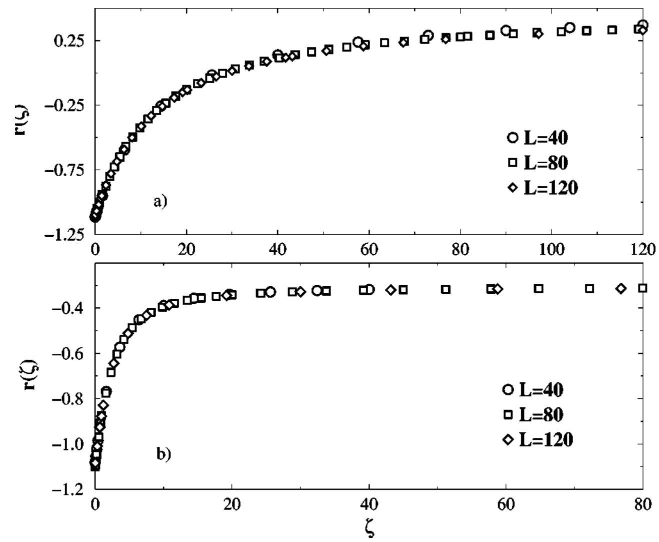

FIG. 1. The cumulant ratio as a function of *dimensionless* scaling variable $\zeta = LH_1^2$: (a) the ''++'' BC (b) the ''+−'' BC. Notice that the convergence of ratio to its limit value is much faster for ''+−'' than for ''++.'' For the latter case, the saturation is achieved for $\zeta \approx 500$ (outside the range of plot).

Limiting values of these functions (i.e., for $\zeta = 0$ and $\zeta \to \infty$) are fully consistent with our more precise calculations, although convergence of ratio to its limit value is much faster for ''wall+−'' than for ''wall++.'' It is interesting to examine asymptotic properties of $r(\zeta)$ for $\zeta\to\infty$. We have checked two simplest possibilities $r(\zeta) \approx r + A\exp(-B\zeta)$ and $r(\zeta) \approx r + A\zeta^{-B}$, for some constants A,B. Our data allowed us to exclude the first possibility, and to verify that the second one is fulfilled with good accuracy. By use of least-square fitting in the log-log scale, we obtained the values $A = 1.57(2)$, $B = 1.25(1)$ for the +− case, and $A = 80(10)$, $B = 1.28(10)$ for the ++ case. On the base of these results, we conjecture that the value of the exponent B is common for both cases and equal to 1.25. At this moment, we are not able to explain it theoretically, and we postpone it to the future.

As far as we know, scaling functions for cumulants have been almost not studied so far. The only exception is paper [21]; however, the authors consider scaling functions different from ours.

VIII. SUMMARY

We have calculated cumulant ratios for Ising strips with three natural boundary conditions, almost not studied so far: ''free,'' ''wall++,'' and ''wall+−'' situations. We have applied the density-matrix renormalization-group method followed by numerical differentiation and extrapolation $L \to \infty$. We claim that our results are very precise (three or four significant digits). The precision is comparable with three other ''top quality'' methods used in similar calculations: Monte Carlo [12], some versions of renormalization group

[13], and analysis of high-temperature series [10].

Some of our results (for the ''wall++'' case) can be interesting in the context of rigorous results for cumulants, namely, those obtained by Newman and Shlosman [22]. They proved general inequality for Ursell functions in ferromagnetic Ising systems at zero bulk magnetic field H: $(-1)^{n-1}U_{2n}\geqslant 0$. Our cumulant r corresponds to U_4. For the ''free'' and ''wall+−'' systems, this inequality *is fulfilled*, whereas in the ''wall++'' case is *not*. This does not contradict the Newman and Shlosman inequality, because the ''wall++'' system is calculated at $H\neq 0$ [remember $H_0(L)\sim L^{-\Delta/\nu}$]. It shows, however, that the Newman and Shlosman inequality cannot be fulfilled if the assumption $H=0$ is relaxed. It would be very interesting to generalize their results for the ''wall-type'' cases.

We have also calculated the quantity which has apparently escaped attention so far, namely, the scaling functions for cumulants. Such functions provide information how finite surface fields influence values of cumulants. This influence is significant—in one case (''++'') even the sign of the cumulant changes upon growth of the surface field.

Natural lines of continuation of our investigations are: testing of universality of cumulants and scaling functions (for other models in the two-dimensional Ising universality class, for example, the hard squares model) and calculation of higher cumulants. This work is currently in progress.

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