Critical Binder cumulant of two–dimensional Ising models

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Abstract. The fourth-order cumulant of the magnetization, the Binder cumulant, is determined at the phase transition of Ising models on square and triangular lattices, using Monte Carlo techniques. Its value at criticality depends sensitively on boundary conditions, details of the clusters used in calculating the cumulant, and symmetry of the interactions or, here, lattice structure. Possibilities to identify generic critical cumulants are discussed.

PACS. 05.50.+q Ising model, lattice theory – 05.10.Ln Monte Carlo method, statistical theory

1 Introduction

In the field of phase transitions and critical phenomena, the fourth order cumulant of the order parameter [1], the Binder cumulant U, plays an important role. Among others, the cumulant may be used to compute the critical exponent of the correlation length, and thence to identify the universality class of the transition, characterised , e.g., by the values of the bulk critical exponents [2].

The value of the Binder cumulant at the transition temperature in the thermodynamic limit, U^*, the critical Binder cumulant, has received much attention as well [3], being a measure of the deviation of the corresponding distribution function of the order parameter from a Gaussian function. However, there seem to be conflicting statements about its 'universality'. For concreteness and simplicity, let us consider here and in the following results within the universality class of the two–dimensional Ising model, with the magnetization as the order parameter. In particular, in the case of the isotropic spin-1/2 Ising model with ferromagnetic nearest–neighbour couplings on a square lattice with L^2 spins, the critical cumulant has been determined very accurately in numerical work, applying Monte Carlo techniques [4] and transfer-matrix methods [5] augmented by finite–size extrapolations to the thermodynamic limit, $L \longrightarrow \infty$. The resulting value, employing full periodic boundary conditions, is $U^* = 0.61069...$ [5]. For other related two-dimensional models on square lattices, including the nearest-neighbour XY-model with an easy axis and the spin-1 Ising model, estimates of U^* have been reported which seem to be consistent with this value [4,5,6,7,8, 9,10,11,12]. Actually, the quoted value for U^* has been sometimes believed to be 'universal', i.e. to be generic for the two–dimensional Ising universality class.

On the other hand, the possible dependence of the critical cumulant, for instance, on boundary conditions has been noted already by Binder in his pioneering work [1].

Indeed, different values of U^* have been obtained when considering various boundary conditions, lattice structures (or anisotropic interactions) as well as aspect ratios, staying in the universality class of the two–dimensional Ising model [3,5,13,14,15,16]. Some of the results can be related to each other by suitable transformations. For instance, applying periodic boundary conditions, the critical cumulant of the nearest–neighbour Ising model with different vertical and horizontal couplings may be mapped onto that of the isotropic model on a rectangular lattice with aspect ratio r [5,16]. Such a scale transformation, keeping rectangular symmetry and employing periodic boundary conditions, does not exist, however, for Ising models with nearest neighbour and *anisotropic* next–nearest neighbour interactions on a square lattice (with the triangular lattice being a special case of that anisotropy [16,17]). This fact has been demonstrated by Chen and Dohm [17] using renormalization group arguments, and it has been confirmed in Monte Carlo simulations [16,18]. It shows a violation of the two–scale factor universality for finite–size effects [19], in general, and, specifically, of the universality of the critical Binder cumulant.

The aim of this paper is, to study spin-1/2 Ising models with nearest neighbour interactions on square and triangular lattices in order to analyse in a systematic way possible dependences of the critical Binder cumulant on boundary conditions, clusters used in calculating the cumulants, and lattice structure (or anisotropy of the interactions).

The paper is organized as follows: In the next section, the model and the method are introduced, and the Binder cumulant is defined. Then, simulational results will be presented, arranged according to boundary conditions. Finally, the findings will be summarized briefly.

2 Model and method

We consider spin-1/2 Ising models on square and triangular lattices with nearest neighbour ferromagnetic interactions, J. The Hamiltonian reads

$$\mathcal{H} = -J \sum_{(x,y),(x',y')} S_{x,y} S_{x',y'} \qquad (1)$$

where $S_{x,y} = \pm 1$ is the spin at site (x, y). Sums are taken over all pairs of nearest–neighbour sites (x, y), (x', y'). x and y refer to symmetry axes of the lattices. Usually, lattices of linear dimensions L and $K = rL$ will be simulated, r is the aspect ratio. As indicated above, the triangular case is isomorphic to an anisotropic Ising model on a square lattice with nearest–neighbour couplings augmented by half of the next–nearest neighbour couplings, also of strength J, along one diagonal direction of the lattice [16,17,20].

Our aim is to study the Binder cumulant at the phase transition temperature T_c. For both lattice structures, the exact critical temperature is known. For the square lattice, one gets [21]

$$k_B T_c / J = 2 / \ln(\sqrt{2} + 1) = 2.26918... \qquad (2)$$

For the triangular lattice, the critical temperature is given by [22]

$$k_B T_c / J = 2 / \ln(\sqrt{3)} = 3.64095.. \qquad (3)$$

The fourth order cumulant of the magnetization, i.e. the Binder cumulant, for a spin cluster C is defined by [1]

$$U(T, C) = 1 - < M^4 >_C / (3 < M^2 >_C^2) \qquad (4)$$

where $< M^2 >_C$ and $< M^4 >_C$ denote the second and fourth moments of the magnetization in that cluster, taking thermal averages. In principle, clusters of various sizes or shapes and systems with different boundary conditions may be studied. In the Ising case, the cumulant approaches in the thermodynamic limit (with the cardinal number $|C| \longrightarrow \infty$) the value 2/3 at temperatures $T < T_c$, while it tends to zero, reflecting a Gaussian distribution of the magnetization histogram, at $T > T_c$ [1]. At T_c, $U^* = U(T_c, |C| \longrightarrow \infty)$ acquires a nontrivial value, the critical Binder cumulant.

To study systematically the possible dependence of the critical cumulant for two-dimensional Ising models on boundary conditions, the choice of clusters C as well as the lattice type (or, more basically [17], the anisotropy of interactions), we performed Monte Carlo simulations for both lattice types at criticality.

Note that simulational data of high accuracy are needed, to obtain reliable estimates for U^*. We computed systems of various shapes and sizes, usually with up to about 4×10^3 spins. In general, the (moderate) system sizes already seem to allow for a smooth extrapolation to the thermodynamic limit. Using the standard Metropolis algorithm (a cluster flip algorithm becomes significantly more efficient for larger system sizes), Monte Carlo runs with up to 10^9 Monte Carlo steps per site, for the largest systems, were performed, averaging then over several, up to

about ten, of these runs to obtain final estimates, and to determine the statistical error bars shown in the figures. We computed not only the cumulant, but also other quantities like energy and specific heat, to check the accuracy of our data. Of course, for sufficiently small lattices thermal averages may be obtained exactly and easily by direct enumeration.

3 Results

The critical Binder cumulant depends sensitively on the boundary conditions. In fact, Ising systems with periodic and free boundary conditions will be analysed here. In addition, the Ising model on a square lattice with mixed, free and periodic, boundary conditions will be considered.

3.1 Periodic boundary conditions

Employing full periodic boundary conditions, with the cluster C comprising the entire system, U^* has been determined accurately before, both for square and triangular lattices. For the square lattice, one gets $U_s^* = 0.61069...$ [4,5,16], and for the triangular lattice, one finds a slighty different, but distinct value, $U_t^* = 0.61182...$ [5,16].

Less attention has been paid in the past, however, to different choices of clusters. In his pioneering work [1], Binder considered square subblocks for the Ising model on a square lattice. In particular, for systems of L^2 spins, the clusters then correspond to subblocks of size L'^2, where $L' = bL$, with the subblock factor $b \leq 1$. The finite–size dependence of the cumulant at criticality has been discussed as well. For the two–dimensional Ising model, the leading correction term to the critical cumulant is argued [1] to behave like $U^* - U_c(T_c, L) \propto 1/L$.

In the original analysis [1], the subblock sizes L' have been enlarged at fixed L. We pursue a somewhat different strategy in computing cumulants at T_c by fixing the subblock factor b and then enlargening the linear dimension of the lattice with L^2 spins (applying periodic boundary conditions). In particular, we set $b = 1, 1/2, 1/4$, and 1/8. Some representative data of our simulations are depicted in Fig. 1. Increasing the system size L, the cumulant at criticality allows for a smooth and reliable extrapolation to the thermodynamic limit, yielding U_b^*. U_b^* is observed to decrease with decreasing subblock factor b, and we estimate $U_b^* = 0.5925 \pm 0.0005, 0.577 \pm 0.001$, and 0.568 ± 0.0015 for $b = 1/2, 1.4$, and 1/8, respectively. Plotting now U_b^* against b, we obtain, in the limit $b \longrightarrow 0$, the critical cumulant, $U_{b=0}^* = 0.560 \pm 0.002$. This estimate may be checked by fixing L' and increasing L to estimate $U_{L'}^*$, see Fig. 2. $U_{L'}^*$ is found to depend only rather weakly on L', $L' \geq 4$. Taking into account estimates for $L' = 4$, 8, and 16, we arrive at a value for $U_{b=0}^*$, which agrees nicely with the one quoted above. Note that the critical cumulant in the limit $b \longrightarrow 0$ refers to arbitrarily large clusters or subblocks being eventually embedded in their indefinitely larger 'natural' heat bath. In that sense, the clusters themselves are subject to a 'heat bath boundary
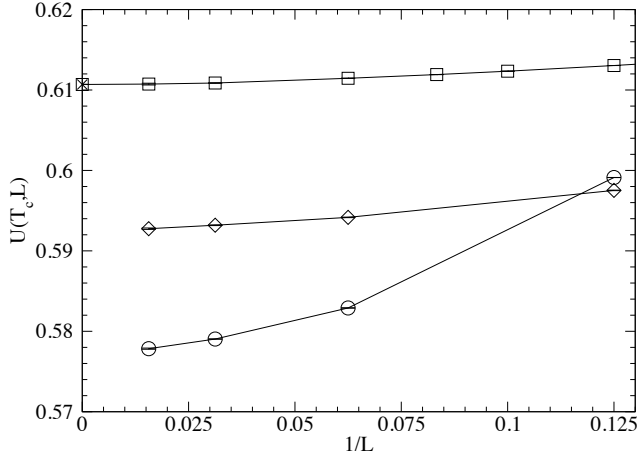
Fig. 1. Binder cumulant $U(T_c, L)$ vs. $1/L$ using subblocks of linear size $L' = bL$ for $b= 1$ (squares), $1/2$ (diamonds), and $1/4$ (circles) in the Ising model with L^2 sites on a square lattice, employing full periodic boundary conditions. The square with a cross, at $1/L = 0$, refers to the result of Ref. 4.
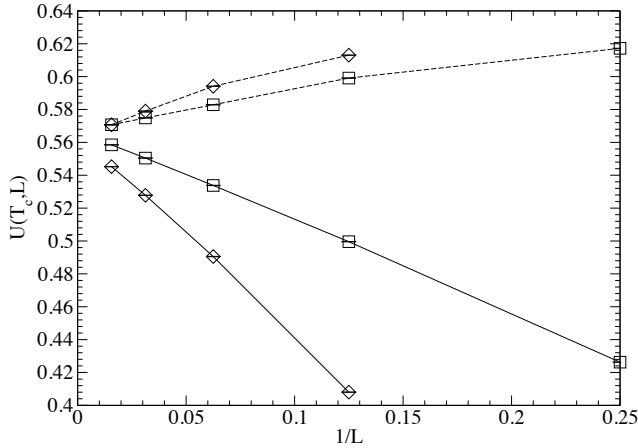

Fig. 2. Fourth–order cumulant $U(T_c, L)$, using subblocks of linear size $L'= 4$ (squares) and 8 (diamonds) as clusters, versus $1/L$ for square lattices of linear dimension L, employing periodic (broken lines) and free (solid lines) boundary conditions.

condition'. This boundary condition is expected to perturb the intrinsic bulk fluctuations of the magnetization of the cluster only very mildly. Therefore, $U_{b=0}^*$ may be a candidate for a critical Binder cumulant, which is robust against various modifications of the model. Indeed, within the accuracy of the simulations, one obtains the same estimate for the critical cumulant, $b \longrightarrow 0$, when one replaces the periodic boundary conditions by free boundary conditions, as will be discussed below.

The critical cumulant for the heat bath boundary condition of the clusters, $b = 0$, is found to depend for rectangular subblocks, $L' \times r_C L'$, on their aspect ratio r_C, tending to decrease significantly, as r_C deviates more and more from one.

Moreover, when going from square to triangular lattices, using periodic boundary conditions and subblocks

of L'^2 spins, the critical cumulant $U_{b=0}^*$ is observed to be very close to that for the square lattice. The possible difference occurs, perhaps, in the third digit. But already for $b = 1$, the difference between U_s^* and U_t^* is quite small. Here, the heat bath boundary condition for the clusters, $b = 0$, tends to reduce such differences furthermore, and one has to be careful in drawing definite conclusions. Indeed, on physical grounds I tend to believe that also under heat bath boundary conditions for the subblocks, there is a difference in the value of the critical cumulant for the triangular and the square lattice, unless one uses subblocks of special shapes, as will be discussed below.

3.2 Mixed boundary conditions

We study the Ising model on a square lattice consisting of L lines, running from left to right, having L sites or spins in each line. At the bottom and top, free boundary conditions are employed, while the left and right hand sides are connected by periodic boundary conditions. The Hamiltonian, eq. (1), is slightly extended by still assuming ferromagnetic nearest neighbour interactions, which now may be different in the two surface lines at the top and bottom, J_s, as compared to those, J_b, in the bulk, i.e. when at least one spin of the nearest neighbour pair of spins is not in a surface line, as usually assumed [23,24, 25,26].

Let us first consider $J_s = J_b$. To compute the critical cumulant, U_{mixed}^*, we take clusters C consisting of all, L^2, thermally excitable spins. Results for various system sizes are depicted in Fig. 3. Again, the data may be smoothly extrapolated to the thermodynamic limit, $L \longrightarrow \infty$, leading to the estimate $U_{mixed}^* = 0.514 \pm 0.001$.

When varying J_s/J_b, the cumulant appears to depend strongly on the ratio of the surface to the bulk coupling, considering systems of fairly small sizes, see Fig. 3 for $J_s/J_b= 0.1$. 1.0, and 2.0. However, in the thermodynamic limit, the critical cumulant seems to approach a unique value, independent of J_s/J_b, as may be inferred also from that figure.

It is well known that the critical behaviour of the bulk is distinct from that of the surface [23,24,25,26]. In particular, in the two–dimensional case, the vanishing of the surface magnetization, on approach to T_c, is described by a power law with an exponent $1/2$, while the exponent of the bulk magnetization is $1/8$ [26,27,28]. Thence, it may be interesting to restrict the clusters C to the surface lines at the bottom and top of the lattice, in analogy to what has been done before for Ising films in three dimensions [29]. Here, we find that the critical cumulant tends to vanish in the thermodynamic limit, reflecting a Gaussian distribution of the histograms for the surface magnetization. The vanishing may be explained by the fact that the surface is one–dimensional in our case.
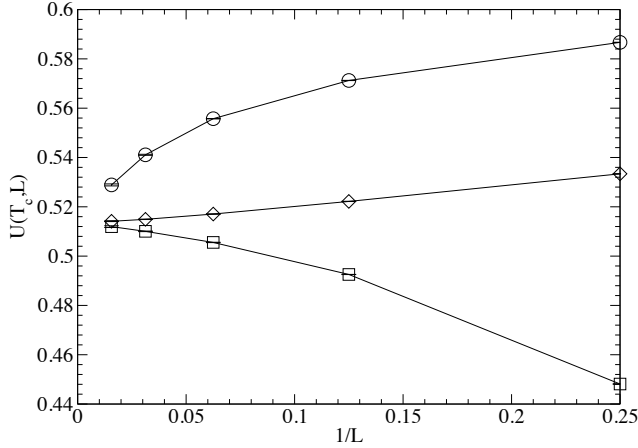
Fig. 3. Binder cumulant $U(T_c, L)$ for the Ising model with mixed boundary conditions and L^2 spins on a square lattice as a function of $1/L$, varying the ratio $J_s/J_b = 0.1$ (squares), 1.0 (diamonds), and 2.0 (circles).

Fig. 4. Binder cumulant $U(T_c, L(_R))$ at criticality for square (squares) and triangular (triangles) lattices with free boundary conditions along two symmetry axes of the lattices (broken lines) and along discretized circles (solid lines) as a function of $1/L$ and $1/L_R$, respectively.

3.3 Free boundary conditions

Free boundary conditions allow one to study arbitrary shapes of the lattice. Moreover, when compared to periodic boundary conditions, they are more realistic.

Let us first consider square and triangular lattices with L^2 spins, i.e. with aspect ratio $r = 1$, applying free boundary conditions at the four sides of the system. The clusters C are comprising all spins, $b = 1$. As may be inferred from Fig. 4, the critical cumulant, in the thermodynamic limit, may be estimated from a smooth extrapolation of the simulational data. The resulting values deviate appreciably for the two different lattice structures: For the square lattice, we find $U^*_{fbc,s} = 0.396 \pm 0.002$, while for the triangular lattice, we obtain $U^*_{fbc,t} = 0.379 \pm 0.001$. Accordingly, free boundary conditions are very useful to show the relevant influence of the lattice type (or anisotropy of the interactions) on the critical Binder cumulant. In comparison, the difference in the critical cumulant for the Ising model on square and triangular lattices is rather small in the case of periodic boundary conditions, see above.

The critical cumulant is expected to depend on the aspect ratio, as we confirmed by considering square lattices with the aspect ratio $r = 1/2$. The critical cumulant U^* is estimated to be 0.349 ± 0.002.

We also computed the cumulant, for the square lattice, with the clusters C being square subblocks of fixed linear dimension L', to study the effect of heat bath boundary conditions, with the subblock factor $b \longrightarrow 0$. As illustrated in Fig. 2, by increasing L, the resulting critical cumulant $U^*_{fbc}(L')$ tends to approach the same value as in the case of periodic boundary conditions using the same subblocks L'. The finite–size correction term of the cumulant has opposite sign for the two boundary conditions, see Fig. 2. We conclude that there is strong evidence that the critical cumulant acquires the same value for free and periodic boundary conditions, when the clusters are embedded in their natural heat bath. We tend to suggest, that the very same value holds for other boundary conditions as well.
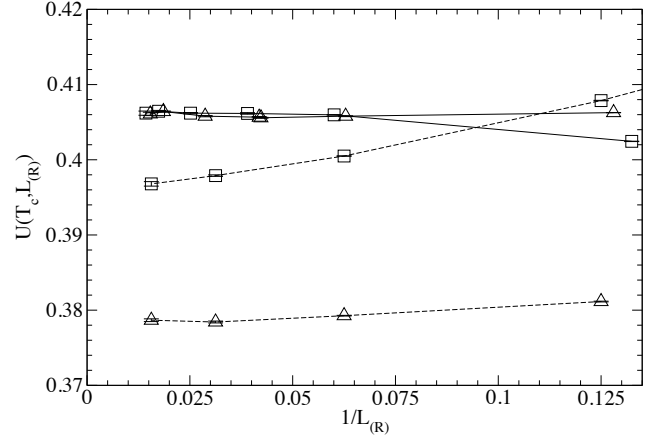
On the other hand, as discussed above, the critical cumulant U^*, in the limit $b \longrightarrow 0$, still depends on the shape of the clusters and, presumably, on the lattice type (or anisotropy of interaction).

The ('non–universal') dependences of U^* may be partly explained by the fact, that the shape of the cluster C does not fit to the spatial structure of the spin correlation function. Indeed, we propose that an appropriate cluster shape follows from the Wulff construction at criticality [30], which determines equilibrium shapes and preserves the intrinsic symmetry of the correlations. In the case of square and triangular lattices, this consideration leads to free boundary conditions of circular shape. Interpreting the Ising model on the triangular lattice as a model with anisotropic next–nearest neighbour interactions on a square lattice, the circle would transform into an ellipse, rotated with respect to the principal axes, on the square lattice. Obviously, for finite radii, the circular shape may be approximated by a discretization. More concretely, we define a radius R from the center of the square or triangular lattice, and we keep all spins, N_R, within this radius as active, thermally excitable spins, while the remaining spins are set to be equal to zero. From that construction, an effective linear dimension L_R may be defined by $L_R = \sqrt{N_R}$ (being proportional to an effective radius of the cluster). In the thermodynamic limit, $R \longrightarrow \infty$, one arrives at a perfect circle. Certainly, an analogous approach is feasible for clusters with heat bath boundary conditions, $b = 0$, being, however, more cumbersome, because one had to take, at each given radius, the thermodynamic limit $L \longrightarrow \infty$.

Simulational data for both lattices with discretized circular free boundary conditions are depicted in Fig. 4. In contrast to the case of free boundary conditions along symmetry axes of the lattices, the critical cumulants for both lattices now tend to approach close-by, if not identical values, $U^*_{circle} = 0.406 \pm 0.001$. Of course, further numerical

Table 1. Selected critical Binder cumulants of the two–dimensional Ising model with periodic (pbc), free (fbc), mixed, and heat bath (hbbc), $b = 0$, boundary conditions on the square or triangular (tri) lattice, considering various system shapes, see text.

boundary	lattice	shape	U^*
pbc	square	square	0.61069... [5]
pbc	tri	rhombus	0.61182... [5]
fbc	square	square	0.396 ± 0.002
fbc	tri	rhombus	0.379 ± 0.001
mixed	square	square	0.514 ± 0.001
hbbc	square	square	0.560 ± 0.002
fbc	square, tri	circle	0.406 ± 0.001

as well as analytical work will be very useful to clarify this interesting aspect.

4 Summary

In this article, we estimated, using Monte Carlo techniques, the critical Binder cumulant U^* for Ising models with nearest neighbour interactions on square and triangular lattices, employing various boundary conditions, types of clusters, and aspect ratios. Selected examples are listed in Tab. 1.

In particular, in the case of periodic boundary conditions we considered square clusters with decreasing subblock factor b. In the limit $b = 0$, we estimate, for the square lattice, $U^*_{b=0} = 0.560 \pm 0.002$. The critical cumulant is observed, when studying clusters of rectangular shapes, to depend on their aspect ratio. The, presumably, rather weak dependence of $U^*_{b=0}$ on the lattice structure for these 'heat bath boundary conditions' for the clusters is not resolved in our simulations.

For the Ising model with mixed boundary conditions, analysing square lattices with the aspect ratio $r = 1$ and clusters comprising all spins, the strength of the surface coupling is found to be irrelevant for the critical cumulant. For clusters containing only the surface spins, the fluctuations of the surface magnetization seem to be of Gaussian form with vanishing U^*. This behaviour reflects the fact that the surface is a one-dimensional object here.

Applying free boundary conditions, the critical Binder cumulants U^* for systems with the aspect ratio $r = 1$ and clusters including all spins, $b = 1$, are cleary different for square and triangular lattices ($U^*_{fbc,s} = 0.396 \pm 0.002$, $U^*_{fbc,t} = 0.379 \pm 0.001$). They differ significantly from the known corresponding values for periodic boundary conditions. In the limit $b = 0$, we obtain for the square lattice an estimate for $U^*_{b=0}$ which agrees, within the error bars, with the one for periodic boundary conditions. Perhaps most interestingly, employing free boundary conditions for clusters of circular form, we find numerical evidence for a unique value, both for square and triangular lattices, $U^*_{circle} = 0.406 \pm 0.001$. In general, we suggest that the dependence of the critical cumulant on the anisotropy of interactions or the lattice structure may be overcome by using cluster shapes obtained from the Wulff construction at criticality.

Certainly, previous standard analyses of the critical cumulant, using especially periodic boundary conditions with the subblock factor $b = 1$, are not invalidated by our study, when they are interpreted properly. In particular, when comparing critical cumulants on different models, one has to make sure that the models satisfy the same symmetries determined by, for instance, the interactions and/or lattice structure. In other words, for such analyses universality of the critical cumulant holds in a rather restricted sense, when compared to universality of critical exponents. In any event, care is needed in applying the critical Binder cumulant when one tries to identify universality classes or the location of the phase transition.

In general, a finite-size scaling theory including boundary conditions, system shapes and anisotropy of interactions would be desirable, extending previous descriptions [19,3,31,17].

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