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LETTER TO THE EDITOR

Critical Binder cumulant in two-dimensional anisotropic Ising models

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Online at stacks.iop.org/JPhysA/38/L739**Abstract**

The Binder cumulant at the phase transitions of Ising models on square lattices with various ferromagnetic nearest- and next-nearest-neighbour couplings is determined using mainly Monte Carlo techniques. We discuss the possibility of relating the value of the critical cumulant in the isotropic, nearest neighbour and in the anisotropic cases to each other by means of a scale transformation in rectangular geometry to pinpoint universal and nonuniversal features.

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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.

The value of the Binder cumulant at the transition temperature, $U(T_c)$, the critical Binder cumulant, has received much attention, too, indicating the universality class as well [2]. For instance, in the case of the spin-1/2 Ising model with ferromagnetic nearest-neighbour couplings the critical cumulant has been determined very accurately in numerical work, applying Monte Carlo techniques [3] and transfer-matrix methods augmented by finite-size extrapolations to the thermodynamic limit [4]. The resulting value, $U(T_c) = 0.61069\dots$ [4], has been observed to hold also for various other Ising-type models on a square lattice [3, 4].

Quite recently, it has been demonstrated by Chen and Dohm [5] that the critical Binder cumulant may display non-universal features, when the couplings on the square lattice are anisotropic. More specifically, they have studied critical effects of the anisotropy matrix of the Landau–Ginzburg–Wilson Hamiltonian, consisting of the coefficients in front of the leading, second-order gradient term of the Hamiltonian. A nondiagonal matrix is shown to imply

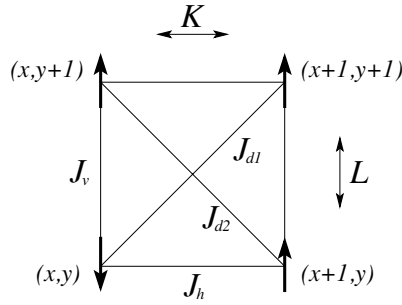


Figure 1. Sketch of the interactions in the anisotropic Ising model.

that the isotropic case cannot be restored by a rescaling of lengths, i.e. in choosing suitable aspect ratios on a rectangular geometry. Such a scale transformation is possible in the case of a diagonal anisotropy matrix, for instance, for nearest-neighbour Ising models with two different couplings along the axes of the square lattice [4–6].

In this letter, we shall present results of rather extensive Monte Carlo simulations for a variety of anisotropic Ising models on a square lattice, corresponding to diagonal and nondiagonal anisotropy matrices. Our data agree qualitatively with the recent results by Chen and Dohm [5] on nonuniversality in the case of a nondiagonal matrix. They confirm quantitatively the scale transformation given by Kamieniarz and Blöte [4] in the case of a diagonal matrix.

2. Results

We consider spin-1/2 Ising models on a square lattice with anisotropic nearest- and next-nearest neighbour interactions. The Hamiltonian reads

$$\mathcal{H} = - \sum_{x,y} S_{x,y} (J_h S_{x+1,y} + J_v S_{x,y+1} + J_{d1} S_{x+1,y+1} + J_{d2} S_{x+1,y-1}), \quad (1)$$

where $S_{x,y} = \pm 1$ is the spin at site (x, y) (see figure 1). In most cases, we take all couplings to be positive, i.e. ferromagnetic. In the Monte Carlo simulations, systems with KL spins, subject to full periodic boundary conditions, are analysed, where $K(L)$ corresponds to the $x(y)$ -direction. The aspect ratio, r , is defined by $r = K/L$.

The critical Binder cumulant is defined by [1]

$$U(T_c) = 1 - \langle M^4 \rangle / (3 \langle M^2 \rangle^2) \quad (2)$$

taking the thermodynamic limit, $L, K \rightarrow \infty$; $\langle M^2 \rangle$ and $\langle M^4 \rangle$ denote the second and fourth moments of the magnetization, $M = \sum_{x,y} S_{x,y} / (KL)$.

We studied especially two types of anisotropy. In the first case, where both diagonal next-nearest-neighbour couplings vanish, $J_{d1} = J_{d2} = 0$, and the anisotropy matrix is diagonal [5].

In the second case, where $J_v = J_h$, $J_{d1} = J_d$, and $J_{d2} = 0$, one encounters nondiagonality [5]. Indeed, we consider the two-dimensional variant of a three-dimensional model which had been analysed by Chen and Dohm [5] and subsequently investigated using Monte Carlo techniques [7]. The simulations, however, may have been hampered by the fact that the critical phase transition temperature is not known exactly, in contrast to the present situation.

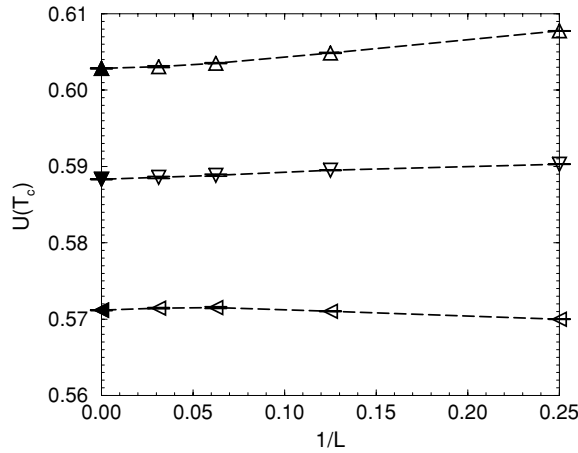


Figure 2. The critical Binder cumulant $U(T_c)$ for Ising models of size L^2 with $J_v/J_h = 4.0, 3.0$ and 2.0 (from bottom to top). Open symbols denote Monte Carlo data, full symbols, at $1/L = 0$, result from the scale transformation [4] as described in the text. Lines are guides to the eye.

Note that data of high accuracy are needed. We computed systems of sizes, K, L , ranging typically from 4 to 64 for square lattices, $K = L$. Using the standard Metropolis algorithm (a cluster flip algorithm becomes significantly more efficient for larger system sizes), Monte Carlo runs with up to 5×10^8 Monte Carlo steps per site, for the largest systems, were performed, averaging then over several, 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 such as energy and specific heat, to check the accuracy of our data. Of course, sufficiently small lattices may be solved easily by direct enumeration.

2.1. Diagonal anisotropy matrix

We consider the anisotropic Ising model, equation (1), with vanishing next-nearest-neighbour interactions and different horizontal, J_h , and vertical J_v , nearest-neighbour interactions (see figure 1). Then the anisotropy matrix is diagonal [5]. The exact transition temperature is given by [8, 9]

$$\sinh(2J_h/k_B T_c) \sinh(2J_v/k_B T_c) = 1, \quad (3)$$

where k_B is the Boltzmann constant. Following Kamieniarz and Blöte [4], the critical Binder cumulant for the anisotropic model on a square lattice, $K = L$, in the thermodynamic limit, can be obtained from that of the isotropic case, $J_h = J_v$, on a rectangular lattice with the aspect ratio $r = K/L$ using a ‘scale transformation’:

$$\sinh(2J_h/k_B T_c) = 1 / \sinh(2J_v/k_B T_c) = r. \quad (4)$$

The critical cumulant $U(T_c)$ of the isotropic case with arbitrary aspect ratio r has been calculated before, extrapolating to the thermodynamic limit, with a high degree of accuracy resulting in a polynomial representation of $U(T_c)$ in r [4]. Note that this critical cumulant decreases monotonically from its maximal value at $r = 1$ to 0 when the aspect ratio is increased to infinity [4] (or lowered to zero, because of the obvious symmetry when replacing r by $1/r$), i.e. when approaching the one-dimensional limit of the model.

In figure 2 we display results of our check on that scale transformation, showing our Monte Carlo results of $U(T_c)$ for anisotropic Ising systems, $J_h \neq J_v$, of small and moderate

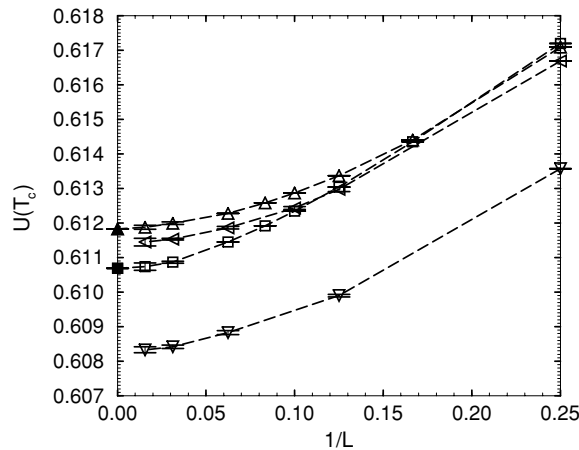


Figure 3. The critical cumulant of the anisotropic triangular Ising model for sizes L^2 , with $J_d/J = 0.0$ (squares), 1.0 (triangles up), 1.5 (triangles left) and 2.5 (triangles down). Open symbols denote our Monte Carlo (as well as numerically exact data for small lattices), full symbols, at $1/L = 0$, denote previous estimates following from finite-size extrapolations [4].

sizes, $K = L$. We also include the values we obtained by evaluating the previously reported polynomial results for the isotropic case with the appropriate (see equation (4)) aspect ratio r [4]. We find a very good, quantitative agreement between our Monte Carlo data and the values based on the scale transformation and the polynomial representation [4].

This observation confirms the universality of the critical Binder cumulant in the case of a diagonal anisotropy matrix.

2.2. Nondiagonal anisotropy matrix

Now, we consider the case where $J_v = J_h = J$, and $J_{d1} = J_d$, while $J_{d2} = 0$ (see figure 1). The model has been called, albeit being defined on a square lattice, the ‘anisotropic triangular model’ [9], because of an obvious isomorphy. Its anisotropy matrix is nondiagonal [5]. Again, the exact transition temperature is known [9, 10] as

$$(\sinh(2J/k_B T_c))^2 + 2 \sinh(2J/k_B T_c) \sinh(2J_d/k_B T_c) = 1, \quad (5)$$

where J and J_d are supposed to be ferromagnetic in the following, unless stated otherwise (a weakly antiferromagnetic J_d does not destroy the ferromagnetic order at low temperatures [9]). Some of our simulational results for the Binder cumulant at T_c for square lattices, $L = K$, with ferromagnetic couplings are shown in figure 3, together with highly accurate estimates based on finite-size extrapolations to the thermodynamic limit [4] in the cases $J_d = 0$ being the isotropic nearest-neighbour square Ising model, and $J_d = J$ being the isotropic nearest neighbour triangular Ising model. The Monte Carlo data seem to allow a smooth extrapolation to the thermodynamic limit, providing reliable and accurate estimates (we refrained from a quantitative finite-size analysis, because, in general, the form of the corrections to scaling seems to be unknown).

Results for extrapolations to the thermodynamic limit are depicted in figure 4. Most importantly, the critical Binder cumulant $U(T_c)$ is seen to increase from its value in the

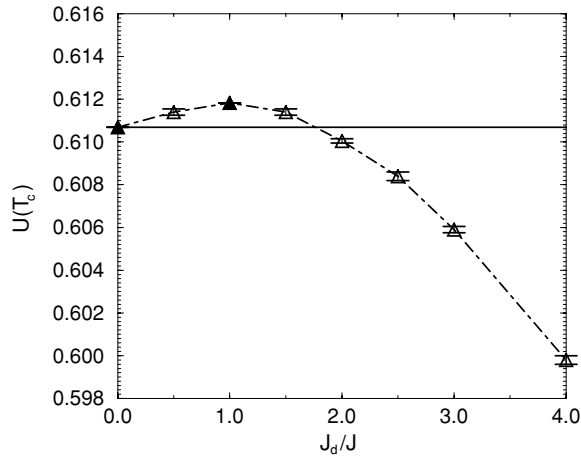


Figure 4. The critical Binder cumulant, extrapolated to the thermodynamic limit (see figure 3) for the anisotropic triangular Ising model as function of the anisotropy J_d/J . Full symbols denote estimates taken from [4]. The solid line corresponds to the isotropic case on a square lattice, $J_d = 0$.

isotropic, $J_d = 0$, case when introducing the diagonal interaction $J_d > 0$. $U(T_c)$ seems to reach a maximum at about $J_d/J = 1.0$, decreasing then, crossing the isotropic value at about $J_d/J \approx 1.74$ (possibly at $\sqrt{3}$, as one might speculate), and finally approaching the one-dimensional limit, where $U(T_c)$ tends to zero, when J becomes indefinitely weak compared to J_d . As has been just emphasized, $U(T_c)$ is initially, for $0 < J_d/J \lesssim 1.74$, larger than in the isotropic limit. Now, varying the aspect ratio and keeping the rectangular geometry in the isotropic Ising model, this can only lead to a decrease in the critical Binder cumulant [4]. Therefore, it is not possible to obtain the critical Binder cumulant in the anisotropic case, $K = L$ and $0 < J_d/J \lesssim 1.74$, by a scale transformation from the isotropic case, in contrast to the situation discussed in the previous subsection. Obviously, this finding is in accordance with the analysis by Chen and Dohm [5]. Our findings do not rule out the possibility that special cases of the triangular and square models, choosing suitable aspect ratios and anisotropies, may be mapped onto each other, having the same critical cumulants [4].

Note that the critical cumulant seems to decrease monotonically when taking a weak antiferromagnetic coupling J_d , as we find in preliminary simulations.

Perhaps quite interestingly, the critical Binder cumulant displays a non-monotonic behaviour when varying the aspect ratio for the anisotropic triangular model, when J_d/J is sufficiently large. Starting with the square lattice, $r = 1$, and then, say, enlarging (or, equivalently due to symmetry, lowering) the aspect ratio, $U(T_c)$ first becomes larger, before finally decreasing again as one approaches the one-dimensional geometry.

In summary, the Monte Carlo simulations show that for a diagonal anisotropy matrix, the critical Binder cumulant in the anisotropic and isotropic cases are connected by a scale transformation keeping rectangular geometry. In marked contrast, such a scale transformation does not exist, in general, in the anisotropic triangular model described by a nondiagonal anisotropy matrix, for reasons which have been discussed recently by Chen and Dohm, demonstrating non-universal features in the critical Binder cumulant [5]. Thence, care is needed in identifying universality classes and in estimating phase transition temperatures in using the critical Binder cumulant.

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