Critical Binder cumulant in a two-dimensional anisotropic Ising model with competing interactions

W. Selke

JARA-SIM, Institut für Theoretische Physik, RWTH Aachen, 52056 Aachen, Germany

L. N. Shchur

*Landau Institute for Theoretical Physics, 142432 Chernogolovka, Russia and Moscow University of Physics and Technology (MFTI),
Dolgoprudny, Russia*

The Binder cumulant at the phase transition of Ising models on square lattices with ferromagnetic couplings between nearest neighbors and with competing antiferromagnetic couplings between next-nearest neighbors, along only one diagonal, is determined using Monte Carlo techniques. In the phase diagram a disorder line occurs separating regions with monotonically decaying and with oscillatory spin-spin correlations. Findings on the variation of the critical cumulant with the ratio of the two interaction strengths are compared to related recent results based on renormalization-group calculations.

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. In particular, the cumulant may be used to locate the phase transition from the intersection of the cumulant for different system sizes. The cumulant also allows to compute the critical exponent of the correlation length, and thence to identify the universality class of the transition.

However, care is needed when attempting to identify the universality class from the value of the Binder cumulant, in the thermodynamic limit, at the transition, U^*. Indeed, that value is known to depend, in a given universality class, on various aspects including the boundary conditions, the shape of the system (being extrapolated to the thermodynamic limit), and the anisotropy of the correlations or interactions [1–7]. On the other hand, U^* may not depend on other details of the system like the spin value [8] or the lattice structure [6].

In recent years, based on renormalization-group (RNG) calculations of Dohm and Chen [4,7] and subsequent Monte Carlo simulations [5,6,9,10], the influence of anisotropic interactions on the critical Binder cumulant U^* has been elucidated. Much attention has been focused on the Ising model with nearest-neighbor (nn) couplings, J, where the anisotropy is introduced by the next-nearest-neighbor (nnn) couplings along only one diagonal of the lattice, J_d [4,5,7]. One encounters a "nondiagonal anisotropy matrix" [4]. Then, in general, there is no simple transformation relating U^*, for given boundary condition and shape, to that of the isotropic model by adjusting the shape [4]. Such a transcription may be easily performed in the case of a diagonal anisotropy matrix, as it occurs, for instance, for the nn Ising on a square lattice with different vertical and horizontal ferromagnetic interactions, where U^* of the anisotropic model on lattices with square shape may be expressed by U^* of the isotropic model on lattices with rectangular shapes [2,5].

In this contribution, we shall extend our previous Monte Carlo study for anisotropic nn and nnn Ising models on square lattices with only ferromagnetic interactions,

$J, J_d > 0$, to the case of competing nnn antiferromagnetic couplings, $J_d < 0$, with J remaining ferromagnetic. Thereby, spatially modulated, oscillatory spin-spin correlations may occur, adding an interesting feature to the phase diagram. The present study has been partly motivated by related recent quantitative renormalization-group calculations of $U^*(J_d/J)$ for a closely related model, showing intriguing symmetry properties [7], as will be discussed below.

The Hamiltonian of the model may be written in the form

$$\mathcal{H} = -\sum_{x,y} S_{x,y}[J(S_{x+1,y} + S_{x,y+1}) + J_d S_{x+1,y+1})] \qquad (1)$$

where $S_{x,y} = \pm 1$ is the Ising spin at site (x, y). $J > 0$ is the ferromagnetic nn coupling along the principal axes of the square lattice, while the nnn coupling, J_d acts along only one diagonal, i.e., along the [11] direction of the lattice. J_d may be ferromagnetic, $J_d > 0$, as has been studied before [5], or antiferromagnetic, $J_d < 0$.

Before turning to the critical Binder cumulant, we shall first discuss the phase diagram, exhibiting interesting features, especially for antiferromagnetic nnn couplings.

At $J_d/J > -1$, there is a ferromagnetic phase at low temperatures. The exact transition temperatures, $k_B T_c/J$, are known to be determined by [11,12]

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

The line is depicted in Fig. 1. The transition temperature T_c goes to zero on approach to $J_d/J = -1$. At that point, the ground state is highly degenerate, with the energy per site being $E_0 = -J$. The degenerate configurations include the ferromagnetic structures, uncoupled antiferromagnetic Ising chains along the [11] direction, and horizontal and vertical ferromagnetic stripes of spins with alternating sign corresponding to coupled modulated Ising chains along the [11] direction. A rather large degeneracy, due to the uncoupled antiferromagnetic chains along the [11] direction, persists at $J_d/J < -1$. Indeed, it has been argued that there is no long-
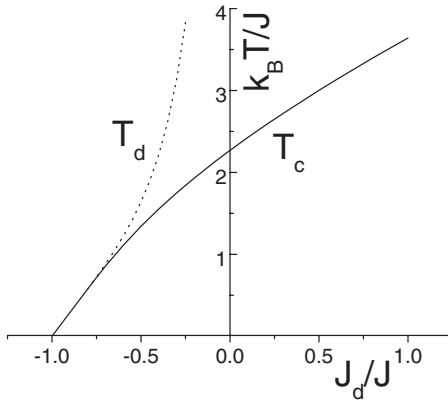
FIG. 1. Phase diagram of Hamiltonian (1), showing the exact boundary line of the ferromagnetic phase [12] (solid line) and the disorder line [14] (dashed line).

range ordering at low temperatures in that part of the phase diagram [13]. Actually, in the following we shall consider $J_d/J \geq -1$.

Due to the competing ferro- and antiferromagnetic couplings, at $J_d/J < 0$, a disorder line, $T_d(J_d/J)$, separates, above T_c, the region with only monotonically decaying spin-spin correlations from the one with oscillatory correlations [14]. The disorder line of the model, Eq. (1), has been calculated exactly as well [14,15]. It is determined by

$$\cosh(2J/k_B T_d) = \exp(-2J_d/k_B T_d). \qquad (3)$$

The line $T_d(J_d/J)$ is also shown in Fig. 1. It arises from the highly degenerate point at $(J_d/J = -1, \ T = 0)$, reflecting the spatially modulated configurations occurring there as ground states. At low temperatures, $-J_d$ being not far from J, the disorder line T_d follows closely the phase-transition line, T_c, eventually moving away from it toward higher temperatures, as J_d gets weaker, and finally approaching infinite temperature at vanishing nnn antiferromagnetic couplings, see Fig. 1. Of course, there is no disorder line for ferromagnetic nnn interactions, $J_d > 0$.

The different types of correlations at temperatures below and above the disorder line, fixing J_d/J, are illustrated in Fig. 2, displaying Monte Carlo data for spin-spin correlations along the [11] direction, $G_1(r) = \langle S_{x,y} S_{x+r,y+r} \rangle$, along the prin-
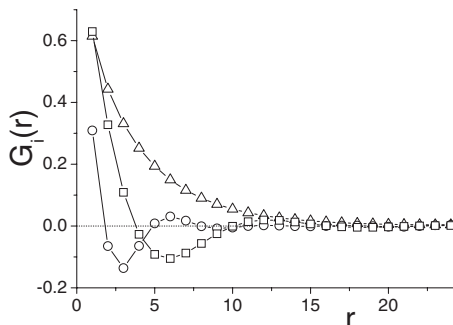

FIG. 2. Simulated spin-spin correlation function G_i, with $i = 1$ (circles), 2 (squares), 3 (triangles), as described in the text, at $J_d/J = -3/4$ and $k_B T/J = 0.9$, for lattices with 48^2 spins.
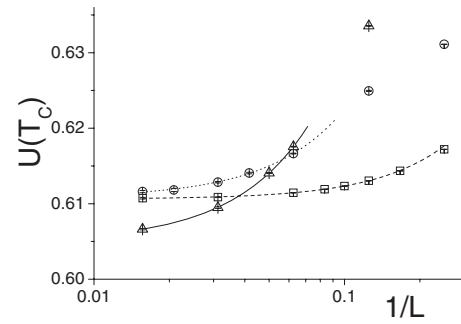

FIG. 3. Binder cumulant at T_c, $U(T_c)$, versus inverse system size $1/L$, including least square fits to the Monte Carlo data (lines) and the resulting estimates for the critical Binder cumulant, U^*. The cases $J_d/J = -0.316$ (squares) and $-5/9$ (circles) are shown.

cipal axes, $G_2(r) = \langle S_{x,y} S_{x,y+r} \rangle = \langle S_{x,y} S_{x+r,y} \rangle$, and perpendicular to the [11] direction, $G_3(r) = \langle S_{x,y} S_{x+r,y-r} \rangle$. At $T > T_d$, G_1 and G_2 decay, for sufficiently large distances r, exponentially and in an oscillatory, purely sinusoidal manner, with the wave number depending on J_d/J and temperature [14]. At and below the disorder line, the correlations along the principal axes and along the [11] direction decay monotonically. In addition, our simulations suggest that G_3 decays also above T_d monotonically (and exponentially) with distance, indicating that the competing interactions do not affect qualitatively correlations perpendicular to the [11] direction.

Note that disorder lines also exist in other Ising models with competing interactions, for instance, in the much studied axial next-nearest neighbor Ising (ANNNI) model [16,17].

Let us now turn to the Monte Carlo findings on the critical Binder cumulant U^* of the model, Eq. (1). U^* is defined by [1]

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

taking the thermodynamic limit; $\langle M^2 \rangle$ and $\langle M^4 \rangle$ denote the second and fourth moments of the order parameter, the magnetization M.

To estimate $U^*(J_d/J)$, we simulated the model for square shapes with L^2 sites or spins, employing full periodic boundary conditions, using the standard Metropolis algorithm (note that, e.g., cluster flip algorithms are usually rather inefficient in case of competing ferro- and antiferromagnetic interactions). Monte Carlo runs with, typically, 5×10^8 Monte Carlo steps per site were performed, averaging then over several, up to ten, of these runs to obtain final estimates and to determine statistical error bars. L ranged from 4 to 64. Larger system sizes would require an enormous amount of computer time to get data of the needed very high accuracy.

To extrapolate to the thermodynamic limit, $L \to \infty$, least square fits were done. The procedure is exemplified in Fig. 3. The final error bars result from the fits. One may emphasize that the finite-size behavior of the Binder cumulant is not known in the anisotropic case. As depicted in the figure, we did not include in the fits the data for small system sizes, to improve the quality of the fits. Actually, the fits are stable, within the error bars, when excluding merely data for $L=4$, independent of including data for other small sizes, $L=8$ and
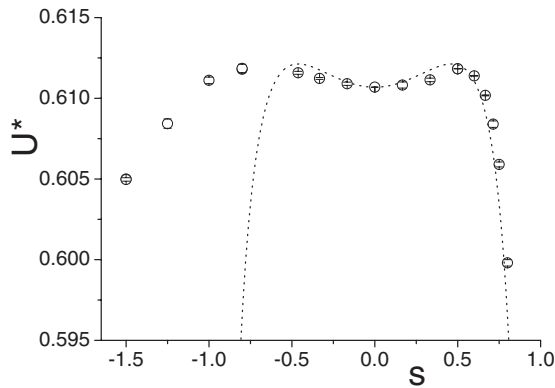
FIG. 4. Critical Binder cumulant, $U^*(s)$, versus $s=1/(1+(J/J_d))$. The result of a renormalization-group analysis [7], see text, is included as dashed line.

16. Obviously, corrections to the asymptotic behavior, are quite large for $L=4$. Note that results of such fits, for $J_d>0$, agree very well with our previous estimates using a somewhat subjective 'smooth extrapolation' to the thermodynamic limit [5] (the agreement being also true in this case, $J_d<0$). These previous estimates, in turn, agree very well with highly accurate numerical findings [2], so that we expect the present results to be reliable.

In Fig. 4, we plot U^* against $s=1/(1+(J/J_d))$, following a recent renormalization-group analysis [7], with $s<0$ for $J_d<0$ and $s>0$ for $J_d>0$. The reason for this choice will be discussed below. We also include our previous estimates [5] of U^* for $J_d\geq0$, adding one additional new point at $s=1/6$. Obviously, the critical Binder cumulant depends, both in the case of only ferromagnetic interactions and also in the case of competing antiferromagnetic couplings, continuously on s (or J_d/J). The transition at $T_c(s)$ is always in the Ising universality class, as we confirmed by monitoring, especially, the, asymptotically, logarithmic size dependence of the specific heat at T_c. Thence, U^*, for given boundary condition and shape, changes, within the Ising universality class, with the anisotropy, J_d/J.

Interestingly, $U^*(s)$ is (almost) symmetric around the isotropic situation, $s=0$, at small values of $|s|$. However, for larger values of $|s|$, there is a pronounced asymmetry. This may be understood by the fact that the model reaches one-dimensional limits, where $U^*\rightarrow0$, for $s=1$ or $J_d/J=\infty$ at positive s, and for $s=-\infty$ or $J_d/J=-1$ at negative s. The nonmonotonicity of U^* for fairly small values of $|s|$ is worth mentioning. It has been found for $s>0$ in a previous Monte Carlo study [5]. It also holds for $s<0$, in agreement with a recent suggestion [7].

The previous Monte Carlo data [5] on $U^*(s)$ at $s\geq0$ agree closely with results of a recent renormalization-group analysis by Dohm, as has been already discussed there [7]. That analysis has been done for the model, Eq. (1), augmented by a ferromagnetic interlayer nn coupling J_l on a cubic lattice, with $J_l=J+J_d$. The interlayer coupling has been chosen to preserve essential features of the anisotropy matrix of the model on the square lattice [7]. Indeed, this choice allows to describe well, in the framework of RNG theory, the simulational data on $U^*(s)-U^*(0)$ for the two-dimensional model

with ferromagnetic nnn interactions, $s\geq0$ [7]. Certainly, the critical Binder cumulant in the isotropic case, $s=0$, is different for square and cubic lattices, thereby motivating to look at the difference, $U^*(s)-U^*(0)$, of the critical cumulants [7]. The RNG study yields a perfect symmetry of $U^*(s)-U^*(0)$ around $s=0$, and an interesting nonmonotonic behavior in s.

To compare the present Monte Carlo data to the RNG findings, we prefer to plot, see Fig. 4, the RNG results in the form $U^*_{RNG}(s)U^*(s=0)/U^*_{RNG}(s=0)$, with the critical Binder cumulant of the two-dimensional isotropic Ising model, $U^*(0)$, being [2] 0.610 69…. Of course, the perfect symmetry and nonmonotonicity found in the RNG study is preserved by this choice, as displayed in Fig. 4. As follows from that figure, the symmetry, suggested by the RNG analysis, is approximated closely in the two-dimensional Ising model with antiferromagnetic nnn interactions only for small values of $|s|$. But there are pronounced deviations at stronger antiferromagnetic nnn couplings.

In fact, for competing antiferromagnetic couplings the phase diagrams of the models in two and three dimensions, and thence the corresponding critical Binder cumulants, may be expected to differ substantially. In particular, in two dimensions there is, as discussed above, a phase transition of Ising type down to $J_d/J=-1$, with spatially modulated correlations occurring only in the disordered phase above the disorder line. In contrast, in three dimensions, the transition line of Ising type between the ferro- and paramagnetic phases may be expected to extend only up to a Lifshitz point [18–20] at $(J_d/J)_{LP}$ (>-1) or s_{LP}, at which the ferromagnetic, the spatially long-range ordered modulated, and the disordered phases meet, similar to the well-known situation in the ANNNI model [16].

Indeed, a standard mean-field calculation shows that the Lifshitz point occurs, for $J_l=J+J_d$, at $J_d/J=-1/2$, corresponding to $s_{LP}=-1$. In the modulated phase close to the transition to the paramagnetic phase, at $J_d/J<(J_d/J)_{LP}=-1/2$, the magnetization along the x- and y-axes change in a sinusoidal manner. The modulated, long-range ordered phase seems to arise from the highly degenerate ground states at $J_d/J=-1$, with the transition line between the ferromagnetic and the modulated phases, at $-1<s<-1/2$, being of first order. The vicinity of that degenerate point may be explored by systematic low-temperature series expansions [21], being however, well beyond the scope of the present study. Because there are modulated magnetization pattern along two principal axes of the cubic lattice, the x- and the y-axes, we are dealing here with a 'biaxial Lifshitz point' ($m=2$ in the standard notation [18]).

The existence of a Lifshitz point at $s=-1$, has been argued to allow for the complete symmetry of $U^*(s)$ around $s=$ in the RNG analysis [7]. Going beyond mean-field theory, the location of the biaxial Lifshitz point may shift somewhat. To determine accurately the position of the Lifshitz point, high-temperature series may be very helpful, as has been found, for instance, in the case of the ANNNI and related models [22,23,25]. Obviously, it is an open problem, in which way the possible shift in the Lifshitz point may affect the proposed perfect symmetry of $U^*(s)$. Note that the lower critical dimension of a biaxial Lifshitz point is three [18,24], excluding its existence at nonzero temperatures for the square lattice, but not for the cubic lattice.

Certainly, it is desirable to determine $U^*(s)$ of the three-dimensional model in simulations. However, neither $T_c(s)$ nor the location of the Lifshitz point are known. To get then data on U^* of the required high accuracy, a huge amount of computer time would be needed, being hardly feasible at present.

In summary, the critical Binder cumulant U^* of an anisotropic two-dimensional Ising model with competing ferro- and antiferromagnetic interactions has been determined. Because the transition is known exactly, one arrives at accurate estimates based on extensive Monte Carlo simulations. Employing full periodic boundary conditions and considering square shapes, U^* is found to vary continuously with changing anisotropy s. A remarkably close agreement of our findings on $U^*(s)$, at positive values of s and, in case of compet-ing interactiosn, for small negative values of s with the results of a recent renormalization-group analysis is observed. Differences at stronger competing anisotropy are explained by the absence of a biaxial Lifshitz point at nonzero temperatures in two dimensions.

[1] K. Binder, Z. Phys. B: Condens. Matter **43**, 119 (1981); Phys. Rev. Lett. **47**, 693 (1981).

[2] G. Kamieniarz and H. W. J. Blöte, J. Phys. A **26**, 201 (1993).

[3] W. Janke, M. Katoot, and R. Villanova, Phys. Rev. B **49**, 9644 (1994).

[4] X. S. Chen and V. Dohm, Phys. Rev. E **70**, 056136 (2004).

[5] W. Selke and L. N. Shchur, J. Phys. A **38**, L739 (2005).

[6] W. Selke, Eur. Phys. J. B **51**, 223 (2006); J. Stat. Mech.: Theory Exp. **2007**, P04008.

[7] V. Dohm, Phys. Rev. E **77**, 061128 (2008).

[8] D. Nicolaides and A. D. Bruce, J. Phys. A **21**, 233 (1988).

[9] M. Schulte and C. Drope, Int. J. Mod. Phys. C **16**, 1217 (2005).

[10] M. A. Sumour, D. Stauffer, M. M. Shabat, and A. H. El-Astal, Physica A **368**, 96 (2006).

[11] A. N. Berker and K. Hui, Phys. Rev. B **48**, 12393 (1993).

[12] R. M. F. Houtappel, Physica **16**, 425 (1950).

[13] K. Y. Lin and F. Y. Wu, Z. Phys. B **33**, 181 (1979).

[14] J. Stephenson, Phys. Rev. B **1**, 4405 (1970); J. Math. Phys. **11**, 413 (1970).

[15] I. Peschel and V. J. Emery, Z. Phys. B: Condens. Matter **43**, 241 (1981).

[16] W. Selke, Phys. Rep. **170**, 213 (1988).

[17] M. Beccaria, M. Campostrini, and A. Feo, Phys. Rev. B **73**, 052402 (2006).

[18] R. M. Hornreich, M. Luban, and S. Shtrikman, Phys. Rev. Lett. **35**, 1678 (1975).

[19] W. Selke in *Phase Transitions and Critical Phenomena*, edited by C. Domb and J. L. Lebowitz (Academic, New York, 1992), Vol. 15, p. 1.

[20] H. W. Diehl, Pramana-J. Phys. **64**, 803 (2005).

[21] M. E. Fisher and W. Selke, Phys. Rev. Lett. **44**, 1502 (1980).

[22] S. Redner and H. E. Stanley, Phys. Rev. B **16**, 4901 (1977).

[23] J. Oitmaa, J. Phys. A **18**, 365 (1985).

[24] H. W. Diehl and M. Shpot, Phys. Rev. B **62**, 12338 (2000).

[25] P. Butera and M. Pernici, Phys. Rev. B **78**, 054405 (2008).