Revisiting the field-driven edge transition of the tricritical two-dimensional Blume-Capel model

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We reconsider the tricritical Blume-Capel model on the square lattice with a magnetic field acting on the open boundaries in one direction. Periodic boundary conditions are applied in the other direction. We apply three types of Monte Carlo algorithms, local Metropolis updates, and cluster algorithms of the Wolff and geometric type, adapted to the symmetry properties of the model. Statistical analyses of the bulk magnetization, the bulk Binder ratio, the edge magnetization, and the connected product of the edge and bulk magnetizations lead to new results confirming the presence of a singular edge transition at $H_{sc} \approx 0.68$, as we reported earlier [Phys. Rev. E **71**, 026109 (2005)]. We provide a plausible answer concerning a discrepancy between the behavior of the edge Binder ratio reported in that work and our new results.

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I. INTRODUCTION

The Blume-Capel model [1,2] was introduced as a spin-1 Ising model system, displaying a tricritical point that separates the critical and the first-order parts of a line of phase transitions. In addition to the values ± 1, the spins can also be vacant, i.e., take the value 0. Nearest-neighbor spins interact as $-Ks_is_j$, and we consider the case of ferromagnetic interactions, i.e., $K > 0$. The model includes a per-site reduced potential Ds_k^2. For $D = -\infty$, the spin-zero state is excluded and the model reduces to spin-1/2 Ising model. With increasing D, the density of the spins in the spin-zero state increases, so that also K has to increase in order to reach the phase transition between the disordered state and the long-range ordered state. The critical point remains Ising-like until K and D reach their tricritical values. The tricritical point has previously [3] been determined at $K_{tr} = 1.6431759(1)$, $D_{tr} = 3.2301797(2)$.

Some time ago we investigated the particular case of the tricritical model on the square lattice with periodic boundary conditions in one direction, and open edges in the other direction [4]. Conformal boundary theory predicts the existence of new critical phases in the presence of a boundary field and edge enhancements [5,6]. Here we specialize to a slightly less general case without edge enhancements, described by the reduced Hamiltonian

$$\mathcal{H}/k_BT = \sum_{x=1}^{L}\sum_{y=1}^{L}\left[-K(s_{x,y}s_{x+1,y} + s_{x,y}s_{x,y+1}) + Ds_{x,y}^2\right] - H_s\sum_{x=1}^{L}(s_{x,1} + s_{x,L}), \qquad (1)$$

where x and y are Cartesian coordinates of the spins which take the values $s_{x,y} = 0, \pm 1$. By definition, $s_{L+1,y} \equiv s_{1,y}$ and $s_{x,L+1} \equiv 0$. Thus Eq. (1) describes an $L \times L$ system on a cylinder with open ends.

In Ref. [4] we defined, on the basis of the spins $s_{x,1}$ and $s_{x,L}$, the edge magnetization density m_s and the associated Binder [7] ratio

$$Q_s \equiv \langle (m_s - \langle m_s \rangle)^2 \rangle^2 / \langle (m_s - \langle m_s \rangle)^4 \rangle. \qquad (2)$$

Using Monte Carlo data taken at the estimated tricritical point, we reported [4] that finite-size scaling of Q_s showed the existence of a critical edge transition at $H_{sc} = 0.6772(10)$. This edge transition can be seen as a "surface" transition of the two-dimensional system.

However, as pointed out by Francesco Parisen Toldin [8] to one of us, the validity of this result is not clear. The analysis of the Binder ratio uses the assumption that the singular contribution of $\langle (m_s - \langle m_s \rangle)^2 \rangle \propto L^{2y_s - 1}$ dominates over the analytic background, of which the finite-size dependence behaves as L^0. Since the value of the critical exponent $2y_s$ describing the surface transition is known [5,6] as $y_s = 2/5$, the assumption is only valid if the amplitude of the analytic background is zero or negligible. We are thus left with the task to find out if our result for the edge transition is still valid, and if so, how we could possibly have arrived at that result. The present work is intended to answer these questions.

While a reanalysis of the old data would logically seem to be the first step, it is unfortunately not possible because of the discontinuation of the Computational Physics Section by the Faculty of Applied Physics of the Delft University of Technology, which took place around the time of the publication of Ref. [4]. All simulation data and backups were lost. We therefore performed new calculations and analyses, described in Sec. II, with a conclusion following in Sec. III.

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II. NUMERICAL RESULTS AND ANALYSIS

A. Location of the tricritical point

The tricritical point was previously [4] determined at $K_{\rm tr} = 1.6431759(1)$, $D_{\rm tr} = 3.2301797(2)$, on the basis of transfer-matrix calculations for finite system sizes up to $L = 16$. This result may be compared to a more recent Monte Carlo result by Kwak *et al.* [9] which translates into $K_{\rm tr} = 1.6447(3)$, $D_{\rm tr} = 3.2335(7)$. These results are consistent if somewhat wider error margins are employed. We extended the old transfer-matrix calculations up to $L = 18$. Subsequent fit procedures did not lead to a revision of the result of Ref. [4], while the confidence levels of the quoted uncertainty margins improved. As a consistency check we calculated the free-energy densities $f(K_{\rm tr}, D_{\rm tr}, L)$ of $L \times \infty$ systems in cylindrical geometries with $L = 2$ to 18 at $K_{\rm tr} = 1.6431759$, $D_{\rm tr} = 3.2301797$, and applied fits according to

$$f(K_{\rm tr}, D_{\rm tr}, L) = f_{\rm tr} + \frac{\pi c_{\rm a}}{6L^2} + p_1 L^{y_1} + \cdots , \qquad (3)$$

with correction terms having exponents of L equal to even negative integers. This enables the estimation of the conformal anomaly $c_{\rm a}$ [10,11], for which we obtain $c_{\rm a} = 0.700000(1)$, in a good agreement with the exact value 7/10 [12] for the tricritical Ising model.

B. Monte Carlo algorithms

The existing results for the surface transition [4] were obtained by means of a Metropolis-type algorithm. The efficiency of these simulations with local updates is limited by critical slowing down. We attempted to improve the efficiency by means of two types of cluster updates: first, a Wolff-type cluster algorithm, acting only on the ± 1 spin states, and, second, a geometric cluster algorithm that can also move the vacancies.

The Wolff algorithm for the Ising model essentially uses the $+/-$ symmetry of the model, which is broken by the surface magnetic field $H_{\rm s}$. We therefore replace the interaction of the edge spins with the magnetic field $H_{\rm s}$ by a coupling of those spins with a "ghost spin" [13]. The $+/-$ symmetry is restored in the Hamiltonian of the resulting system, but the nature of the Wolff algorithm is such that it can also change the sign of the ghost spin and thus, in effect, the sign of the field. In order to obtain data that apply to positive $H_{\rm s}$, we may simply multiply the magnetizations by the value of the ghost spin at sampling time.

Due to the introduction of the couplings with the ghost spin for $H_{\rm s} > 0$, the cluster formation process moves away from the percolation threshold, and the algorithm loses part of its efficiency, depending on the magnitude of $H_{\rm s}$. In comparison with the Metropolis algorithm, it does still significantly decrease the autocorrelation times of the larger systems.

Due to the absence of translational symmetry in the y direction, the set of useful geometric symmetry operations for the geometric cluster algorithm [14] is limited. We used lattice inversions centered at $(x, y) = (k/2, L/2 + 1/2)$, where $k = 1, 2, 3, \ldots, 2L$. The algorithm can, e.g., swap groups of spins and/or vacancies along the x direction and also between the upper ($y > L/2 + 1/2$) and lower ($y < L/2 + 1/2$) halves of the system. It appears that this algorithm leads to another small increase of the speed of computation, especially for larger system sizes.

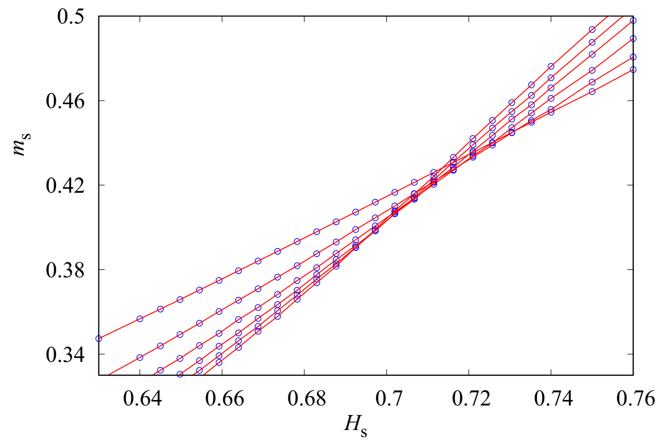

FIG. 1. Edge magnetization density $m_{\rm s}$ versus the surface field $H_{\rm s}$. Data are shown for system sizes $L = 4$, 8, 16, 32, 60, and 120. Larger systems correspond with steeper curves. The intersections indicate the presence of an edge transition.

C. Monte Carlo results

All simulations took place at the tricritical point, at several values of the surface field $H_{\rm s}$, for 22 system sizes ranging from $L = 4$ to 120. For each system size, roughly 10^9 samples were taken, separated by about $L/2$ Metropolis sweeps, $L/5$ Wolff cluster steps, and $L/3$ geometric cluster steps. The sampled quantities included the edge magnetization density $m_{\rm s}$, the bulk magnetization density $m_{\rm b}$, and moments of their distributions and cross products. We thus obtained the surface Binder ratio defined in Eq. (2) and the bulk ratio $Q_{\rm b} \equiv \langle m_{\rm b}^2\rangle^2/\langle m_{\rm b}^4\rangle$. Unlike $m_{\rm s}$, $m_{\rm b}$ vanishes in the thermodynamic limit, and therefore no subtraction of the average bulk magnetization was involved.

The results for the surface magnetization are shown in Fig. 1 for several values of the surface field $H_{\rm s}$ in the vicinity of the critical point reported in Ref. [4]. At a surface critical point, $m_{\rm s}$ should approach a nonzero constant for $L \to \infty$, and the relevance of the surface field should lead to intersections of the $m_{\rm s}$ vs $H_{\rm s}$ curves. The results in Fig. 1 thus confirm the presence of a surface transition near the location given in Ref. [4].

The expected scaling behavior of $Q_{\rm s}$ is found using finite-size scaling of the free-energy function [15], taking into account the analytic part of the free energy, and expressing the moments of $m_{\rm s} - \langle m_{\rm s}\rangle$ in derivatives to the edge field $H_{\rm s}$. The result is as follows:

$$Q_{\rm s}(L) = \frac{aL^{4y_{\rm s}} + bL^{2y_{\rm s}+1} + cL^2}{a'L^{4y_{\rm s}} + b'L^{2y_{\rm s}+1} + c'L^2}. \qquad (4)$$

The amplitudes a, a', b, b' depend on the singular part of the free energy, whereas c, c' are due to the analytic part. Thus $a = a_0 + a_1(H_{\rm s} - H_{\rm sc})L^{y_{\rm s}} + \ldots$, and similarly for a', b, b'. The latter dependence on $H_{\rm s}$ would, if $2y_{\rm s} > 1$, lead to intersections of the $Q_{\rm s}$ versus $H_{\rm s}$ curves, converging to a/a' at

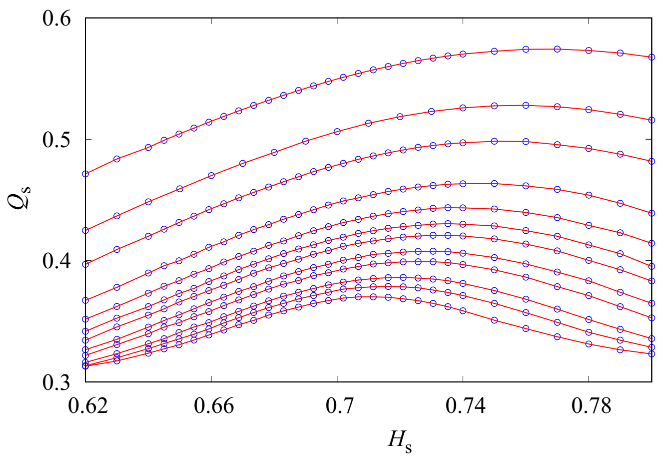

FIG. 2. Binder ratio Q_s defined on the moments of the distribution of the edge magnetization m_s versus the surface field H_s. Data are shown for system sizes $L = 4$ (above), 6, 8, 12, 16, 20, 24, 32, 40, 60, 80, and 120 (below).

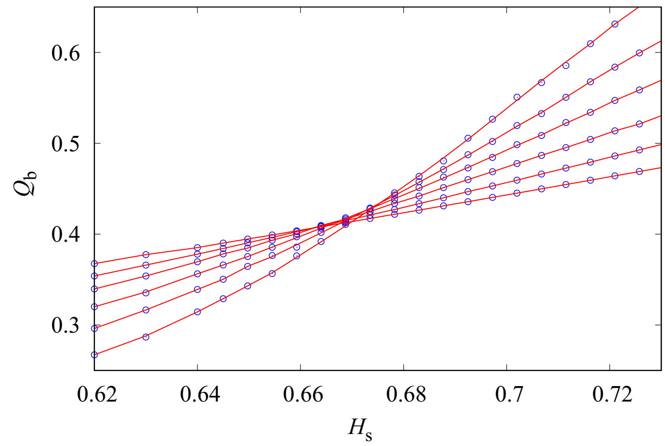

FIG. 3. Binder ratio Q_b defined on the moments of the distribution of the bulk magnetization density m_b, versus the surface field H_s. Data are shown for system sizes $L = 4,\ 8,\ 16,\ 32,\ 60,$ and 120. Steeper curves apply to larger systems. One-sigma statistical error margins are at most equal to the symbol size.

the critical point. If, however, $2y_s < 1$, then the terms with amplitudes c and c' dominate for sufficiently large L, so that Q_s converges to an analytic function c/c' of H_s that is independent of L.

Results for the surface ratio Q_s are shown in Fig. 2. There are no intersections in the range of interest, and the results clearly correspond with the case $2y_s < 1$, in agreement with the existing result $y_s = 2/5$. The data in this figure are therefore not consistent with the behavior of Q_s as reported in Ref. [4].

Next, we analyzed the bulk Binder ratio Q_b defined as $Q_b \equiv \langle m_b^2\rangle^2/\langle m_b^4\rangle$. After expression of the bulk magnetization moments in derivatives of the free energy, and expansion of the finite-size scaling equation at the surface transition point, one finds the leading terms in the scaling behavior of Q_b as

$$Q_b(H_s, L) = Q_b + \sum_{k=1,2\ldots} g_k(H_s - H_{sc})^k L^{ky_s} + b_1 L^{2-2y_b} + b_2 L^{y_2} + b_3 L^{y_3} + \cdots . \quad (5)$$

Since the leading tricritical bulk magnetic exponent equals $y_b = 77/40$ [16], the analytic contribution with amplitude b_1 is subdominant. Thus, the Q_b data near the surface critical point of the tricritical model should display intersections converging to the surface critical point. Monte Carlo results for Q_b, shown in Fig. 3, confirm this expectation. Least-squares fits were applied according to Eq. (5), with correction exponents $y_1 = 2 - 2y_b = -1.85$, $y_2 = -1$, and $y_3 = -2$. These fits yielded $H_{sc} = 0.6770(5)$ and $Q_b = 0.442(2)$. One-sigma error margins are quoted between parentheses. Note that the estimated edge critical point lies close to that given in Ref. [4] and that the new result for the bulk ratio Q_b is close to the old result for the surface ratio which was given as $Q_s = 0.4419(10)$.

We have also applied least-squares fits to analyze the surface magnetization m_s as a function of H_s. Finite-size scaling predicts its behavior in the vicinity of the surface transition as

$$m_s(H_s, L) = \sum_{k=0,1,\ldots} m_k(H_s - H_{sc})^k + L^{y_s-1}[a_0 + a_1(H_s - H_{sc})L^{y_s} + a_2(H_s - H_{sc})^2 L^{2y_s} + \ldots + b_1 L^{y_1} + b_2 L^{y_2}], \quad (6)$$

where the terms with m_k describe the analytic contribution, and we have used correction exponents $y_1 = -1$, which is the irrelevant exponent of the tricritical Ising model [16], and $y_2 = -2$. This fit yielded $H_{sc} = 0.682(2)$.

Next we consider the connected correlation of the surface and bulk magnetization, i.e., $\langle\langle m_s m_b\rangle\rangle = \langle m_s m_b\rangle - \langle m_s\rangle\langle m_b\rangle$. After multiplication by the system size L, the analytic contribution in the result is independent of L, and one expects the following finite-size scaling behavior near the surface transition:

$$c_{sb} \equiv L\langle\langle m_s m_b\rangle\rangle = \sum_{k=0,1,\ldots} p_k(H_s - H_{sc})^k + L^{y_s+y_b-2}[a_0 + a_1(H_s - H_{sc})L^{y_s} + a_2(H_s - H_{sc})^2 L^{2y_s} + \ldots + b_1 L^{y_1} + b_2 L^{y_2}]. \quad (7)$$

with the bulk tricritical magnetic exponent [16] fixed at $y_b = 77/40$ and the surface magnetic exponent at $y_s = 2/5$ [5,6]. Thus, the quantity c_{sb} should be divergent at the surface transition. This agrees well with the numerical finite-size data shown in Fig. 4. Least-squares fits, with y_s left free, to the data for $L \geqslant 5$ lead to the results $H_{sc} = 0.6801(4)$ and $y_s = 0.400(5)$.

Finally, we analyzed the bulk magnetization as a function of H_s. One expects

$$m_b(H_s, L) = L^{y_b-2}[a_0 + a_1(H_s - H_{sc})L^{y_s} + a_2(H_s - H_{sc})^2 L^{2y_s} + \ldots + b_1 L^{y_1} + b_2 L^{y_2}]. \quad (8)$$

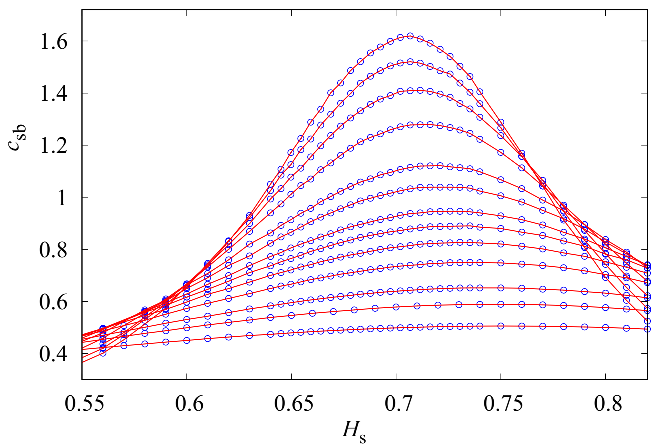

FIG. 4. Scaled connected correlation function c_{sb} versus edge field for system sizes $L = 4$, 6, 8, 12, 16, 20, 24, 32, 40, 60, 80, 100, and 120. Larger system sizes display higher maxima. These data illustrate the divergent nature of c_{sb}.

The result for H_{sc} is listed in Table I, together with the critical fields as obtained from other quantities.

III. CONCLUSION

We confirm the existence of the field-induced edge transition of the tricritical Blume-Capel model. The newly found results for the bulk Binder ratio Q_b are close to those presented in Ref. [4] for the surface Binder ratio Q_s, while the new results for the surface Binder ratio Q_s disagree with the behavior reported in Ref. [4]. We therefore suspect that the results obtained from the bulk Binder ratio have been mislabeled as surface results in Ref. [4]. The new result for the surface critical field H_{sc} obtained from Q_b is practically the same as the old result as quoted from Q_s. However, the differences with the other results for H_{sc} are rather large in comparison with the statistical errors quoted, perhaps due to the presence of an unresolved correction to scaling. Whereas the presence of another correction with exponent $y_4 = -0.6$ would improve the consistency of the result obtained from Q_b with the other results in Table I, our data are insufficient to clearly resolve such a correction. Taking into account that the one-sigma errors quoted above are too small, and the possible presence of another correction as mentioned, we propose a more reasonable final estimate $H_{sc} = 0.679(2)$.

TABLE I. Summary of the results for the location of the surface transition H_{sc} as obtained from the data for the quantities listed in the first column. One-sigma errors are quoted between parentheses.

Quantity	H_{sc}	Source
Q_s	0.6772 (10)	Ref. [4]
Q_s	No result	Present work
Q_b	0.6770 (5)	Present work
$\langle m_s \rangle$	0.682 (2)	Present work
$\langle\langle m_s m_b \rangle\rangle$	0.6801 (4)	Present work
$\langle m_b \rangle$	0.6805 (11)	Present work

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