Ising cubes with enhanced surface couplings

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Using Monte Carlo techniques, Ising cubes with ferromagnetic nearest-neighbor interactions and enhanced couplings between surface spins are studied. In particular, at the surface transition, the corner magnetization shows nonuniversal, coupling-dependent critical behavior in the thermodynamic limit. Results on the critical exponent of the corner magnetization are compared to previous findings on two-dimensional Ising models with three intersecting defect lines.

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I. INTRODUCTION

In the thermodynamic limit, critical phenomena may occur not only in the bulk of a system, but also at its surfaces, edges, and corners. To be specific, let us consider Ising magnets with short-range interactions. Then, there are two typical scenarios: (a) bulk m_b, surface m_1, edge m_2, and corner m_3 magnetizations may order at the same temperature (''ordinary transition''), but with different power laws and (b) surface, edge, and corner magnetizations may order simultaneously first (''surface transition'') due to enhanced, strong surface couplings, followed by ordering of the bulk magnetization at the lower bulk transition temperature (''extraordinary transition''). Surface singularities at ordinary and surface transitions have been studied extensively, theoretically [1,2] as well as experimentally [3]. Most of the rather few studies on edge critical behavior dealt with the ordinary transition [4–7]. Only very recently, edge criticality both at the surface transition [8] and at the normal transition [9] has been investigated.

Similarly, corner criticality in three-dimensional Ising systems has been analyzed, to our knowledge, only at the ordinary transition, applying mean-field theory [10] and Monte Carlo simulations [7]. However, that case deserves to be studied at the surface transition as well for various reasons. For magnetic properties of nanostructured materials, corners are expected to play an important role [11,12]. In addition, magnetism may be enhanced at surfaces, especially at step edges and corners of, e.g., metals by increased local magnetic moments and/or couplings [13,14]. More detailed future investigations on this aspect, using, for instance, density functional methods, are encouraged. Last, but not least, the problem is of genuine theoretical interest. At the surface transition, the critical fluctuations are essentially two dimensional. Edges are local perturbations acting then similar to defect lines in two-dimensional Ising models leading to interesting nonuniversal critical phenomena [10,8]. Accordingly, corners, say, of an Ising cube may be interpreted as intersection points of three defect lines. At such points, one also expects intriguing nonuniversal behavior of local quantities, such as the corner magnetization, following exact analytical work on two-dimensional Ising systems with intersecting defect lines [15].

II. MODEL, METHOD AND RESULTS

We study nearest-neighbor Ising models on simple cubic lattices with $L \times M \times N$ spins (usually we shall consider Ising cubes, i.e., $L=M=N$) and ferromagnetic interactions. The Hamiltonian may be written in the form

$$\mathcal{H} = -\sum_{\text{bulk}} J_b S_{xyz} S_{x'y'z'} - \sum_{\text{surface}} J_s S_{xyz} S_{x'y'z'} - \sum_{\text{edge-surface}} J_{es} S_{xyz} S_{x'y'z'} - \sum_{\text{edge}} J_e S_{xyz} S_{x'y'z'} \qquad (1)$$

with spins $S_{xyz} = \pm 1$ at sites (xyz); the sums run over bonds between neighboring spins with coupling constants to be specified below; $x(y,z)$ going from 1 to $L(M,N)$ (setting the lattice constant equal to one). Free boundary conditions hold for the spins in the surface planes. The pairs of neighboring spins in the Hamiltonian (1) are located either on edge sites with the edge coupling J_e, on edge and surface sites coupled by J_{es}, on surface sites with the interaction J_s, or on sites with at least one of the spins in the interior of the system interacting with the bulk coupling J_b. We refrained from assigning another coupling strength to pairs of spins on corner and edge sites, which is taken to be equal to J_e.

To study the behavior at the surface transition T_s, we chose $J_s = 2J_b$, where $k_B T_s / J_b \approx 4.975$ [8], while the bulk transition T_c occurs at $k_B T_c / J_b \approx 4.5115$ [16,17]. The effect of the edge couplings was studied by considering the three cases (i) of equal surface couplings, i.e., $J_e = J_{es} = J_s$, (ii) of reduced edge couplings, especially $J_{es} = J_s$, $J_e = J_b$, and (iii) of reduced edge-surface couplings, especially $J_e = J_s$, $J_{es} = J_b$.

The size of the Ising cubes wih L^3 spins ranged from $L=5$ to $L=80$. In the Monte Carlo simulations, we used the efficient single-cluster-flip algorithm. Thermal averages were obtained from an ensemble of at least 10^2 realizations, using different random numbers. In each realization, several 10^4 clusters were taken into account, after equilibration.

The quantity of main interest is the corner magnetization, or more general, the local magnetization $m_l(x,y,z)$ at site (xyz). $m_l(x,y,z)$ may be defined by the correlation function

$$m_l(x,y,z) = \sqrt{\langle S_{xyz} S_{x'y'z'} \rangle}, \qquad (2)$$

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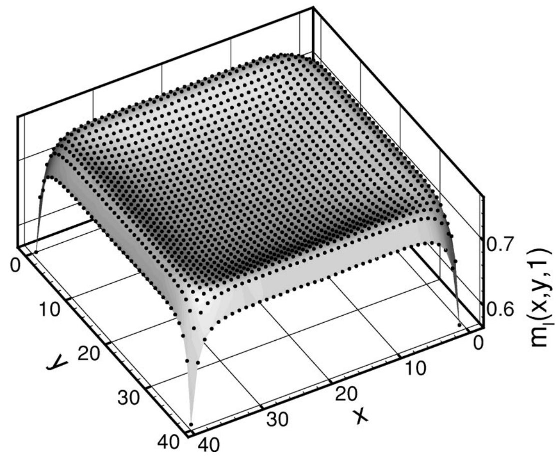

FIG. 1. Simulated profile of the local magnetization at the surface, $m_l(x,y,1)$, for an Ising model of 40^3 spins with equal surface couplings, $J_e = J_{es} = J_s = 2J_b$, at $k_BT/J_b = 4.9$.

where (xyz) and $(x'y'z')$ are topologically equivalent sites with maximal separation distance; brackets denote the thermal average. In the thermodynamic limit, $L \to \infty$, one recovers the standard definition of the local magnetization $m(x,y,z) = \langle S_{xyz} \rangle$. $m_l(x,y,z)$ approaches closely $m(x,y,z)$ provided the separation distance between the two equivalent spins is large compared to the correlation length. Certainly, finite-size effects are most severe near criticality, as usual. The deviation of m_l from m may be monitored by varying the size of the cubes L and by considering the correlation function between spins on equivalent sites with different separation distances (for instance, two corner spins may be connected either by an edge, by a surface diagonal, or by the bulk diagonal).

In Fig. 1 the intriguing profile of the local magnetization at the surface, $m_l(x,y,1)$, of a 40^3 Ising cube with equal surface couplings, case (i), is depicted, at $k_BT/J_b = 4.9$, i.e., $T \approx 0.985T_s$. The nonmonotonic behavior along paths from the edges or corners towards the center of the surface reflects the influence of bulk spins, as has been discussed before [8]. Crossover to monotonicity of the profile, with the largest magnetization at the corners, is expected to occur even closer to T_s in sufficiently large systems. At lower temperatures, roughly $T < T_c$, the profile is monotonic as well, with the smallest magnetization at the corners due to the different coordination numbers at corners, edges, and surfaces, see Fig. 2.

Near the surface transition, T_s, the corner magnetization, say, $m_3 = m_l(1,1,1)$, is expected to vanish, in the thermodynamic limit, as $m_3 \propto t^{\beta_3}$, where t is the reduced temperature $t = |T - T_s|/T_s$. To estimate β_3, we consider the effective exponent [7,8,18] $\beta_{\rm eff}(t) = d \ln m_3 / d \ln t$. When analyzing the Monte Carlo data, the derivative is replaced by a difference at discrete temperatures. As $t \to 0$, $\beta_{\rm eff}$ approaches β_3, provided finite-size effects can be neglected.

The temperature dependence of the effective exponent $\beta_{\rm eff}$ for the three different sets of couplings, (i), (ii), and (iii), is shown in Fig. 3, displaying only data which were checked to be unaffected by finite–size effects. Error bars stem from the ensemble averaging performed to determine m_3. The resulting estimates for the asymptotic critical exponent β_3 are (i) 0.06 ± 0.01 at $J_e = J_{es} = J_s = 2J_b$, (ii) 0.14 ± 0.015 at $J_{es} = J_s = 2J_b$ and $J_e = J_b$, and (iii) 0.26 ± 0.02 at $J_e = J_s = 2J_b$ and $J_{es} = J_b$. In addition, we estimated β_3 at the ordinary transition, $J_e = J_{es} = J_s = J_b$ to be $\beta_3 = 1.77 \pm 0.05$, confirming and refining our previous estimate based on computing the corner magnetization from metastable states [7]. Error bars are inferred from ''reasonable'' extrapolations of the effective exponent, see Fig. 3.

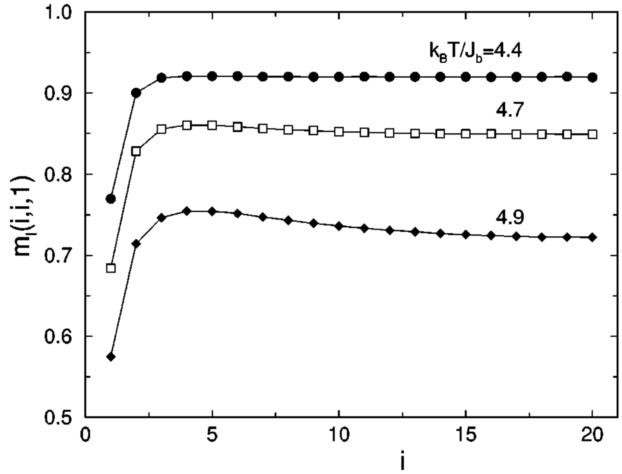

FIG. 2. Magnetization profile $m_l(i,i,1)$ along the diagonal of the surface for an Ising model of 40^3 spins with equal surface couplings $J_e = J_{es} = J_s = 2J_b$, at $k_BT/J_b = 4.9, 4.7$, and 4.4 (from bottom to top). Error bars are smaller than the size of the symbols.

To explain the Monte Carlo findings on β_3, note that the critical fluctuations at the surface transition are essentially two dimensional and that corners are intersection points of the edges. Now, as had been shown before [8], at the surface transition edges act as ladder- or chain-type defect lines [19–21,10]. The critical exponent β_2 of the edge magnetization is nonuniversal [being nontrivial even in case (i) of equal surface couplings, due to the coupling to bulk spins], varying with the edge J_e and edge-surface J_{es} couplings [8]. To a given set of interactions J_e and J_{es}, one may assign roughly an effective defect coupling of ladder or chain type $J_d^{\rm eff}$, yielding the same critical exponent for the defect mag-

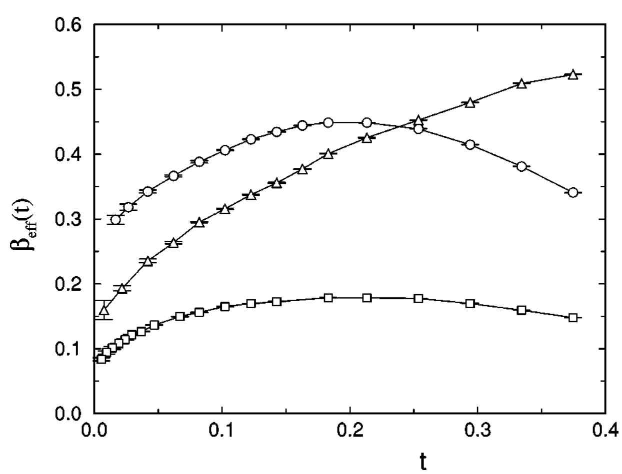

FIG. 3. Effective exponent $\beta_{\rm eff}$ versus reduced temperature t for (i) $J_e = J_{es} = J_s$ (squares), (ii) $J_{es} = J_s$, $J_e = J_b$ (triangles), and (iii) $J_e = J_s$, $J_{es} = J_b$ (circles). Ising cubes with up to 80^3 spins were simulated, circumventing finite-size effects.

netization in the two-dimensional Ising model β_l and for the edge magnetization at the surface transition of the three-dimensional Ising model β_2. Specifically, for a ladder-type defect, the critical exponent of the magnetization in the ladder rows β_l is given by [20,21]

$$\beta_l = 2\,\arctan^2(\kappa_l^{-1})/\pi^2 \tag{3}$$

with $\kappa_l = \tanh[J_l/(k_B T_{2d})]/\tanh[J/(k_B T_{2d})]$, where T_{2d} is the transition temperature. Comparing β_2 and β_l, one may interpret the defect coupling J_l of the two-dimensional model as the desired effective coupling J_d^{eff} (J is the coupling constant away from the defect line, corresponding to J_s in the three-dimensional systems).

Following this analogy, the critical exponent of the corner magnetization, β_3, can be related to that of the magnetization at the intersection of three defect lines in the two-dimensional Ising model β_i, with effective defect couplings J_d^{eff}. Indeed, in the two-dimensional Ising model, the value of β_i has been calculated exactly for three intersecting ladder defects by Henkel *et al.* [15], showing a nonuniversal behavior, with β_i depending on the strength of the defect couplings J_l. If those couplings are weaker than in the rest of the system, then β_i will increase with decreasing $J_l (<J)$, $\beta_i > 1/8$, 1/8 being the well-known Onsager value in the isotropic two-dimensional Ising model. In turn, if the defect couplings get stronger, then β_i will get smaller. The concrete expression for β_i is quite lengthy [15] and will not be reproduced here, but it can be evaluated in a straightforward way.

The effective ladder-type defect couplings J_d^{eff} in the three cases we considered are (i) $J_d^{\mathrm{eff}} \approx 1.22 J_s$ corresponding to $\beta_2 \approx 0.095$ [8] in the case of equal surface couplings, i.e., an effective enhancement of the couplings at the edges due to the influence of bulk spins, (ii) $J_d^{\mathrm{eff}} \approx 0.99 J_s$ corresponding to $\beta_2 \approx 0.127$ [8] for weakened edge couplings, i.e., the enhancement is now approximately compensated by the weakening of J_e, and (iii) $J_d^{\mathrm{eff}} \approx 0.74 J_s$ corresponding to $\beta_2 \approx 0.176$ [8] for weakened edge-surface couplings, overcompensating the enhancement by the reduction in J_{es} (note that the values of β_2 differ significantly from those of β_3). Using these estimates of J_d^{eff}, one obtains from the exact expression [15] for the two-dimensional Ising model with three intersecting ladder defects of those strengths the following values for β_i (i) 0.082, (ii) 0.128, and (iii) 0.21, in satisfactory agreement with the Monte Carlo findings on β_3. Of course, a more refined analysis had to take into account, e.g., the rather complicated (see also the nonmonotonic profiles in Figs. 1 and 2) nature of the edge as a simultaneously ladder- and chain-type defect line as well as the effect of the bulk spin next to the corner on the corner magnetization. Indeed, the good agreement between β_3 and β_i in case (ii) may be related to the fact that the chainlike character is rather weak in that situation. The bulk spin is expected to strengthen the effective coupling at the corner especially in case (i), giving rise to the reduction in β_3 as compared to β_i.

Certainly, bulk properties will become critical only at the extraordinary transition, at $k_B T_c/J_b \approx 4.5115$. For instance, the specific heat C is expected to diverge there, in the thermodynamic limit. For finite, L^3 Ising cubes, one observes that a maximum in C near T_c shows up only for systems with at least a few thousands spins, getting more pronounced as the system size increases [we studied case (i) with equal surface couplings and $J_s = 2J_b$]. On the other hand, the maximum in C near the surface transition T_s dominates for small cubes, becoming more and more suppressed as one increases the size L. For cubes of moderate size, say $15 < L < 60$, the temperature dependence of the specific heat is characterized by an easily detectable two-peak structure, with maxima close to T_c and T_s. The height of the two peaks may be easily varied by replacing the Ising cubes by slabs.

In summary, the corner magnetization at the surface transition of Ising cubes has been found to display nonuniversal critical behavior, with the critical exponent β_3 of the corner magnetization (being distinct from the corresponding edge exponent β_2) depending on the strength of the edge and edge-surface couplings. The concrete value of β_3 may be approximated rather well from the exactly known value of the critical exponent of the magnetization at the intersection point of three defect lines in the two-dimensional Ising model by estimating effective defect couplings from the edge critical behavior.

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