

## Surface Critical Behavior of Two-Dimensional Dilute Ising Models

W. Selke,<sup>1</sup> F. Szalma,<sup>2</sup> P. Lajkó,<sup>2</sup> and F. Iglói<sup>3</sup>

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Ising models with nearest neighbor ferromagnetic random couplings on a square lattice with a (1, 1) surface are studied, using Monte Carlo techniques and a star-triangle transformation method. In particular, the critical exponent of the surface magnetization is found to be close to that of the perfect model,  $\beta_1 = 1/2$ . The crossover from surface to bulk critical properties is discussed.

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**KEY WORDS:** Random Ising model; surface magnetization; Monte Carlo simulations.

### 1. MODEL AND METHODS

The bulk critical behavior of the two-dimensional dilute Ising model has been studied extensively in recent years.<sup>(1-4)</sup> According to renormalization group calculations, the randomness leads, at least in the limit of weak dilution, to logarithmic modifications of the asymptotic power-laws for various quantities in the perfect model, in agreement with results of Monte Carlo simulations (however, also conflicting interpretations of numerical results have been suggested and discussed).<sup>(3, 5)</sup> In particular, the bulk magnetization,  $m_b$ , is expected to vanish as

$$m_b \propto t^{1/8} |\ln t|^{-1/16} \quad (1)$$

where  $t$  is the reduced temperature  $t = (T_c - T)/T_c$ .

In this Communication we shall present findings on surface critical properties of nearest neighbor random spin-1/2 Ising models on a square

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<sup>1</sup> Institut für Theoretische Physik B, Technische Hochschule, D-52056 Aachen, Germany.

<sup>2</sup> Institute for Theoretical Physics, Szeged University, H-6720 Szeged, Hungary.

<sup>3</sup> Research Institute for Solid State Physics, H-1525 Budapest, P.O. Box 49, Hungary, and Institute for Theoretical Physics, Szeged University, H-6720 Szeged, Hungary.

lattice with a surface. Randomness is introduced by allowing the nearest neighbor ferromagnetic couplings to take two values,  $J_1$  and  $J_2$ , where  $J_1$  is greater or equal to  $J_2$ . If both couplings occur with the same probability, then the model is self-dual.<sup>(6)</sup> The self-dual point is located at

$$\tanh(J_1/T_c) = \exp(-2J_2/T_c) \quad (2)$$

determining the critical temperature, if the model undergoes one phase transition. Indeed, results of simulations<sup>(7)</sup> strongly support that assumption.

Most of our findings are based on extensive Monte Carlo (MC) simulations, using single-spin and cluster-flip algorithms. To facilitate comparison of the simulational data with those of our numerical evaluation of the star-triangle transformation (ST) method,<sup>(8,9)</sup> we study the Ising model with a surface in the diagonal or (1, 1) direction. In that case, the coordination number of the surface spins is two. (Indeed, we believe the critical properties at this ordinary surface transition to be the same for the (1, 1) and the (1, 0) direction, as it is known to be the case in the perfect model). In the simulations, we consider lattices consisting of  $K$  columns and  $L$  rows, where the first and last columns are surface lines; the first and last rows are connected by periodic boundary conditions. Usually, we set  $L = K/2$ , with  $K$  ranging from 40 to 1280. The ST method, which was originally developed for layered lattices,<sup>(8)</sup> is generalized here to treat general inhomogeneous systems. In these calculations,  $K$  is proportional to the number of iterations and goes to infinity, while  $L$ , the number of surface sites, remains finite. In both methods, MC and ST, one has to average over an ensemble of bond configurations. Typically, the number of realizations ranged, in the simulations, from about 20 to several hundreds, taking more configurations for smaller system sizes. In the single-spin flip algorithm, used away from  $T_c$ , usually runs with a few  $10^4$  Monte Carlo steps per site were performed. Closer to  $T_c$ , the more efficient one-cluster spin flip method was applied, taking into account several  $10^4$  clusters per realization. Note that the statistical errors during a MC run turned out to be significantly smaller than those resulting from the ensemble averaging. We tested different random number generators to avoid inaccuracies due to a, possibly, unfortunate choice of the generator.<sup>(10)</sup>

The crucial quantity, computed in the MC simulations, is the magnetization per column,  $m(i) = \langle |\sum s_{i,j}| \rangle / L$ , where  $s_{i,j}$  denotes the spin in column  $i$  and row  $j$ , with  $i = 1, 2, \dots, K$ , and summing over  $j = 1, 2, \dots, L$ . Applying the ST method, we calculated, in particular, the surface magnetization  $m_s = m(1)$ .

In the following, we discuss the results of the MC simulations. The, so far rather preliminary, findings obtained from the ST method are in very

good agreement, demonstrating the correctness and accuracy of the two approaches.

## 2. RESULTS

The simulations were performed at  $r = J_2/J_1 = 1, 1/4,$  and  $1/10,$  monitoring the effect of increasing randomness on the critical surface properties.

In all cases, the magnetization per column,  $m(i)$ , decreases as one moves from the bulk towards the surface, as illustrated in Fig. 1. For sufficiently wide systems,  $K$ , the magnetization profile  $m(i)$  displays a plateau around the center,  $i = K/2$ , with the height being near the bulk magnetization,  $m_b$ . The bulk magnetization is expected to be approached very closely at a distance  $l$  from the surface, with the bulk correlation length determining that distance.<sup>(11)</sup>

In the thermodynamic limit, on approach to the bulk critical temperature,  $T_c$ , equation (2),  $m(i)$  goes to zero. Close to  $T_c$ , one may describe  $m(i)$  by an effective power-law behavior,  $m(i) \propto t^{\beta(i)}$ . Asymptotically, for sufficiently small values of  $t$ , one has  $\beta(1) = \beta_1$ , and  $\beta(i) = \beta$  for  $i > l$  and

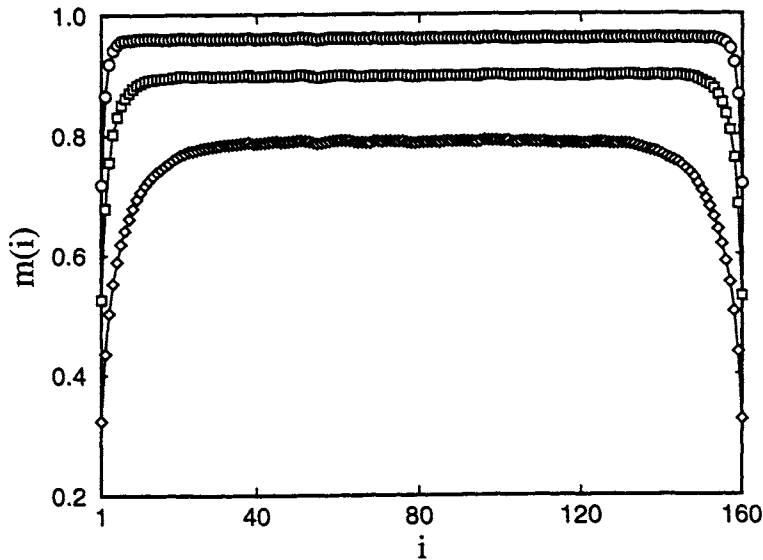


Fig. 1. Magnetization profiles for  $J_2/J_1 = 1/4$ , at various temperatures,  $t = 0.05, 0.15,$  and  $0.3$ , from bottom to top. MC systems of sizes  $L = 80$  and  $K = 160$  were simulated.

$i < K - l$ . In general, one may define an effective, temperature dependent critical exponent,  $\beta(i)_{\text{eff}}$ , by

$$\beta(i)_{\text{eff}} = d \ln[m(i)] / d \ln[t] \quad (3)$$

with the effective exponent becoming the asymptotic exponent as  $t$  vanishes. Certainly, in the MC study,  $\beta(i)_{\text{eff}}$  can be only approximated from data at discrete temperatures, say,  $t$  and  $t + \Delta t$ . The resulting value of the effective exponent is ascribed to the temperature  $t + (\Delta t/2)$  (examples are shown in Fig. 2). Since we are interested in the behavior in the thermodynamic limit, the linear dimensions  $K$  and  $L$  have to be sufficiently large compared to the bulk and surface correlation lengths. Actually, to avoid finite size effects, we chose system sizes with  $L$  increasing approximately linearly with  $1/t$  as one moves towards  $T_c$ .

In the perfect case,  $r = 1$ , our MC data for the magnetization  $m(i)$  as well as the estimates for  $\beta(1)_{\text{eff}}$ ,  $\beta(2)_{\text{eff}}$ , and the effective exponent of the bulk magnetization,  $\beta_{\text{eff}}$  agree excellently with the exact results,<sup>(12, 13)</sup> see Fig. 3 (where we did not include the simulational data), approaching smoothly, in the limit of small  $t$ , the asymptotic exponents for the surface  $\beta(1) = \beta_1 = 1/2$  and the bulk  $\beta = 1/8$ . Note that  $\beta(i)_{\text{eff}}$  decreases with  $i$ , at

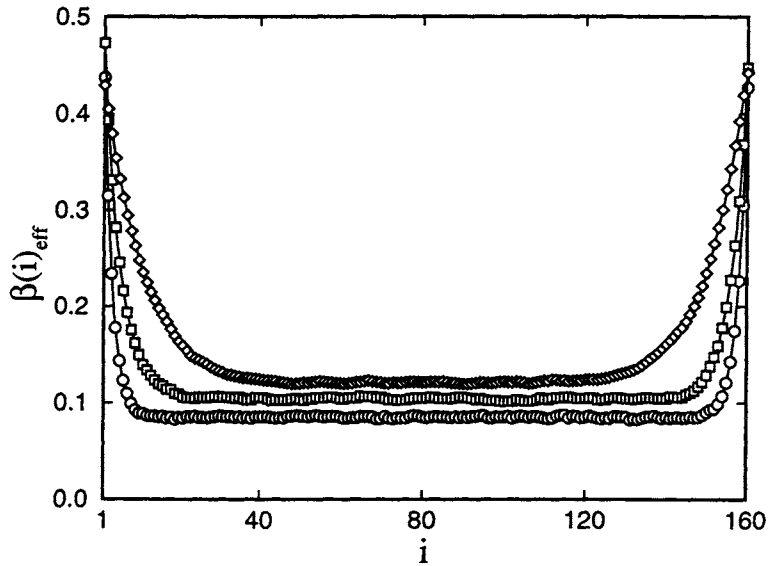


Fig. 2. Effective exponent of the magnetization per column, for  $J_2/J_1 = 1/4$ , at reduced critical temperatures  $t = 0.275, 0.175$  and  $0.075$ , from bottom to top. Systems with  $K = 160$  have been simulated.

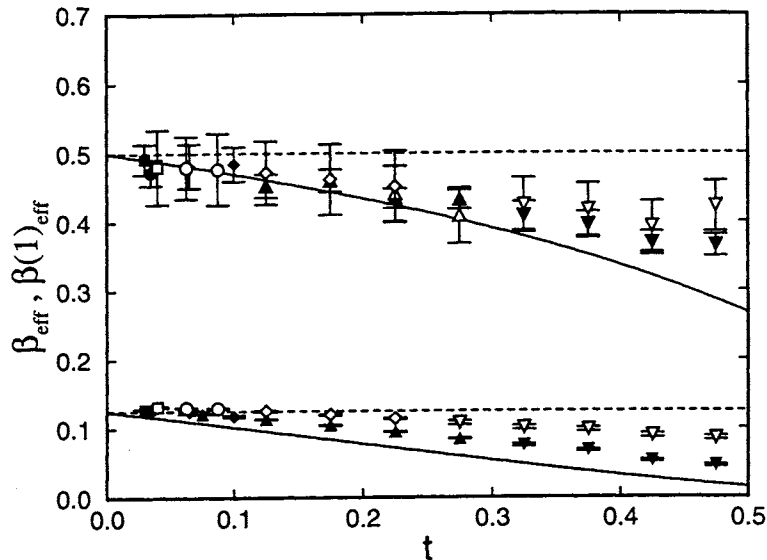


Fig. 3. Effective exponents for the surface and bulk magnetizations, for  $J_2/J_1 = 1$  (solid lines, exact results),  $1/4$  (full symbols), and  $1/10$  (open symbols). The dotted lines denote the asymptotic values of the perfect case. Systems with  $K=80$  (down triangles),  $160$  (up triangles),  $320$  (diamonds),  $640$  (circles), and  $1280$  (squares) have been simulated. The error bars result from ensemble averaging.

fixed temperature,  $t > 0$ . There is an interesting crossover phenomenon (which has not, to our knowledge, been studied exactly, so far) in that effective exponent, being asymptotically either  $1/2$  or  $1/8$ , see Fig. 2. The crossover occurs at a distance from the surface reflecting the bulk correlation length (that length diverges asymptotically like  $1/t$ , i.e. in the same fashion as the surface correlation length).

The effective exponents of the bulk and surface magnetizations, as obtained from the simulations, for the dilute cases  $r = J_2/J_1 = 1/4$  and  $1/10$  are shown in Fig. 3. For  $r = 1/4$ , the values of the exponents, especially of  $\beta(1)_{\text{eff}}$ , follow near criticality rather closely those of the perfect model,  $r = 1$ , as a function of reduced temperature. However, perhaps most noticeably, the bulk critical exponent  $\beta_{\text{eff}}$  superceeds the asymptotic critical value of the perfect case,  $\beta = 1/8$ , at  $t < 0.05$ , as had been observed before.<sup>(7, 14)</sup> Actually, the bulk magnetization data coincide with the previous simulational results obtained for the two-dimensional random-bond Ising model with full periodic boundary conditions. Accordingly,  $m_b$  can be fitted to the ansatz<sup>(7)</sup>

$$m_b = m_0 t^{1/8} (1 + at) ((1 + b \ln[1/t])^{-1/16}) \quad (4)$$

with  $m_0 = 1.203$ ,  $a = -0.183$  and  $b = 0.279$ , where  $b$  determines the cross-over temperature to the critical region dominated by randomness. On the other hand, the effective critical exponent of the surface magnetization  $m_s$  continues to change gradually and smoothly, towards a value close to  $1/2$ , as one enters that region. An asymptotic exponent  $\beta_1 = 1/2$ , as in the perfect case, seems to be conceivable, without any logarithmic corrections to the simple power-law.

At  $r = 1/10$ , i.e. at increased randomness, the effective exponent  $\beta(1)_{\text{eff}}$  tends to change only mildly over a wide range of temperatures,  $0.25 < t < 0.65$ , see Fig. 3. Going closer to  $T_c$ , the exponents starts to increase more visibly. Again, an asymptotic value of  $\beta_1 = 1/2$  is conceivable (certainly, strictly speaking, each extrapolation to the limit of vanishing  $t$ , requiring exceedingly large lattice sizes, is speculative). Note that  $\beta_{\text{eff}}$  superceeds the bulk exponent of the perfect case,  $1/8$ , now already at  $t < 0.12$ . Accordingly, we may safely argue to monitor, on further approach to  $T_c$ , randomness-dominated critical behavior in the bulk and surface properties as well. Obviously, in the case  $J_2/J_1 = 1/10$ , the results of the MC simulations do not indicate that the critical exponent of  $m_s$  is strongly affected by randomness. A “reasonable” guess seems to be  $\beta_1 = 0.49$ , with an error bar of about 0.02. Note that the error bars depicted in Fig. 3 are very pessimistic, resulting from comparing the unfavorable  $\sigma$ -deviations of the magnetizations at consecutive temperatures. Standard, more optimistic, error analyses would reduce the size of the error bars by an appreciable amount.

In summary, we conclude that our extensive MC simulations on two-dimensional random-bond Ising models with a  $(1, 1)$  surface provide no compelling evidence for asymptotic critical exponents depending strongly on the degree of dilution, i.e. the ratio of the strength of the two different coupling constants. It seems well conceivable that the surface magnetization follows the same power-law behavior as in the perfect case, with  $\beta_1 = 1/2$ , without any logarithmic modifications. A detailed analysis, including results from the star-triangle method for the surface magnetization and the critical surface spin correlations, will be published elsewhere.

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