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Logarithmic corrections in the two-dimensional Ising model in a random surface field

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Abstract

In the two-dimensional Ising model weak random surface field is predicted to be a marginally irrelevant perturbation at the critical point. We study this question by extensive Monte Carlo simulations for various strengths of disorder. The calculated effective (temperature or size-dependent) critical exponents fit with the field-theoretical results and can be interpreted in terms of the predicted logarithmic corrections to the pure system's critical behaviour.

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1. Introduction

In an inhomogeneous system the local critical behaviour near localized or extended defects may differ considerably from the bulk critical behaviour in the regular lattice (for a review, see [1]). One possible source of inhomogeneity is quenched (i.e., time-independent) randomness, which can be localized at the surface of the system (fluctuating surface coupling constants [2–6], microscopic terraces at the surface [7]) or at a grain boundary in the bulk of the system. It is known experimentally [8–10] that impurities may diffuse from inside the sample and segregate on the surface or at grain boundaries. In adsorbed systems, quenched disorder is naturally present since adatoms may bind randomly on equivalent surface sites [11].

In a theoretical description of the local critical behaviour of these systems, close to the bulk critical point, one can use a coarse-grained picture in which quenched randomness couples to some local operator. The local operator considered in this paper is the surface order parameter, hence the perturbation is described by the introduction of random fields (RFs) localized at the

surface. Usually the RF has zero mean and its variance is used to characterize the strength of disorder.

In the weak-disorder limit, the relevance or irrelevance of the perturbation can be analysed by making use of a Harris-type criterion [12]. The condition for the irrelevance of RFs on a defect with dimension $d - 1$ can be expressed in terms of the decay exponent for the local order parameter correlations in the pure system [2] as

$$\eta_{\parallel} \geq 1. \quad (1)$$

A plane of RFs in the bulk often constitutes a relevant perturbation as it is the case for the two-dimensional (2D) Ising model with $\eta = 1/4$. Thus a new fixed point appears, which controls the local critical behaviour. This fixed point is expected to be a surface one since RFs tend to destroy the local order and the bulk defect then acts as an effective cut.

Surface RFs are irrelevant for the 3D Ising model as noted and demonstrated through Monte Carlo (MC) simulations [13]. Curiously, in the case of a system with continuous symmetry, like the 3D Heisenberg model, surface RFs destroy the bulk long-range order [14] according to Imry–Ma arguments [15], although the perturbation is irrelevant at the ordinary surface transition according to (1). Among 2D systems the Ising model represents the borderline case, since $\eta_{\parallel} = 1$ [16]. For this model, field-theoretical investigations [11, 17] predict that the weak surface RF is a marginally irrelevant perturbation. Consequently, the surface critical properties of the random model are characterized by the critical singularities of the pure model supplemented by logarithmic corrections to scaling.

These theoretical predictions have not yet been confronted with the results of numerical calculations. In general, the observation and characterization of logarithmic corrections to scaling by numerical methods are notoriously difficult tasks, particularly in systems with quenched disorder. In this respect, a well-known example is the diluted 2D ferromagnetic Ising model, for which the accurate form of the singularities was long debated [18–23].

In this paper we present the results of a numerical study of the surface critical behaviour of the 2D Ising model in the presence of random surface fields. In section 2 we present the model and the known results about its critical properties. Then, through intensive Monte Carlo simulations, we determine effective surface magnetization exponents in two different ways. In section 3, they are obtained as a function of the deviation from the critical temperature. In section 4, we use a small homogeneous surface field at the critical point to deduce size-dependent exponents from the magnetization profiles. In section 5 we discuss the agreement between theoretical and numerical results.

2. The model and its predicted surface critical properties

We consider the Ising model on a $L \times M$ square lattice with the Hamiltonian

$$\mathcal{H} = -J \sum_{i=1}^{L-1} \sum_{j=1}^M (s_{i,j} s_{i+1,j} + s_{i,j} s_{i,j+1}) - \sum_{j=1}^M (h_1(j) s_{1,j} + h_L(j) s_{L,j})$$

$$s_{i,M+1} = s_{i,1}, \quad h_i(j) = \begin{cases} h_s + h & \text{with probability } p = 1/2 \\ h_s - h & \text{with probability } p = 1/2, \end{cases} \quad (2)$$

where $s_{i,j} = \pm 1$. J is the first-neighbour exchange interaction. The RF $h_s \pm h$ acts on the surface spins in the columns at $i = 1$ and $i = L$ and periodic boundary conditions are used in the vertical direction. Our main interest is to calculate the averaged magnetization per column, $m_i = \langle |\sum_j s_{i,j}| \rangle / M$.

For the pure system, i.e. with vanishing surface field, the surface magnetization, $m_s = m_1 = m_L$ is exactly known in the thermodynamic limit ($L, M \rightarrow \infty$) [16]:

$$m_{s,\text{pure}} = \left[\coth(2K) \frac{\sinh(2K) - 1}{\cosh(2K) - 1} \right]^{1/2}, \quad (3)$$

in terms of $K = J/k_B T$, where T is the temperature. At the critical point with $\sinh(2K_c) = 1$ the surface magnetization vanishes as

$$m_{s,\text{pure}} \approx m_0 t^{1/2}, \quad (4)$$

in terms of the reduced temperature, $t = (T_c - T)/T_c$, and $m_0^2 = 4(\sqrt{2} + 1)K_c \ln(2K_c)$. The relevant length scale is the bulk correlation length which, for $t > 0$, is given by [24]

$$\xi = [2 \ln(\sinh(2K))]^{-1}, \quad (5)$$

with the lattice constant for unit length. The correlation length diverges at the critical point as $\xi \approx [2\sqrt{2}K_c t]^{-1}$. Thus the reduced temperature and the length scale are related by

$$-\ln t \simeq 0.913 + \ln \xi. \quad (6)$$

In the presence of random surface fields there are no exact results available. In this case one can use the replica trick to transform the semi-infinite system with a random surface field into n semi-infinite replicas, coupled two-by-two through their surface spins, via nearest-neighbour interactions proportional to h^2 . The average properties of the random system are obtained in the limit $n \rightarrow 0$.

The surface critical properties of the system have been studied via two different methods, both using the differential renormalization group (RG) techniques where the lengths are rescaled by a factor e^l . The surface coupling between the replicas transforms as

$$h^2(l) = \frac{h^2}{1 + \kappa h^2 l}. \quad (7)$$

In the first approach [17] a conformal mapping is used at the bulk critical point, with $h_s = 0$, to transform the n semi-infinite replicas into n infinite strips with width L , which are coupled to each other at both surfaces through h^2 . The behaviour of the inverse correlation length is studied using degenerate perturbation theory to second order in h^2 . From the transformation of the inverse correlation length on the strips under rescaling by $e^l = L$, with $n = 0$, and using the gap-exponent relation [25], one can identify the L -dependent, effective decay exponent η_{\parallel} which is given by

$$\eta_{\parallel} = 1 + \frac{1}{\ln L}, \quad (8)$$

to leading logarithmic order.

In the second approach [11] the behaviour under rescaling of the homogeneous part of the surface field is determined as

$$h_s(l) = \frac{h_s e^{l/2}}{(1 + \kappa h^2 l)^{1/2}}. \quad (9)$$

The surface free energy density transforms as

$$f_s(t, h_s, h^2) = e^{-l} f_s[e^{l/\nu} t, h_s(l), h^2(l)], \quad (10)$$

where ν is the correlation length exponent. Using (9), the surface magnetization reads

$$m_s(t, h^2) = \left. \frac{\partial f_s}{\partial h_s} \right|_{h_s=0} = \frac{e^{-l/2}}{(1 + \kappa h^2 l)^{1/2}} m_s[e^{l/\nu} t, h^2(l)]. \quad (11)$$

With $e^l = \xi \sim t^{-\nu}$ and $\nu = 1$ according to (5), ignoring higher order correction, one obtains

$$m_s(t, h^2) \sim \frac{t^{1/2}}{(1 - \kappa_1 h^2 \ln t)^{1/2}}, \quad 0 < t \ll 1. \quad (12)$$

Thus the critical singularity of the pure model is supplemented by a logarithmic correction to scaling. From a practical point of view, one can define temperature-dependent effective exponents through

$$\beta_s(t) = \frac{\ln[m_s(t(1+\delta))/m_s(t(1-\delta))]}{\ln[(1+\delta)/(1-\delta)]} = \frac{1}{2} \left(1 + \frac{1}{|\ln t|} + \dots \right), \quad (13)$$

with $\delta \rightarrow 0$. The last expression gives the leading logarithmic correction following from equation (12).

Taking into account the scaling relation $\eta_{\parallel} = 2\beta_s/\nu$ with $\nu = 1$, the effective exponents in equations (13) and (8) correspond in terms of the relevant length scales, $L \rightarrow \xi \sim 1/t$.

The following two sections are devoted to a numerical test of the validity of these theoretical results.

3. Effective exponents

The surface critical exponents are deduced from the temperature dependence of the magnetization m_i in the surface layers (for a review, see [26]). We set the homogeneous surface field to zero, $h_s = 0$, the strength of the random surface field ranging from $h = 0.6$ to $h = 1.5$, and take a finite reduced temperature, $t > 0$. Systems of square and rectangular shapes containing $L \times M$ spins, with L and M ranging from 50 to 1000, have been studied using the standard single-spin-flip method. Although systems with rectangular shapes ($M < L$) lead to reduced finite-size effects, the fraction of surface spins is smaller than for a square system and more runs are needed to achieve the same accuracy for the surface magnetization which is self-averaging. Thus we worked with square systems to spare computer time. The final data are obtained after averaging over at least 1000 different runs with different realizations of the random surface field. For every run, time average has been taken over a few 10^4 Monte Carlo steps per spin after equilibration.

As an illustration we present m_i at $t = 0.05$ and $t = 0.02$ in figure 1 for different strengths of the RF. The profile of the pure system is shown for comparison. For a given t and different values of h , m_i displays a plateau around $i = L/2$ for large enough systems. It corresponds to the bulk magnetization, m_b , since its height is independent of h . If we approach the surfaces close enough, $i, L - i < \xi$, we enter in the surface region where the value of the magnetization is rapidly decreasing to its surface value, m_s . As seen in figure 1, for a given t the surface magnetization m_s and the inverse size of the surface region are decreasing with increasing disorder strength h .

According to finite-size scaling, in a large but finite system, sufficiently close to its critical point, $m_s(t)$ behaves as $(-t)^{\beta_s} f(\xi/L)$, where the scaling function, $f(x)$, tends to a constant for small values of its argument. In the actual calculations, we approach the transition point only to such a distance that the finite-size effects remain negligible and effective surface exponents are calculated using (13). In practice, finite-size effects have been circumvented by adjusting the size of the sample in a standard approach [4]. For a given value of t , data obtained for different system sizes are compared. Away from the critical point these data agree as long as the correlation length is less than the extent of the smaller system. Closer to T_c the correlation length increases and at some stage it gets comparable to the size of the smaller system. Finite-size effects then show up by a characteristic fast drop of the effective

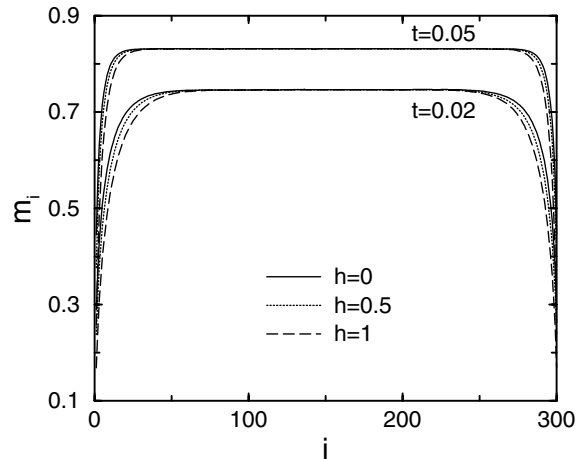


Figure 1. Magnetization profiles with random surface fields $h = 0, 0.5$ and 1 at $t = 0.05$ and $t = 0.02$. The data have been obtained for a system with 300×300 spins.

exponent [4]. The smaller system is then discarded and the procedure is continued with two system sizes which still yield identical data at that temperature. This approach is somehow cumbersome but assures that the final data are essentially free of finite-size effects.

The effective exponents are shown in figure 2 for different values of the strength of the RF. Here, in order to check the form of the logarithmic corrections in equations (8) and (12), β_s is plotted as a function of $1/|\ln t|$. For a given t the effective exponents are increasing with h as expected since RFs decrease local order. On the other hand, for a given h , $\beta_s(t)$ first shows a monotonic increase when t decreases and its value passes over the pure system's surface exponent, $\beta_s = 1/2$. Then, by further decreasing the reduced temperature, $\beta_s(t)$ seems to approach a maximum value. This saturation effect is more evident for large values of h . Unfortunately, the size limitation did not allow us to approach the transition point close enough to follow the predicted decrease of the effective exponent.

Here, in order to compare the numerical results with the theoretical predictions and to extrapolate our data to $t \rightarrow 0$, we use the following expression,

$$m_s(t) = m_0 t^{1/2} \frac{1 + at}{(1 + b \ln t)^{1/2}}, \quad (14)$$

which contains the leading analytic correction which follows from equation (3) and the leading logarithmic corrections to the fixed-point singularity given by (12). Note that the two corrections have different signs and their competing effect results in the non-monotonic temperature dependence of the effective exponent, $\beta_s(t)$. For a given RF, we have fitted the surface magnetization data to the form given in (14) with the amplitudes a and b as free parameters. From this, the effective surface magnetization exponent was calculated and used to extrapolate the data points in figure 2. The data extrapolate to the value of the pure system $\beta_{s,\text{pure}} = 1/2$ after an 'overshooting effect'. A quite similar tendency was observed in [20] for the bulk magnetization exponent of the 2D random bond Ising model. In our calculations, however, the maximum value is almost reached for $h \geq 1$, which was not possible for the random bond model.

In order to check the leading logarithmic correction to the effective exponent, we have calculated the difference of $\beta_s(t)$ and its value in the pure system, $\beta_{s,\text{pure}}(t)$, as calculated from (3) via equation (13). This difference, which is plotted in the inset of figure 2, no longer

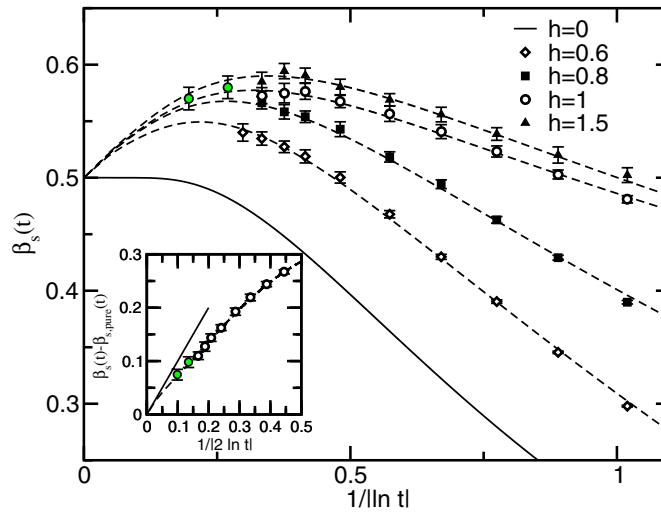


Figure 2. Effective surface exponent for different strengths of the random surface field. The two first points (grey circles) for $h = 1$ were deduced from the short-distance behaviour of the critical profiles discussed in section 4. The broken lines fitting the numerical data correspond to the formula in equation (14), with $a = -0.60, b = -0.23$ ($h = 0.6$), $a = -0.53, b = -0.40$ ($h = 0.8$), $a = -0.40, b = -0.47$ ($h = 1.0$) and $a = -0.47, b = -0.72$ ($h = 1.5$). The inset gives the difference between the effective exponents for the random ($h = 1$) and the pure systems. The straight line gives the predicted leading logarithmic correction.

contains the leading analytic correction; therefore, we expect to be able to compare it with the theoretical prediction in equation (13). As seen in the inset for the random surface field, $h = 1$, the corrections are compatible with theory, although much larger systems are needed in order to reach the asymptotic regime.

The form of the logarithmic corrections has been analysed in still another way by forming the ratio, $r(t, h) = m_{s,\text{pure}}/m_s$, of the surface magnetizations in the pure and in the disordered systems. In this way the leading analytic correction to scaling is eliminated. As shown in figure 3, the square of $r(t, h)$ has an asymptotic linear dependence on $\ln t$, the slope of which is proportional to h^2 , as shown in the inset of figure 3. This is in complete agreement with the theoretical prediction in equation (12).

4. Critical profiles

In this section we study the system at the critical point, $t = 0$; however, in the presence of a small homogeneous surface field, $h_s \ll h$. A typical magnetization profile in the system with $M \ll L$ is shown in the inset of figure 4. These data have been obtained with the Swendsen–Wang algorithm with a layer of ghost spins next to the surface [27]. At least 1000 runs with different realizations of the random surface field were performed, the time average of every run resulting from typically 3×10^5 MC updates.

As known from an analysis of the non-random system [27] the profile first increases close to the surface and then decreases in the bulk. The surface critical exponent, β_s , influences the form of the initial part and can be extracted from it. The non-vanishing surface field h_s introduces a new surface length scale, l_s , which in 2D is given by $l_s \sim h_s^{-1/(1-\eta_0/2)}$ and scales as $\sim h_s^{-2}$ for the Ising model.

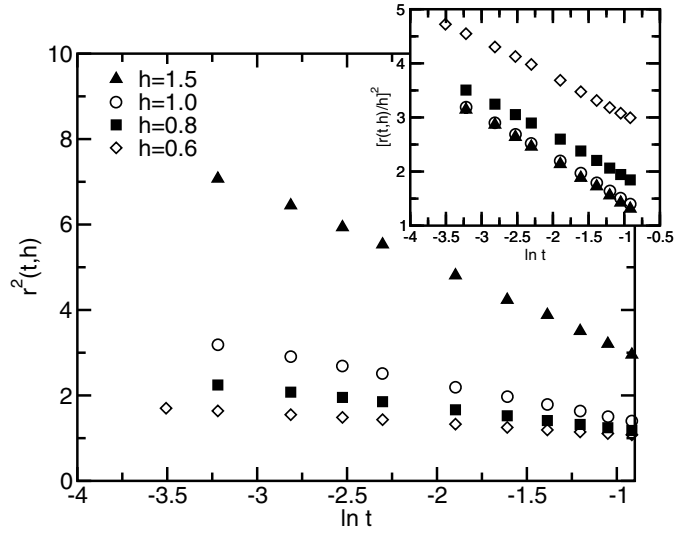


Figure 3. Square of the ratio $r(t, h)$ of the surface magnetizations in the pure and in the disordered Ising model as a function of $\ln t$. The slopes are proportional to h^2 as shown in the inset. Error bars are much smaller than the symbol sizes.

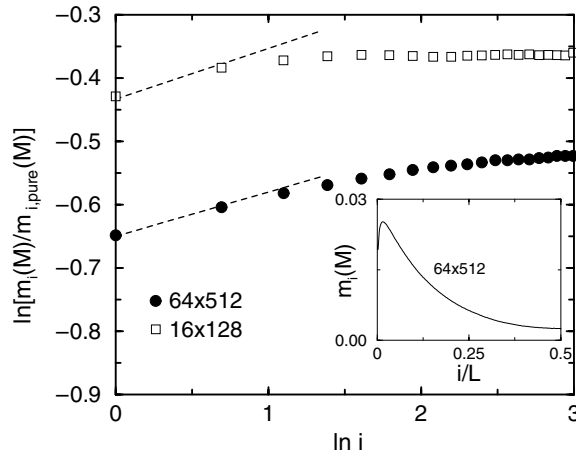


Figure 4. Ratio of the initial part of the critical magnetization profiles calculated in the random and in the pure system in the presence of a small homogeneous magnetic field. The initial slope in the log-log plot corresponds to the difference in the effective magnetization exponents (see the text). Inset: one half of the magnetization profile in the random system.

The initial part of the profile is restricted to $i \ll M, l_s$ and, according to finite-size scaling theory it behaves as

$$m_i(M, l_s) = i^{-x_m} g(i/M, i/l_s), \quad (15)$$

where $x_m = \beta/\nu = 1/8$ is the bulk magnetization scaling dimension. For small values of its arguments the scaling function g is expected to factorize as $g_0(i/M)g_s(i/l_s)$. For the pure 2D Ising model the second term is logarithmic [28], $g_s(i/l_s) \sim \ln(i/l_s) \sim \ln(ih_s^2)$, which makes

the numerical analysis difficult. For the Ising model with RF on the surface, the first term is expected to behave as

$$g_0(y) \sim \frac{y^{1/2}}{(1 + \kappa h^2 \ln y)^{1/2}}. \quad (16)$$

This form incorporates logarithmic corrections which, with $i = 1$ and $M \sim \xi$, are in agreement with the form of the surface magnetization given in equation (12). Now, in analogy with (13), an effective surface magnetization exponent can be defined as

$$\frac{\beta_s(y)}{\nu} = \frac{\ln[g_0(y(1 - \delta))/g_0(y(1 + \delta))]}{\ln[(1 + \delta)/(1 - \delta)]} \quad (17)$$

which, finally when $y \ll 1$, will be a function $\beta_s(M)$ of the characteristic length of the problem.

In order to get rid of the logarithmic factor, $g_s(i/l_s)$, we have calculated the ratio $m_i(M)/m_{i,\text{pure}}(M)$ of the initial profiles in the random and pure systems. Assuming that g_s has the same logarithmic singularity for both, we arrive at the conclusion that the ratio of profiles scales with the difference of the effective exponents, $\Delta\beta_s(M) = \beta_s(M) - \beta_{s,\text{pure}}(M)$.

In the actual calculation we set $h_s = 0.01$ and $h = 1$, and performed MC simulations on systems with sizes $M = 16$ and 64 and different aspect ratios $\alpha = L/M$. For $\alpha = 4$ and 8 , the initial part of the profiles turned out to be indistinguishable. The ratios calculated for the largest α are presented in figure 4 and, from the extrapolated initial slopes in a log–log plot, the differences of the effective exponents take the values $\Delta\beta_s(16) = 0.08(1)$ and $\Delta\beta_s(64) = 0.07(1)$. In order to compare these estimates with the effective exponents obtained in section 3 with a finite t , we use the correspondence of equation (6) with $M = \xi$. The data points obtained in this way are inserted in figure 2. They seem to fit very well with the predicted theoretical curve and are located in the descending part of the curve. Therefore this calculation gives further support to the theoretical results about the form of the logarithmic corrections.

5. Discussion

Marginally irrelevant operators are responsible for logarithmic corrections to scaling, the form of which can often be predicted by field theory and conformal invariance. According to the second-order perturbation theory, the random surface field is expected to be such a marginally irrelevant operator at the surface fixed point of the 2D Ising model. This conjecture, which is made on the basis of the replica trick and in the weak disorder limit, is confronted here with the results of extensive MC simulations for varying strength of the disorder. The calculated effective surface magnetization exponent, which depends either on the distance t from the critical point or on the finite size M of the critical system, varies with these parameters. Since this variation is non-monotonic, a direct extrapolation to the fixed-point values cannot be made from the data available on finite systems. However, the variation of the effective exponents is in good agreement with the theoretical form, which contains the predicted logarithmic correction to scaling to the pure systems critical behaviour. For the largest systems and for the strongest random fields, the numerical results are not too far from that obtained perturbatively in linear order. Therefore we interpret our results as numerical evidence in favour of the validity of the field-theoretical predictions.

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