Magnetization Profile in the $d = 2$ Semi-Infinite Ising Model
and Crossover between Ordinary and Normal Transition

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Abstract

We theoretically investigate the spatial dependence of the order parameter of
the two-dimensional semi-infinite Ising model with a free surface at or above
the bulk critical temperature. Special attention is paid to the influence of
a surface magnetic field $h_1$ and the crossover between the fixed points at
$h_1 = 0$ and $h_1 = \infty$. The sharp increase of the magnetization $m(z)$ close
to the boundary generated by a small $h_1$, which was found by the present
authors in the three-dimensional model, is also seen in two dimensions. There,
however, the universal short-distance power law is modified by a logarithm,
$m(z) \sim z^\kappa \ln z$, where $\kappa$, the difference between the scaling dimensions of
$h_1$ and the bulk magnetization, has the exact value $3/8$. By means of a
phenomenological scaling analysis, the short-distance behavior can be related
to the logarithmic dependence of the surface magnetization $m_1$ on $h_1$. Our
results, which are corroborated by Monte Carlo simulations, provide a deeper
understanding of the existing exact results concerning the local magnetization
and relate the short-distance phenomena in two dimensions to those in higher
dimensionality.

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I. INTRODUCTION

In systems at or close to a critical point the asymptotic power laws governing the behavior of thermodynamic quantities are modified in the vicinity of surfaces or other inhomogeneities. The characteristic distance within which changes occur is given by the bulk correlation length $\xi$. In general each bulk universality class splits up in several surface universality classes, depending upon whether the tendency to order in the surface is smaller or larger than or the same as in the bulk. In the case of the two-dimensional (2-d) Ising model in a semi-infinite geometry there exist two surface universality classes. Since the boundary is one-dimensional and, thus cannot become critical itself, the surface generally reduces the tendency to order. More precisely, for any positive starting value the exchange coupling between surface spins $J_1$ is driven to zero by successive renormalization-group transformations. The relevant field pertaining to the surface is the magnetic field $h_1$, which acts on surface spins only and which for instance may take into account the influence of an adjacent noncritical medium. The two universality classes then are labelled by $h_1 = 0$, the “ordinary” transition, and $h_1 = \infty$, the “normal” transition, where the former is an unstable fixed point and the latter is a stable fixed point of the renormalization-group flow.

In this work we are mainly concerned with order-parameter profiles for finite $h_1$ in the crossover region between the fixed points. Nonetheless, let us first recapitulate the situation at the fixed points. For the sake of simplicity, in the Introduction our considerations remain restricted to bulk criticality $T = T_c$, but the extension to the critical region is straightforward and will be done below. At the critical point and $h_1 = 0$, the order-parameter (or magnetization) profile $m(z)$ is zero for any distance $z \geq 0$ from the surface. In the other extreme, $h_1 = \infty$, it is well known that at macroscopic distances from the surface the magnetization decays as $\sim z^{-x_\phi}$, where $x_\phi = \beta/\nu$ is the scaling dimension of the bulk order-parameter field, with the exact value $1/8$ in the 2-d Ising model.

What do we expect, when $h_1$ takes some intermediate value, i.e., in the crossover region between the fixed points? Now, $h_1$ will certainly generate a surface magnetization $m_1$. As far as the profile $m(z)$ is concerned, a first guess would perhaps be that the magnetization should decay from that value as $z$ increases away from the surface. This guess is supported by mean-field theory, where one can calculate $m(z)$ and indeed finds a monotonously decreasing function of $z$.

In Ref. [5] the present authors have shown that, contrary to the naive (mean-field) expectation, fluctuations may cause the order parameter to steeply increase to values $m(z) \gg m_1$ in a surface-near regime. The range within which this growth occurs (at bulk criticality) is determined by $h_1$, the characteristic length scale being $l_1 \sim h_1^{-1/y_1}$, where $y_1 = \Delta_1/\nu$ is the scaling dimension of $h_1$. As further demonstrated by the present authors in Ref. [5], the growth of order in the near-surface regime $z \ll l_1$ is described by a universal power law

$$m \sim z^\kappa \quad \text{with} \quad \kappa = y_1 - x_\phi,$$

i.e., the growth exponent $\kappa$ is governed by the difference between the scaling dimensions $y_1$ and $x_\phi$. For $z \approx l_1$ the profile has a maximum and farther away from the surface, at distances much larger than $l_1$, the magnetization decays as $z^{-x_\phi}$.
Largely analogous results—monotonous behavior at the fixed points and profiles with one extremum in the crossover regime—where previously found by Mikheev and Fisher [6] for the energy density of the 2-d Ising model. The authors also suggested to calculate the order parameter in the crossover region. Below we focus our attention exactly on this problem. The questions posed in this work are the following:

- Does the short-distance growth of $m(z)$, found for instance in the three-dimensional Ising model, also occur in two dimensions?
- Does the simple power law (1) quantitatively describe the magnetization profile in $d = 2$, or are modifications to be expected?
- Is the scenario for the crossover between “ordinary” and “normal” transition, developed for the three-dimensional Ising model, also valid in $d = 2$?

As we will demonstrate below, the answer to the first and third question is “yes”, but the simple power law (1) is modified by a logarithm.

The rest of this paper is organized as follows: In Sec. II the theoretical framework is expounded. We first summarize the results of Ref. [5] and then generalize the scaling analysis by taking into account the available exact results on the dependence of $m_1$ on $h_1$ and on the magnetization profile. In Sec. III, in order to corroborate our analytical findings, we present Monte Carlo (MC) data for $m(z)$ and compare with exact results for the order-parameter profile. In two Appendices exact literature results on the dependence of the surface magnetization on $h_1$ and on the order-parameter profile are briefly reviewed.

II. THEORY

We consider the semi-infinite Ising system with a free boundary on a plane square lattice. The exchange coupling between neighboring spins is $J$. A surface magnetic field $H_1$ is imposed on the boundary spins and bulk magnetic fields are set to zero such that the Hamiltonian of the model reads

$$\mathcal{H} = -J \sum_{\langle ij \rangle \in V} s_i s_j - H_1 \sum_{i \in \partial V} s_i ,$$

where $\partial V$ and $V$ stand for the boundary and the whole system (including the boundary), respectively. As usual, we work with the dimensionless variables

$$K = J/k_B T \quad \text{and} \quad h_1 = H_1/k_B T .$$

The bulk critical point corresponds to $K_c = \frac{1}{2} \ln(1 + \sqrt{2})$. 

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A. Scaling analysis for Ising system in $2 < d < 4$

In the critical regime, where $|\tau| \equiv |(T - T_c)/T_c| \ll 1$, thermodynamic quantities are described by homogeneous functions of the scaling fields. As a consequence, the behavior of the local magnetization under rescaling of distances should be described by

$$m(z, \tau, h_1) \sim b^{-x_\phi} m zb^{-1}, \tau b^{1/\nu}, h_1 b^{y_1}),$$  \hspace{1cm} (4)

where $x_\phi = \beta/\nu$ and $y_1 = \Delta_1/\nu$ is the scaling dimension of $h_1$. In terms of other surface exponents we have $y_1 = (d - \eta_\parallel)/2 \ [2,7]$. In Eq. (4) it was further assumed that the distance $z$ from the surface is much larger than the lattice spacing or any other microscopic length scale. One is interested in the behavior at macroscopic scales, and, for the present, $z$ may be considered as a continuous variable ranging from zero to infinity.

Removing the arbitrary rescaling parameter $b$ in Eq. (4) by setting it $\sim z$, one obtains the scaling form of the magnetization

$$m(z, \tau, h_1) \sim z^{-x_\phi} M(z/\xi, z/l_1),$$  \hspace{1cm} (5a)

where, as already stated,

$$l_1 \sim h_1^{-1/y_1} \hspace{1cm} (5b)$$

is the length scale set by the surface field. The second length scale pertinent to the semi-infinite system and occurring in (5a) is the bulk correlation length $\xi = \tau^{-\nu}$. Regarding the interpretation of MC data, which are normally obtained from finite lattices, one has to take into account a third length scale, the characteristic dimension $L$ of the system, and a finite-size scaling analysis has to be performed. The latter will be briefly described in Sec. II C.

Going back to the semi-infinite case and setting $\tau = 0$, the only remaining length scale is $l_1$, and the order-parameter profile can be written in the critical-point scaling form

$$m(z, h_1) \sim z^{-x_\phi} M_c(z/l_1).$$  \hspace{1cm} (6)

As said above, for $z \to \infty$ the magnetization decays as $\sim z^{-x_\phi}$ and, thus, $M_c(\zeta)$ should approach a constant for $\zeta \to \infty$. In order to work out the short-distance behavior of the scaling function $M_c(\zeta)$, we demand that $m(z) \sim m_1$ as $z \to 0$. This means that in general, in terms of macroscopic quantities, the boundary value of $m(z)$ is not $m_1$. If the $z$-dependence of $m(z)$ is described by a power law, it cannot approach any value different from zero or infinity as $z$ goes to zero. However, the somewhat weaker relation symbolized by “$\sim$” should hold, stating that the respective quantity asymptotically (up to constants) “behaves as” or “is proportional to”. This is in accord with and actually motivated by the field-theoretic short-distance expansion \[\[4,2],\] where operators near a boundary are represented in terms of boundary operators multiplied by $c$-number functions.

In the case of the three-dimensional Ising model the foregoing discussion leads to the conclusion that $m(z) \sim h_1$ because the “ordinary” surface—the universality class to which
also a free surface belongs—is paramagnetic and responds linearly to a small magnetic field \( H \). The consequence for the scaling function in (3) is that \( M_c(\zeta) \sim \zeta^{y_1} \), and, inserting this in (6), we obtain that the exponent governing the short-distance behavior of \( m(z) \) is given by the difference between \( y_1 \) and \( x_\phi \) (as already stated in Eq. (1)). Using the scaling relation \( \eta_\perp = (\eta + \eta_\parallel) / 2 \) among anomalous dimensions, one can reexpress the exponent \( \kappa \) as

\[
\kappa = 1 - \eta_\perp. \tag{7}
\]

In the mean field approximation the value of \( \kappa \) is zero, and one really has \( m(z \to 0) = m_1 \). However, a positive value is obtained when fluctuations are taken into account below the upper critical dimensionality \( d^* \). For instance, the result for the \( n \)-vector model with \( n = 1 \) (belonging to the Ising universality class) in the framework of the \( \epsilon \)-expansion is \( \kappa = \epsilon / 6 \). Thus, the magnetization indeed grows as \( z \) increases away from the surface.

For the 2-d Ising model the exponent \( \eta_\perp \) is known exactly and one obtains \( \kappa = 3/8 \). However, as will be discussed in Sec. II B, the pure power law found in Ref. [5] for \( d = 3 \) is modified in two dimensions by a logarithmic term, and the exponent \( 3/8 \) cannot directly be seen in the profile.

The above phenomenological analysis is straightforwardly extended to the case \( \tau > 0 \). In \( d > 2 \), we may assume that the behavior near the surface for \( z \ll \xi \) is unchanged compared to (1), and, thus, the increasing profiles are also expected slightly above the critical temperature. The behavior farther away from the surface depends on the ratio \( l_1 / \xi \).

In the case of \( l_1 > \xi \) a crossover to an exponential decay will take place for \( z \approx \xi \) and the regime of nonlinear decay does not occur. For \( l_1 < \xi \) a crossover to the power-law decay \( \sim z^{-\beta/\nu} \) takes place and finally at \( z \approx \xi \) the exponential behavior sets in.

Below the critical temperature, the short-distance behavior of the order parameter is also described by a power law, this time governed by a different exponent, however. The essential point is that below \( T_c \) the surface orders even for \( h_1 = 0 \). Hence, in the scaling analysis the scaling dimension of \( h_1 \) has to be replaced by the scaling dimension of \( m_1 \), the conjugate density to \( h_1 \), given by \( x_1 = \beta_1 / \nu \). The exponent that describes the increase of the profile is thus \( x_1 - x_\phi \), a number that even in mean-field theory is different from zero (= \( 1/2 \)).

Phenomena to some extent analogous to the ones discussed above were reported for the crossover between special and normal transition. Also near the special transition the surface field \( h_1 \) gives rise to a length scale. However, the respective exponent, the analogy to \( \kappa \) in (1), is negative, and, thus, one finds a profile that monotonously decays for all (macroscopic) \( z \), with different power laws in the short-distance and the long-distance regime and a crossover at distances comparable to the length scale set by \( h_1 \). However, non-monotonous behavior in the crossover region is a common feature in the case of the energy density in \( d = 2 \) and as well as in higher dimensionality.

The spatial variation of the magnetization discussed so far strongly resembles the time dependence of the magnetization in relaxational processes at the critical point. If a system with nonconserved order parameter (model A) is quenched from a high-temperature initial state to the critical point, with a small initial magnetization \( m^{(0)} \), the order parameter behaves as \( m \sim m^{(0)} t^\theta \), where the short-time exponent \( \theta \) is governed by the difference...
between the scaling dimensions of initial and equilibrium magnetization divided by the dynamic (equilibrium) exponent \( \frac{d}{\kappa} \). Like the exponent \( \kappa \) in (1), the exponent \( \theta \) vanishes in MF theory, but becomes positive below \( d^* \).

B. Scaling analysis in \( d = 2 \)

During the years, initiated by the work of McCoy and Wu [16,17], the 2-d Ising model with a surface magnetic field received a great deal of attention, because many aspects can be treated exactly and it is a simple special version of the 2-d Ising model in an inhomogeneous bulk field, a problem to which an exact solution would be highly desirable. Some of these exact results, namely those considering the vicinity of the critical point [18,19], will be used in the following as a guiding line for our phenomenological scaling analysis and to compare numerical data with.

The dependence of \( m_1 \) on the surface magnetic field (bulk field \( h = 0 \)) in the 2-d Ising model was calculated exactly by Au-Yang and Fisher [18] in a \( n \times \infty \) (strip) geometry. The limit \( n \to \infty \), yielding results for the semi-infinite geometry, was also considered. Whereas above two dimensions at the ordinary transition the surface, in a sense, is paramagnetic, i.e., the response of \( m_1 \) to a small \( h_1 \) is linear, in two dimensions the function \( m_1(h_1) \) has a more complicated form. As summarized in Appendix A (see Eq. (A2)), there is a logarithmic correction to the linear term in \( d = 2 \); for \( h_1 \to 0 \) the surface magnetization behaves as \( \sim h_1 \ln h_1 \).

Further, as shown by Bariev [19] and summarized in Appendix B, the length scale \( l_1 \) determined by \( h_1 \) behaves as \( \sim [\tanh(h_1)]^{-2} \). For small \( h_1 \), where the scaling analysis is expected to be correct, this is consistent with (5b) as \( y_1 = 1/2 \) in the 2-d Ising model. Thus the characteristic length scale that enters the scaling analysis depends in the same way upon \( h_1 \) as in higher dimensions.

The foregoing discussion allows us to generalize our scaling analysis, especially Eqs. (3) and the near-surface law (1), such that the special features of the 2-d Ising model are taken into account. Again, the only available length scale at \( \tau = 0 \) is \( l_1 \), and the magnetization can be represented in the form given in Eq. (1). For \( z \to \infty \) we expect that \( m \sim z^{-1/8} \) and, thus, \( M_\zeta(\zeta) \) should approach a constant for \( \zeta \to \infty \). In order to find the short-distance behavior we assume again that \( m(z) \sim m_1 \) as \( z \to 0 \). Taking into account the logarithmic correction mentioned above and discussed in more detail in Appendix A (see Eq. (A2)), we find that \( M_\zeta(\zeta) \sim \zeta^{1/2} \ln \zeta \) for \( \zeta \to 0 \). Hence, for the short-distance behavior of \( m(z) \) in the semi-infinite system we obtain

\[
m(z, h_1) \sim h_1 z^{\kappa} \ln(h_1 z^{y_1}),
\]

where the exact values of the exponents are \( \kappa = 1 - \eta_\perp = 3/8 \) and \( y_1 = 1/2 \). Thus, for \( z < l_1 \) the magnetization \( m(z) \) for a given value of \( h_1 \) behaves as \( \sim z^{3/8} \ln z \).

The result (8) should hold for any value of the exchange coupling \( J_1 \) in the surface. In our MC analyses to be presented below we implemented free boundary conditions with \( J = J_1 \), but we expect (8) to hold for any value of \( J_1 \) with possible \( J_1 \)-dependent nonuniversal constants leaving the qualitative behavior of the profiles unchanged.
Eq. (8) is the main analytic result of this work. As discussed in the following, it is consistent with Bariev’s exact solution [19] (see Appendix B) and with MC data for the profile. It tells us that the short-distance power law behavior is modified by a logarithmic term. This logarithm can be traced back to the logarithmic singularity of the surface susceptibility [1], which, in turn, causes the logarithmic dependence of $m_1$ on $h_1$, and eventually leaves its fingerprint also on the near-surface behavior of the magnetization. The result (8) provides a thorough understanding of the near-surface behavior of the order parameter and allows to relate special features of the two-dimensional system, which were (as we will discuss in more detail below) previously known from the exact analyses [19], to the somewhat simpler short-distance law in higher dimensions.

C. Finite Size scaling

In order to assess the finite size effects to be expected in the MC simulations, we have to take into account the finite-size length scale $L$, which is proportional to the linear extension $N$ of the lattice (compare Sec. III A below). The generalization of (4) reads [20]

$$m(z, \tau, h_1, L) \sim b^{-x_\phi} m(zb^{-1}, \tau b^{1/\nu}, h_1 b^{\mu_1}, Lb^{-1}) ,$$

and proceeding as before, we obtain as the generalization of (5a) to a system of finite size:

$$m(z, \tau, h_1, L) \sim z^{-x_\phi} M(z/\xi, z/l_1, z/L) .$$

Thus even at $T_c$ there are two pertinent length scales, on the one hand $L$ (imposed by the geometry that limits the wavelength of fluctuations) and on the other hand $l_1$ (the scale set by $h_1$).

It is well known that for large $z \gtrsim L$ we have to expect an exponential decay of $m(z)$ on the scale $L$. In the opposite limit, when $z$ is smaller than both $L$ and $l_1$, we expect the short-distance behavior (8) to occur. However, for $d = 2$ it can be concluded from the finite-size result (A4) that there will be an $L$-dependent amplitude, a prefactor to the function given in (8). But otherwise the logarithmically modified power law (8) should occur. Farther away from the surface, the form of the profile depends on the ratio between $l_1$ and $L$. For $z$ smaller than both $L$ and $l_1$, the behavior is described by (8). In the case of $l_1 > L$ a crossover to an exponential decay will take place for $z \simeq L$. In the opposite case, a crossover to the power-law decay $\sim z^{-x_\phi}$ takes place, followed by the crossover to the exponential behavior at $z \simeq L$. Thus, qualitatively, the discussion is completely analogous to the one in Sec. II A, where the behavior at finite $\xi$ was described.

III. MONTE CARLO SIMULATION

A. Method

The results of the scaling analysis, especially the short-distance law (8), were checked by MC simulations. To this end, we calculated order-parameter profiles for the 2-d Ising model...
with uniform exchange coupling $J$. The geometry of our systems was that of a rectangular (square) lattice with two free boundaries (opposite to each other) and the other boundaries periodically coupled, such that the effective geometry was that of a cylinder of finite length. The linear dimension perpendicular to the free surfaces was taken to be four times larger than the lateral extension in order to keep corrections due to the second surface small [21]. Hence, when we talk about a lattice of size $N$ in the following, we refer to a rectangular $N \times 4N$ system.

In order to generate an equilibrium sample of spin configurations, we used the Swendson-Wang algorithm [22]. It effectively avoids critical slowing down by generating new spin configurations via clusters of bonds, whereby the law of detailed balance is obeyed. For a given spin configuration, a bond between two neighboring spins of equal sign exits with probability $1 - e^{-2K}$. There are no bonds between opposite spins. Then, clusters are defined as any connected configuration of bonds. Also isolated spins define a cluster, such that eventually each spin belongs to one of the clusters. After having identified the clusters, the new configuration is generated by assigning to each cluster of spins a new orientation, with equal probability for each spin value as long as the cluster does not extend to a surface.

In order to take into account $h_1$, we introduced, in the same way as suggested by Wang for taking into account bulk fields [23], two “ghost” layers of spins next to each surface that couple to the surface spins with coupling strength $h_1$ and that all point in the direction of $h_1$. If at least one bond between a surface and a ghost spin exists the cluster has to keep its old spin when the system is updated. This preserves detailed balance. In the practical calculation this rule was realized by a modified (reduced) spin-flip probability

$$p(k) = 1 - \frac{1}{2} \exp(-2h_1 k) \quad (11)$$

for clusters pointing in the direction of $h_1$ (and $1/2$ for clusters pointing in opposite direction), $k$ being the number of surface spins contained in the cluster.

In order to obtain an equilibrium distribution of configurations we discharged several hundred (depending on system size) configurations after the start of the simulation. To keep memory consume low, we used multispin-coding techniques, i.e., groups of 64 spins were coded in one long integer.

**B. Comparison with exact results**

A crucial test for the MC program is the comparison with known exact results. On the other hand, if both MC data an exact results agree, the former can be regarded also as a confirmation of the exact results. Having calculated order-parameter profiles for different values of $h_1$, in particular the magnetization at the boundaries (the ends of the cylinder) can be obtained. In Fig. 1 we show the results for $m_1(h_1)$. The squares respresent our MC data for a system of size $N = 512$. Also depicted is the exact result for the semi-infinite system taken from Ref. [18] (see also Appendix A). It is clear that the MC values approach the exact curve for large $h_1$. Below $h_1 \approx 0.03$, the MC results show a linear dependence on $h_1$, significantly deviating from the exact curve. The linear behavior can be regarded as
a finite-size effect, and it is qualitatively consistent with the result (A4) of Au-Yang and Fisher [18]. The latter was derived in a strip of finite width with infinite lateral extension, however, so that a quantitative comparison with our data is not possible.

Fig. 1: Monte Carlo results for \( m_1 \) as a function of \( h_1 \) for \( N = 512 \) (represented by full squares) compared to the exact result of Ref. [18] (see Appendix A). The statistical errors of the Monte Carlo data are about the same size as the symbols. A detailed discussion and comparison of the data is in the text.

Next we compare with the exact solution obtained by Bariev [19] for the order-parameter profile. The explicit result (B5) holds in the limit \( h_1 \to 0 \). This limit is hard to access in the MC simulation since the signal \( m(z) \) becomes small and is eventually lost in the noise. To obtain a concrete result to compare with, we have calculated the profile numerically from (B4) terminating the series in (B4a) after the third term. It turned out that the series converges rather quickly as long as the distance from the surface is not too small. Only very close to the surface higher orders need to be taken into account. Concretely, we took \( K = 0.999K_c \) (i.e. \( \tau \approx 0.001 \)) and \( h_1 = 0.01 \). Then, employing (B2) and (B4) one obtains \( \xi = 567 \) and \( l_1 = 2069 \), respectively. The result of the numerical evaluation of (B4) is shown in Fig. 2 (dashed curve), where \( m(z) \) versus the distance \( z \equiv n - 1 \) is plotted.

Then, with exactly the same parameters, the MC profiles were calculated, with the size \( N \) varying between 128 and 1024. The results are depicted in double-logarithmic representation in Fig. 2 (solid curves). It is obvious that the MC data approach the (approximated, in principle) exact profile with increasing lattice size. Most importantly, both results show the short-distance behavior anticipated from the scaling analysis above and expressed in (8). This is demonstrated by the dotted line, which depicts the function \( 0.016 n^{3/8} (6.15 - \ln n) \) (the constants were fitted). As expected, it only describes the profile for short distances...
from the boundary and becomes wrong for large distances, completely analogous to the asymptotic form (A2) of \( m_1(h_1) \).

\[ \begin{align*}
\text{Fig. 2: Monte Carlo profiles for } K/K_c &= 0.001 \text{ and } h_1 = 0.01 \text{ for lattices of size 128×512, 256×1024, 512×2048, and 1024×4096 (solid lines from below to above) compared with the numerical evaluation of the exact result (B4). The latter holds for the semi-infinite system. It is clearly visible that the Monte Carlo data approach the exact result for increasing system size. The dotted line represents the asymptotic (\( z \to 0 \)) behavior expressed in Eq. (8) \( \sim z \ln z \) that becomes wrong for large distances.}
\end{align*} \]

C. Monte Carlo results

First we discuss a set of profiles which were obtained with \( N = 512 \) by setting \( h_1 = 0.01 \) and \( K/K_c \) varying between 0.996 to 1.004, in steps of 0.001. The data are depicted in Fig. 3. Depending on the temperature, we averaged over 10000 to 30000 configurations. Especially the shape of the critical profile, marked in Fig. 3, is consistent with the scaling analysis of Sec. II B. It increases up to \( z \approx 60 \), then has a maximum and farther away from the surface it decays. With increasing distance the influence of the second surface (here at \( z = 2047 \)) becomes stronger, such that the profile has a minimum about halfway between the boundaries. (The data of Fig. 3 were not symmetrized after the average over configurations was taken.)

For \( T > T_c \) (curves below the critical profile), the maximum moves towards the surface and the regime of growing magnetization becomes smaller. This is consistent with the scaling analysis of Sec. III A, in this case the growth is limited by the correlation length \( \xi \). On the other hand, for \( T < T_c \), the tendency to decay in between the surfaces becomes weaker, as the the bulk value of the magnetization in the ordered phase grows. As said in Sec. III A, the short-distance growth below \( T_c \) is described by \( z^{x_1-x_\phi} \), where the difference \( x_1 - x_\phi \) takes also the exact value 3/8 [24]. This time, there is no logarithm however, and the growth is steeper than above \( T_c \).
Fig. 3: Order-parameter profiles for various temperatures below and above $T_c$ for fixed $h_1 = 0.01$ and $N = 512$ compared with the critical profile. The three curves above the critical profile were obtained with $K/K_c = 1.001, 1.002, 1.003$. The four profiles below correspond to $K/K_c = 0.999 \ldots 0.996$. The data are not symmetrized.

Fig. 4 shows the MC results for the critical point, for different values of $h_1$ in double-linear representation. In Fig. 5 the same data are plotted double-logarithmically. The lower dashed line shows the short-distance behavior $\sim z^{3/8} \ln z$ according to Eq. (8) and (as already discussed in connection with Fig. 2) the MC profiles confirm the scaling analysis of Sec. IV B. The upper dashed line is the pure power law $z^{-1/8}$ that describes the decay in the regime where $z$ is larger than $l_1$ but still smaller than $L$ or $\xi$. In our simulation this regime is only reached for relatively large values of $h_1 \gtrsim 0.5$. The uppermost profile ($h_1 = 1.0$) obviously goes through this regime for $10 \lesssim z \lesssim 60$. The finite-size exponential behavior (see Sec.II C) can be observed in all curves for $z \gtrsim 100$. The data of Figs. 4 and 5 are symmetrized, i.e., after averaging over configurations we computed the mean value of the left and right halves of the system. Hence, the profiles are only displayed up to halfway between the boundaries (here $z = 1023$).

The location of the maximum of $m(z)$, $z_{\text{max}}$, as a function of $h_1$ is depicted in Fig. 6. The maximum $z_{\text{max}}$ was determined from the profiles by a graphical method. Error bars are estimated. For small values of $h_1$ the near-surface growth is limited by finite-size effects. Up to about $h_1 = 0.03$, the value of $z_{\text{max}}$ is roughly independent of $h_1$. For larger values of $h_1$, $z_{\text{max}}$ moves towards the surface. As indicated by the dashed line, the dependence of $z_{\text{max}}$ on $h_1$ is completely consistent with $l_1 \sim h_1^{-2}$ obtained from the scaling analysis (see (5b)). For $h_1 = 1.0$ (upper curve) the maximum value of $m(z)$ is at the boundary, and the magnetization monotonously decays for $z > 0$. 

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Fig. 4: Monte Carlo profiles for $N = 512$ at $T = T_c$ for $h_1 = 0.005, 0.01, 0.02, 0.03, 0.07, 0.1$, and $1.0$ (from bottom to top). The data are symmetrized and are only shown up to $z = 1023$.

Fig. 5: The same profiles as in Fig. 4 in double-logarithmic representation, pronouncing the short-distance behavior. For small $h_1$ (lower curves) the growth of $m(z)$ described by Eq. (8) is clearly visible. For $h_1 = 1.0$ our Monte Carlo result (upper solid line) is in accord with $m(z) \sim z^{-1/8}$ (dashed line). The behavior of the Monte Carlo data for $z \gtrsim 100$ is described by the (finite-size) exponential decay and corrections to the semi-infinite profiles due to the second boundary become stronger.
Fig. 6: The location of the maximum $z_{\text{max}}$ of $m(z)$ in dependence of $h_1$ as obtained from the data of Fig. 4 and other profiles for the same system (not displayed). The dashed line represents $l_1 \sim h_1^{-2}$. For larger values of $h_1$ we have $z_{\text{max}} \sim l_1$. For small $h_1$ where $l_1$ becomes larger than the finite-size scale $L$, $z_{\text{max}}$ is determined by $L$.

Fig. 7: Order-parameter profiles for $K = K_c$ and $h_1 = 0.01$ for system size $N = 128, 256, 512, 1024, \text{ and } 2048$.

In Fig. 7 profiles for fixed $h_1$ and $T = T_c$ for various system sizes (ranging between $N = 128$ and 2048) are displayed. With increasing $N$, the maximum keeps moving away
from the surface, \( z_{\text{max}} \simeq \) in the largest system. This means that with these parameters we are still in the regime where \( L < l_1 \). When \( h_1 = 0.03 \) is taken instead, the situation is different. The respective MC data are depicted in Fig. 8. For the small system we have again increasing \( z_{\text{max}} \). For the two largest systems \( N = 1024 \) and 2048, however, the maximum is roughly located at the same distance from the surface, signaling that now \( l_1 < L \).

![Fig. 8: Profiles for \( h_1 = 0.03 \) and otherwise the same parameters as in Fig. 7.](image)

**IV. DISCUSSION**

We studied the short-distance behavior of order-parameter profiles in the two-dimensional semi-infinite Ising system at or above the bulk critical temperature. Our main goals were a detailed understanding of the near-surface behavior of the order parameter and a complete scenario for the crossover between “ordinary” and “normal” transition.

With regard to the short-distance behavior, especially for small surface fields \( h_1 \), the Ising model in \( d = 2 \) turned out to be quite special. The functional form is quantitatively not captured by the analysis of Ref. [5], where the main emphasis was put on the situation in \( d = 3 \). Here we demonstrated by means of a scaling analysis that a small \( h_1 \) induces a magnetization in a surface-near regime that grows as \( z^{3/8} \ln z \) as the distance \( z \) increases away from the surface (see Eq. (8)). Our findings are not only consistent with available exact results (to which we made a detailed comparison), but they also allow a detailed understanding of the physical reasons for the growth and its quantitative form. The surface magnetization \( m_1 \) generates in the region that is (on macroscopic scales) close to the surface and that is much more susceptible than the surface itself, a magnetization \( m(z) \) much larger than \( m_1 \). The exponent \( 3/8 \) that governs the power-law part of the growth is the difference between the scaling dimensions \( y_1 \) (of \( h_1 \)) and \( x_\phi \) (of the bulk magnetization). Eventually,
as was demonstrated Sec. II B, the logarithmic factor can be traced back to the logarithmic dependence of \( m_1 \) on \( h_1 \).

The scenario for the crossover between “ordinary” and “normal” developed in Ref. [5] and generalized in this work to include the 2-d Ising model is the following: At \( T = T_c \) a small \( h_1 \) causes the increasing near-surface behavior described above. The magnetization grows up to distances \( l_1 \approx h_1^{-1/2} \) and then the crossover to the power-law decay \( \sim z^{-1/8} \) takes place. With increasing \( h_1 \) the surface-near regime becomes smaller, and eventually for \( h_1 \to \infty \) the length scale \( l_1 \) goes to zero, such that the region with increasing magnetization vanishes completely and the situation of the “normal” transition is reached.

For \( T \) slightly above \( T_c \) our scenario essentially remains valid as long as \( \xi > l_1 \). Only when \( z \) is of the order of \( \xi \) the crossover to the exponential decay takes place. For \( \xi < l_1 \), on the other hand, the growth is limited to the region \( z < \xi \).

Concerning three-dimensional systems several experiments were pointed out in Ref. [5], whose results are possibly related related to the anomalous short-distance behavior [25,26]. It would be an interesting question for the future, whether similar, surface-sensitive experiments in two-dimensional systems are feasible.

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APPENDIX A: EXACT RESULTS FOR THE SURFACE MAGNETIZATION

The boundary magnetization \( m_1(h_1) \) was calculated exactly by Au-Yang and Fisher [18] for the semi-infinite 2-d Ising model at the critical point, in the critical regime, and for a strip of finite width at the bulk critical point. Whereas above two dimensions a free surface near criticality is paramagnetic in the sense that the response of \( m_1 \) on \( h_1 \) is linear, it was found that in \( d = 2 \) the function \( m_1(h_1) \) is modified by logarithmic terms.

In the 2-d Ising model the surface magnetic field \( h_1 \) enters the analysis only through the variable [18]

\[
u = \tanh h_1 ,
\]

which will also play an important role in Appendix B. For \( \tau = 0 \) and small \( u \) (in which case \( u \approx h_1 \)) the asymptotic behavior of \( m_1 \) takes the form [18]

\[
m_1(h_1) \approx B_1 u (b_1 - 2 \ln u) ,
\]

where \( B_1 = 1.5369 \ldots \) and \( b_1 = -1.3201 \ldots \) are constants. There is an exact formula available for \( m_1(h_1) \) (see Eqs. (2.10) and (2.11) of Ref. [18]) but the asymptotic result (A2) was sufficient for carrying out the scaling analysis in Sec. II B. In Sec. II IB, we compare our MC data for \( m_1 \) with the exact result. The lesson learned from (A2) is that in \( d = 2 \) and in semi-infinite geometry the dependence of \( m_1 \) and \( h_1 \) is not simply linear but modified by a logarithmic term: For small \( h_1 \) the surface magnetization behaves as \( h_1 \ln h_1 \). This was not taken into account in Ref. [5], where we focussed on the short-distance behavior in \( d = 3 \).
In the critical region, for $\tau > 0$, the leading contribution to the surface magnetization is given by

$$m_1(h_1, \tau) = B_1 u \left[ \ln(2K_c \tau) + \mathcal{B}(\tau/u^2) \right].$$

(A3)

This tells us that slightly above the critical point the dependence of $m_1$ on $h_1$ is indeed linear, but, different from the situation in $d > 2$, there is a (logarithmic) dependence on the temperature $\tau$. The scaling function $\mathcal{B}$ approaches a constant for $\tau/u^2 \to 0$ and asymptotically goes as $\sim \ln(\tau/u^2)$ for $\tau/u^2 \to \infty$, leading back to (A2).

In Ref. [18] the function $m_1(h_1)$ was also calculated for a strip of finite width $N$ and infinite lateral extension at the (bulk) critical point. This result is of interest for the comparison with our MC data. Similarly to the case $\tau > 0$, the logarithmic term in the limit $u \to 0$ is absent in the strip. The leading contribution can be written in the form

$$m_1(h_1) = B_1 u \left( b_1^* + c_1^* N^{-1} + \ln N \right),$$

(A4)

where $b_1^* = 1.0731 \ldots$ and $c_1^* = \sqrt{2}/2$. Thus, as in (A3) the dependence on $h_1$ is linear, with an $N$-dependent amplitude $\sim \ln N$. Taking this into account in the scaling analysis, it leads to an $N$-dependent amplitude in the profile, an effect that is clearly visible in Figs. 2, 7 and 8, where the profiles for different system sizes were plotted.

**APPENDIX B: EXACT RESULTS FOR THE MAGNETIZATION PROFILE**

In a work by Bariev [19], the local magnetization of the semi-infinite 2-d Ising model with surface magnetic field was represented in terms of a series of multiple integrals. For the system we consider [27] this solution can be written in the form

$$m(n, K, h_1) = \left( 1 - S^2 \right)^{1/8} \mathcal{F}(2n/\xi, l_1/\xi),$$

(B1)

where $S = \sinh(2K)$, the integer $n$ counts the distance (number of spin columns) from the boundary starting with $n = 1$, and $\xi$ is the correlation length defined by

$$\xi = \sqrt{\frac{S}{2}} \frac{1}{1 - S}.$$  

(B2)

The dimensionless variables $K$ and $h_1$ were defined in (3).

The length scale $l_1$ occurring in (B1) represents the distance up to which the short-distance behavior (8) is found. It is explicitly given by [19]

$$l_1 = \frac{\tanh(K)}{2} \frac{1}{u^2}.$$  

(B3)

The main result of Ref. [19] is the scaling function $\mathcal{F}(x, y)$ in (B1) expressed in form of a series of multiple integrals, with distinct solutions above and below the critical temperature.
Since we are interested in the case \( T > T_c \), we here only show the result for the former case. The solution for the scaling function takes the form \[ F(x, y) = \frac{y}{\sqrt{y^2 + 2}} \exp(-x/2) \exp\left(\sum_{k=1}^{\infty} \frac{1}{k} f_k(x, y)\right), \tag{B4a} \]
with
\[
f_k(x, y) = -\frac{1}{\pi^k} \int_0^\infty dw_1 \ldots \int_0^\infty dw_k \prod_{l=1}^k \exp[-x \cosh(w_l)] \times \frac{\cosh(w_l) - 1}{\cosh(w_l) + \cosh(w_{l+1})} \frac{\cosh(w_l) - 1 - y^2}{\cosh(w_l) + 1 + y^2}, \quad w_{k+1} = w_1, \tag{B4b} \]
where we abbreviated \( \cosh \equiv \cosh \).

Several explicit asymptotic solutions were given in Ref. \[19\]. The case \( z < l_1 < \xi \) was not considered, however. Also we ourselves were not able to obtain an explicit solution in the limit where \( \xi \) goes to infinity by \( z/l_1 \) remain at some finite value, the case, where the anomalous short-distance behavior discussed in Sec. II B shows up most clearly. The so far only available explicit exact solution that is consistent with our findings is given by Eq. (28) of Ref. \[19\]. It says that, asymptotically for \( x \ll 1 \) and in the limit \( y \to 0^+ \), the scaling function \( \text{(B4a)} \) is given by
\[
F(x, 0^+) = E_3 |\ln(x/4) + 1| x^{3/8} \left[ 1 + \frac{3}{4} x + O(x^2 \ln x) \right] \tag{B5} \]
with the constant \( E_3 = 0.6987 \ldots \)

The asymptotic result \( \text{(B5)} \) is in agreement with our scaling analysis, which itself provides a deeper understanding of the functional form of \( \text{(B5)} \). Firstly, the exponent \( 3/8 \) occurs and can be attributed to the difference of scaling dimension as discussed in Sec. II B. Secondly, a logarithmic factor shows up, now with an argument \( \sim z/\xi \) instead of \( \sim z/l_1 \), however. That effectively \( \xi \) replaces \( l_1 \) for \( l_1 \to \infty \) can be understood on the basis of our scaling analysis and the results reported in Appendix I, since, as Eq. (A3) tells us, there is no logarithmic dependence of \( m_1 \) on \( h_1 \) for \( h_1 \to 0 \) and finite \( \xi \).

In order to obtain profiles for the whole crossover region between the fixed points, one has to compute the multiple integrals occurring in \( \text{(B4b)} \) numerically to some finite order in the series. The series converges rather quickly such that in most cases the termination after the third term is sufficient. Only very close to the surface corrections due to higher orders become appreciable.

We evaluated \( \text{(B4)} \) numerically for \( K = 0.9999 K_c \). The corresponding correlation length is \( \xi = 567 \) (lattice spacings). In Fig. 9 the results for the order-parameter profiles with the same values of \( h_1 \) as used in Figs. 4 and 5 are displayed in double-logarithmic representation \( (z \equiv n - 1) \). Again the power law \( \sim z^{-1/8} \) is displayed for comparison. The resemblance between the MC results shown in Fig. 5 and the curves of Fig. 9 is striking. One has to bear in mind, however, that in the former case the crossover to the exponential decay was caused by finite-size effects. In Fig. 9, on the other hand, it is attributable to the finite correlation
Fig. 9: Order-parameter profiles calculated from Bariev’s solution Eq. (B4) for the semi-infinite 2-d Ising model, with $K/K_c = 0.999$, and for the same values of $h_1$ as in Fig. 4.
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Below the upper critical dimension \( d^* \), the scaling relation \( y_1 + x_1 = d - 1 \) between the operator dimensions holds. In the 2-d Ising model \( y_1 = 1/2 \) such that \( x_1 \) takes the same value, \( x_1 = 1 - y_1 \). In general \( x_1 \) and \( y_1 \) have different values.

In Ref. [19] a slightly more general system with different coupling strengths in directions parallel and perpendicular to the surface was examined. We restrict our presentation to the isotropic case.