Surface critical exponents at a discontinuous bulk transition

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Systems with a bulk first-order transition can display diverging correlation lengths close to a surface. This surface induced disordering yields a special type of surface criticality. Using extensive numerical simulations we study surface quantities in the two-dimensional Potts model with a large number of states q which undergoes a discontinuous bulk transition. The surface critical exponents are thereby found to depend on the value of q, which is in contrast to prior claims that these exponents should be universal and independent of q. It follows that surface-induced disordering at first-order transitions is characterized by exponents that depend on the details of the model.

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I. INTRODUCTION

The presence of a surface is well known to change locally the critical properties at an equilibrium critical point.[1–5] At the so-called ordinary transition, where only the bulk correlation length diverges, this breaking of spatial translation invariance yields a surface universality class characterized by a set of critical exponents that differ from the corresponding bulk critical exponents. This change of local critical exponents due to the presence of a surface is not restricted to equilibrium phase transitions, but has recently also been revealed at a dynamic phase transition.[6] In addition, enhanced surface couplings in three-dimensional systems may result in a variety of surface phase transitions. Whereas at the special point both the bulk and the surface are critical, at the so-called surface transition only the surface orders whereas the bulk remains disordered. Finally, at the extraordinary transition the bulk orders in the presence of an ordered surface. Additional phenomena, for example, critical wetting, are encountered when external fields are applied.[7]

A special kind of surface critical phenomenon can be encountered in situations where the bulk undergoes a first-order phase transition.[8–13] Due to surface-induced disordering the surface order parameter may go continuously to zero when one approaches the bulk transition temperature from below; i.e., one has a first-order transition in the bulk but a second-order transition at the surface. This surface critical behavior, which is coupled to an interface delocalization phenomenon, is characterized by a set of surface critical exponents. This general scenario has been verified for a range of systems, for example, an effective interface model,[14] face-centered-cubic Ising antiferromagnets,[15,16] body-centered-cubic alloys,[17,18] or two-dimensional Potts models undergoing a discontinuous bulk phase transition.[19,20]

Related surface (or, more appropriately, interface) phenomena are also encountered in nonequilibrium situations where magnetic systems are sheared or magnetic blocks are moved passed each other, thereby giving rise to magnetic friction.[21–26] When the involved bulk systems have an equilibrium first-order transition, as is the case for two-dimensional and three-dimensional Potts systems with a large number of states, nonequilibrium surface transitions of different types (continuous, discontinuous, and tricritical) emerge.[23,26]

Early on, the values of the different local exponents at surface-induced disordering were determined within Landau theory.[9–11] Surface exponents were also determined in an effective interface model that incorporates fluctuations by expanding around the mean-field solution.[14] However, until now only very few attempts have been made to compute for specific systems the surface critical exponents at a discontinuous bulk transition. For instance, in numerical simulations of both face-centered-cubic[16] and body-centered-cubic[18] alloys nonuniversal exponents were observed at surface-induced disordering. In a study[20] of the two-dimensional Potts model, which undergoes a first-order phase transition when the number of states q is larger than 4, the surface exponents were computed exactly in the $q \longrightarrow \infty$ limit. In addition, systems with $q = 7$, 8, or 9 states were studied numerically for small stripes with mixed boundary conditions using Density Matrix Renormalization Group (DMRG). After the data obtained for stripes with width less than 40 rows was extrapolated to infinity, it was concluded that the corresponding surface exponents were universal and identical to those of the $q \longrightarrow \infty$ case.

In this paper we are revisiting surface-induced disordering in the two-dimensional Potts model. Using extensive numerical simulations, we study large systems with up to $q = 100$ states. Our numerical data for a variety of quantities and boundary conditions show in a consistent way that the surface exponents at the bulk first-order transition depend on the number of states. Therefore, while the general scenario of surface-induced disordering is correct, the phenomenon does not yield universal surface exponents, but instead the values of these exponents are nonuniversal and depend on microscopic details like the number of states.

Our paper is organized in the following way. We introduce the model and the quantities of interest in the next section, before briefly reviewing in Sec. III some of the general results obtained for surface-induced disordering, as far as they are relevant for our study. In Sec. IV we present our numerical results and obtain the values of different surface exponents. As we show, the different quantities yield a consistent picture indicating that the surface exponents at the first-order transition in the two-dimensional Potts model depend on the number of states and are therefore not universal. Finally, in Sec. IV we discuss our results and conclude.

II. MODEL AND QUANTITIES

In the following we study the ordering of the two-dimensional Potts model in the presence of a surface, characterized by the Hamiltonian

$$\mathcal{H} = -J_b \sum_{\text{bulk}} \delta(s_{x,y} - s_{x',y'}) - J_s \sum_{\text{surface}} \delta(s_{x,y_s} - s_{x',y_s}), \quad (1)$$

where $\delta(\cdots)$ is the Kronecker δ, with $\delta(x) = 1$ if $x = 0$ and $\delta(x) = 0$ otherwise. In this Hamiltonian the first term describes the interaction between nearest-neighbor Potts spins where at least one of them does not belong to the surface, whereas the second term is the interaction between nearest-neighbor spins that are both located at the surface row y_s. The ferromagnetic bulk and surface coupling constants are given by $J_b > 0$ and $J_s > 0$. Throughout this study we only consider the case $J_s = J_b = J$. Temperatures are measured in units such that $J/k_B = 1$, where k_B is the Boltzmann constant.

Our focus is on cases where the bulk transition is of first order.[27] For that reason we consider at every lattice site (x,y) a Potts spin $s_{x,y}$ that can take on q values, $s_{x,y} = 1, \ldots, q$, with $q > 4$. We thereby probe a wide range of q values, namely, $q = 5, 9, 16$, and 100.

We consider systems composed of $L \times M$ spins, where the values of L and M used in our study are discussed below. We always consider periodic boundary conditions in the x direction. Most of our quantities are obtained for free boundaries in the y direction, yielding systems with two surfaces located at $y = 1$ and $y = M$. In order to make a connection with the data discussed in Ref. 20, we also investigate some systems with symmetry-breaking boundary conditions where the spins along one of the surfaces are at a fixed common value.

Due to the presence of surfaces, local quantities depend on the row index y (Refs. 1–5). Our quantities of interest include the local magnetization, $m(y)$, the surface excess magnetization, m_s, and the spin-spin correlations along and perpendicular to the surface, $C_{ss}(x)$ and $C_{sb}(y)$, respectively, where the index s (b) indicates a surface (bulk) spin.

The magnetization of row y is given by

$$m(y) = (qN_m(y)/L - 1)/(q - 1), \quad (2)$$

where $N_m(y)$ is the average number of majority spins in that row: $N_m(y) = \max(N_1(y), \ldots, N_q(y))$, with $N_k(y)$ being the average number of spins in state k in row y. The surface magnetization m_1 is given by $m_1 = m(1)$ (which equals $m(M)$ in the case of free boundary conditions). From the magnetization profile we can derive the so-called surface excess magnetization associated with the surface located at $y = 1$:

$$m_s = \sum_{y=1} [m_b - m(y)], \quad (3)$$

where m_b is the bulk magnetization. When approaching the q-dependent bulk transition temperature $T_c(q) = 1/\ln(1 + \sqrt{q})$ from below, both the surface magnetization and the surface excess magnetization are displaying close to $T_c(q)$ an algebraic behavior as a function of

temperature:[9,11]

$$m_1 \sim [(T_c(q) - T)/T_c(q)]^{\beta_1}, \quad (4)$$

$$m_s \sim [(T_c(q) - T)/T_c(q)]^{\beta_s}, \quad (5)$$

with the critical exponents β_1 and β_s, respectively.

Surface induced disordering is an anisotropic critical phenomenon, governed by two different correlation length exponents $\nu_\parallel$ and $\nu_\perp$ for correlations parallel and perpendicular to the surface.[10] The corresponding temperature-dependent correlation lengths $\xi_\parallel$ and $\xi_\perp$ can be obtained from the surface-surface and surface-bulk correlators:

$$C_{ss}(x) = \frac{q}{q-1} \left\langle \delta(s_{1,1} - s_{x,1}) - \frac{1}{q} \right\rangle - m_1^2$$
$$\sim \exp(-x/\xi_\parallel), \quad (6)$$

$$C_{sb}(y) = \frac{q}{q-1} \left\langle \delta(s_{1,1} - s_{1,y}) - \frac{1}{q} \right\rangle - m_1 m(y)$$
$$\sim \exp(-y/\xi_\perp), \quad (7)$$

with

$$\xi_\parallel \sim [(T_c(q) - T)/T_c(q)]^{-\nu_\parallel}, \quad (8)$$

$$\xi_\perp \sim [(T_c(q) - T)/T_c(q)]^{-\nu_\perp}, \quad (9)$$

close to $T_c(q)$.

Our aim in the following is to obtain values for the critical exponents β_1, β_s, $\nu_\parallel$, and $\nu_\perp$ as a function of the number of states q. In order to do so we combine two complementary approaches. In the first approach we determine our quantities as a function of temperature and calculate from these data effective exponents that yield the critical exponents in the limit $T \longrightarrow T_c(q)$ (Refs. 5 and 28). For example, for the surface magnetization m_1 we obtain the effective surface exponent via the logarithmic derivative

$$\beta_{1,\text{eff}}(t) = \frac{d \ln m_1}{d \ln t}, \quad (10)$$

with the reduced temperature $t = (T_c(q) - T)/T_c(q)$. We then have

$$\beta_1 = \lim_{t \longrightarrow 0} \beta_{1,\text{eff}}(t). \quad (11)$$

For this approach only data not affected by finite-size effects should be used, which requires the comparison of systems of different sizes. For that reason we study large ranges of L and M, ranging from $L = 80$ to $L = 1280$ and from $M = 40$ to $M = 320$. In the second approach we try to use finite-size effects to our advantage. Following Ref. 20, we consider the surface magnetization at the exactly known bulk transition temperature $T_c(q)$, using symmetry-breaking boundary conditions. For a system with $L = \infty$ and width M, the surface magnetization should then depend algebraically on the scaling dimension $x_1 = \beta_1/\nu_\perp$, i.e., $m_1 \sim M^{-x_1}$. In order to mimic a stripe of infinite length we study systems with L up to $L = 64\,000$. As a drawback, only stripes with rather small widths M can be simulated. Still, comparing our estimates

for the scaling dimension with the independently determined values of β_1 and $\nu_\perp$ using temperature-dependent quantities provides us with an important check whether our different data sets are consistent.

III. SCALING IN THE PRESENCE OF SURFACE-INDUCED DISORDERING

When the bulk undergoes a continuous phase transition, as is, for example, the case for the Ising model, then the surface critical exponents and the relationship between these exponents can be derived from the scaling form of the singular part of the surface free energy.[1–3] As shown in Ref. [10] a similar phenomenology holds in the case of surface-induced disordering. Indeed, as a function of the two scaling fields t (the reduced temperature) and h_1 (a surface field), the singular part of the surface free energy may be written as[10]

$$f_s = |t|^{2-\alpha_s} \Omega(|t|^{-\Delta_1} h_1), \tag{12}$$

with the two independent surface exponents α_s and Δ_1. All surface critical exponents can then be expressed through these two independent exponents. Specifically for some of the exponents at the center of our study one obtains the following:[10]

$$\beta_1 = 2 - \alpha_s - \Delta_1, \tag{13}$$

$$\beta_s = 1 - \alpha_s, \tag{14}$$

$$(d-1)\nu_\parallel = 2 - \alpha_s. \tag{15}$$

Combining Eqs. (14) and (15) yields for two-dimensional systems with $d = 2$ the relationship

$$\nu_\parallel = 1 + \beta_s, \tag{16}$$

which provides an additional check for the consistency of our data.

IV. RESULTS

Due to the surface-induced disordering, bulk and surfaces behave remarkably differently when approaching the first-order bulk transition temperature: whereas the bulk magnetization displays a discontinuous jump at that temperature, the surface magnetization vanishes continuously. This is illustrated in Fig. 1 for two different numbers of states q through the magnetization profiles close to a surface of systems composed of 640×320 spins.

Data like those shown in Fig. 1 allow us to obtain the temperature dependence of both the surface magnetization and the surface excess magnetization (3). From the logarithmic derivative with respect to the reduced temperature $t = (T_c(q) - T)/T_c(q)$, see Eq. (10), we obtain effective exponents that in the limit $t \longrightarrow 0$ yield the values of the critical exponents. The result of this procedure is shown in Fig. 2 for (a) the surface magnetization and (b) the surface excess magnetization. As explained in Sec. II, the use of temperature-dependent effective exponents is only meaningful when data for the semi-infinite system are studied. For that reason we very carefully analyzed finite-size effects by comparing data for a
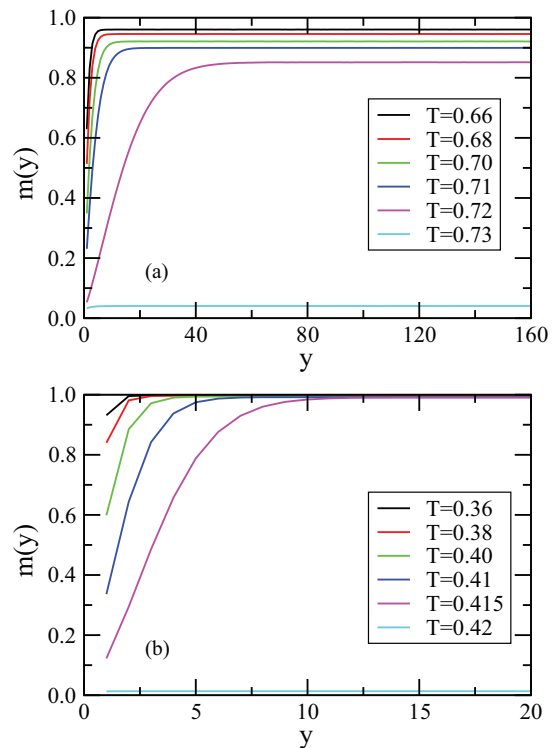

FIG. 1. (Color online) Layer magnetization density as a function of layer index y for (a) $q = 9$ states and (b) $q = 100$ states. The layer $y = 1$ is the surface layer. Approaching the bulk transition temperature from below, the surface magnetization decreases continuously, whereas deep inside the bulk the local magnetization displays a discontinuous jump. The highest temperature included is just above the corresponding bulk transition temperature. The data have been obtained for a system composed of 640×320 spins. Error bars, which result from averaging over typically ten independent runs, are of the order of the thickness of the lines.

range of different system sizes. Only data that were identical for at least two different system sizes have been retained. The curves shown in Fig. 2 for the different values of q are therefore free of any finite-size effects. We first note that the effective exponents do not display a plateau but instead keep changing as a function of the reduced temperature. This is similar to what one observes in situations where the bulk undergoes a second-order phase transition.[28] Extrapolating the data to $t = 0$, we obtain the values for the critical exponents listed in Table I. We note that the exponent β_s of the surface excess magnetization is negative, in agreement with a diverging disordered region at the bulk transition temperature.

As our systems are rather large, we manage to obtain data not affected by finite-size effects up to very close to the phase transition point. Extrapolating the data to the phase transition point itself using different functions yields slightly different values for the critical exponents. Our error bars in Table I are conservative and take these differences in the extrapolated values into account.

The results shown in Fig. 2 and Table I indicate that the surface exponents depend on the number of states q and that their values approach the exactly known value for $q \longrightarrow \infty$ (Ref. [20]) when q increases. This scenario is different from
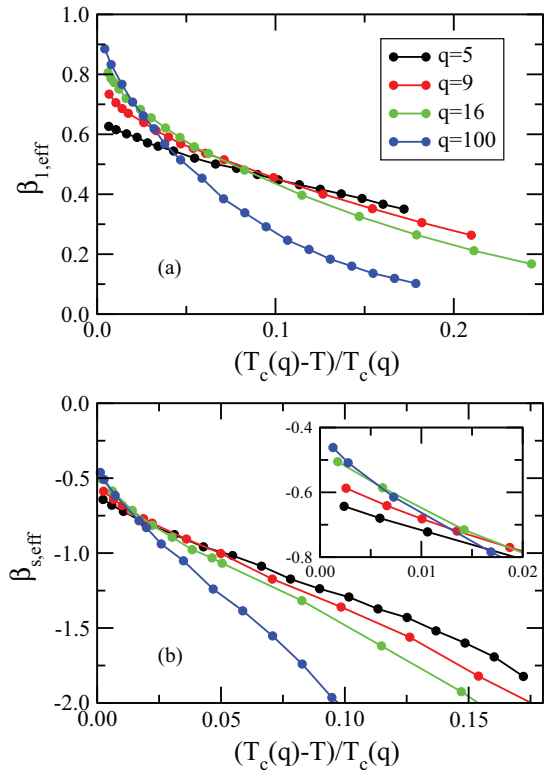
FIG. 2. (Color online) (a) Effective exponent of the surface magnetization and (b) effective exponent of the surface excess magnetization as a function of the reduced temperature $[T_c(q) - T]/T_c(q)$ for systems with different numbers of states q. Here, $T_c(q)$ is the bulk transition temperature for the model with q states. The inset in panel (b) shows a blow-up close to the transition temperature. The values of the exponents obtained from extrapolating to the transition temperature are given in Table I. Only data not affected by finite-size effects are shown. Error bars are of the order of the symbol sizes in the main figures.

that discussed in Ref. 20 where it was claimed that the surface critical exponents are independent of q and identical to the $q \longrightarrow \infty$ case. As we discuss in the following, our data show in a consistent way that the Potts surface critical exponents at a first-order bulk transition are indeed not universal.

In order to capture the expected anisotropy of the critical surface we study the surface-surface and surface-bulk correlations [see Eqs. (6) and (7)]. As shown in Fig. 3 for the example of $q = 9$ states these spatial correlations, after some short-distance regime, rapidly display an exponential

TABLE I. Surface critical exponents for two-dimensional Potts models with q states that have a first-order bulk transition.

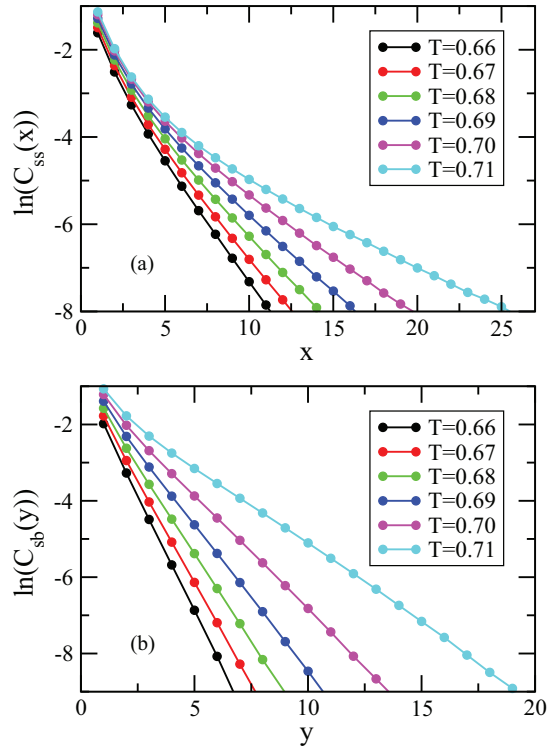| q	β_1	β_s	$\nu_\parallel$	$\nu_\perp$
5	0.64(2)	−0.63(3)	0.42(3)	0.56(5)
9	0.79(1)	−0.54(2)	0.53(4)	0.46(2)
16	0.90(2)	−0.46(3)	0.55(3)	0.43(2)
100	0.95(2)	−0.40(2)	0.59(2)	0.38(2)
∞[20]	1		2/3	1/3

FIG. 3. (Color online) (a) Surface-surface and (b) surface-bulk correlation for the $q = 9$ case and different temperatures below the bulk transition temperature. Both quantities display an exponential decay characterized by a typical temperature-dependent length (see Fig. 4). The data have been obtained for a system with 640×320 spins after averaging over at least 50 independent runs. Error bars are smaller than the size of the symbols.

dependence on the distance. The corresponding correlation lengths, see Eqs. (6)–(9), increase with temperature, as shown in Fig. 4 for the $q = 9$ and $q = 100$ cases. This figure also reveals that we are indeed dealing with strongly anisotropic
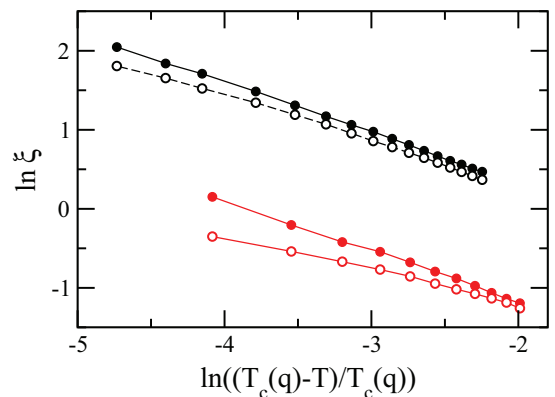

FIG. 4. (Color online) Temperature-dependent correlation lengths as obtained from the spatial correlation functions (see Fig. 3 for examples). The black (red) lines are for the $q = 9$ ($q = 100$) system, with solid (open) symbols indicating the correlation length parallel (perpendicular) to the surface. On approaching the bulk transition temperature the correlation lengths display an algebraic behavior. The values of the correlation length exponents obtained from the slopes in this figure are collected in Table I.

critical systems, governed by direction-dependent correlation length critical exponents; see Table I for our estimates for these exponents.

Table I provides strong indications that the surface critical exponents at the first-order phase transition depend on the number of states. Further support comes from the fact that we have the possibility to do some consistency checks. We first notice from Eq. (16) that the values of $\nu_\parallel$ and β_s should differ by one: $\nu_\parallel - \beta_s = 1$. From our estimates in Table I we obtain the following values for this difference: 1.05 ± 0.06 for $q = 5$, 1.07 ± 0.06 for $q = 9$, 1.01 ± 0.06 for $q = 16$, and 0.99 ± 0.04 for $q = 100$. Therefore the difference between these two exponents is marginally compatible with 1 for the smaller values of q and in full agreement with the scaling relation (16) for the larger values of q.

For a second consistency check we can try to exploit finite-size effects in order to obtain an estimate of the ratio $x = \beta_1/\nu_\perp$. We thereby follow Ref. 20 and consider at the bulk transition temperature $T_c(q)$ systems with mixed boundary conditions where at one edge we keep all the spins at a common value, whereas the other edge is a free edge. For the $q = 7$, 8, and 9 cases Iglói and Carlon[20] used the DMRG method in order to calculate the surface magnetization as a function of the width M of the system and obtained estimates for the scaling dimension $x = \beta_1/\nu_\perp$ for the $\infty \times M$ system, with M going up to 40. In our Monte Carlo simulations we can only simulate finite L. Going up to $L = 64\,000$ sites, we carefully monitor finite-size effects in that direction. Figure 5(a) shows the resulting data for the surface magnetization as a function of the stripe width M for $L = 64\,000$.

We can obtain an effective exponent x_{eff} from these data through the following logarithmic derivative:

$$x_{\text{eff}}(M) = -\frac{d \ln m_1}{d \ln M}. \tag{17}$$

Comparing effective exponents for different values of L, only those data not affected by finite-size effects have been included in Fig. 5(b). We also include as stars the data obtained in Ref. 20 for the $q = 9$ case using DMRG (see Table IV in that paper). We note that for $q = 100$ we are only able to achieve data representative for $L = \infty$ for small values of M. This figure shows as bars on the y axis the estimates for the scaling dimension x that result when using the values for β_1 and $\nu_\perp$ given in Table I. The consistency of these estimates with the effective exponents lends additional support to a q dependence of the surface critical exponents at surface-induced disordering.

V. DISCUSSION AND CONCLUSION

Systems undergoing discontinuous bulk transitions may exhibit diverging correlation lengths at surfaces due to surface induced disordering. While a variety of theoretical studies have verified this general scenario, only very few attempts have been made to determine directly surface critical exponents through numerical simulations. The results have been somewhat contradictory. Whereas DMRG results for stripes of the Potts system[20] seemed to indicate a high degree of universality, with surface exponents that do not depend on the number of states q, simulations of face-centered-cubic[16]
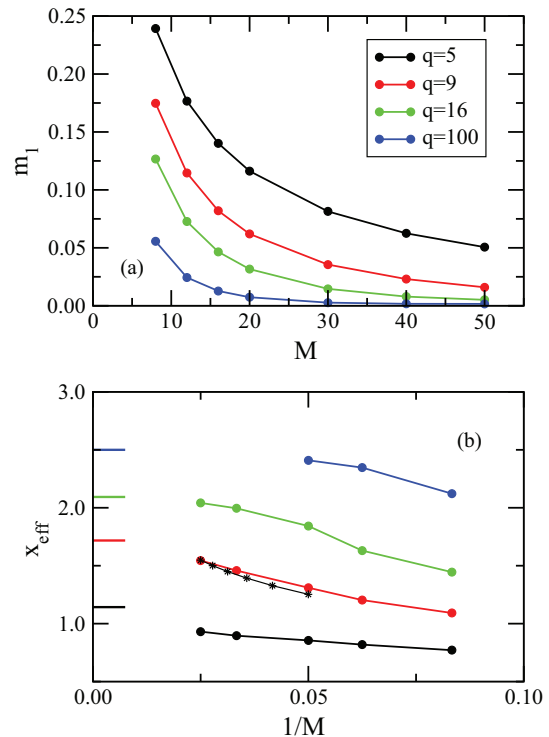

FIG. 5. (Color online) (a) Surface magnetization at the bulk transition temperature for stripes of width M where at one of the surfaces we impose fixed boundary conditions. The different curves correspond to different numbers of states q. The length of the system is $L = 64\,000$. (b) Effective scaling dimension obtained from the data shown in panel (a). Only data not affected by finite-size effects are displayed. The bars on the y axis indicate the values obtained from Table I when assuming the scaling relation $x = \beta_1/\nu_\perp$. The stars are the data given in Table IV of Ref. 20 for the $q = 9$ case using DMRG.

and body-centered-cubic[18] alloys found nonuniversal surface exponents.

In this work we have revisited the two-dimensional q-state Potts model through extensive numerical simulations. Focusing on systems with $q = 5$, 9, 16, and 100 states, we measured the time-dependent magnetization profiles as well as surface-surface and surface-bulk correlation functions. The extracted values of surface critical exponents indicate that the exponents are not universal but depend on the number of states q (see Table I). We verified that our data fulfill a scaling relation connecting the exponent of the surface excess magnetization with the correlation length exponent for correlations parallel to the surface. In addition, data obtained at the bulk transition temperature for systems with mixed boundary conditions are found to yield effective scaling dimensions that are compatible with the exponents obtained from the temperature-dependent quantities. It is this consistency of our data that provides a strong indication that the values of surface critical exponents at the first-order transition of the two-dimensional Potts model depend on the number of states q.

Still, a word of caution is in order, as it is notoriously difficult to make definitive statements for critical systems based solely on numerical results. Thus it is possible that within the accuracy of our numerical data the effective exponents

satisfy scaling laws due to the form of the (unknown) corrections to scaling while at the same time the extrapolation of the effective exponents yields inaccurate values for the critical exponents. This type of behavior has been seen, for example, in the interfacial adsorption of q-state Potts models where the interface critical exponents are universal,[29] whereas this universality is difficult to see in simulations due to subtle finite-size effects.[30]

Our results, together with those obtained in Refs. 16 and 18 for the three-dimensional alloys, indicate that the local critical exponents at surface-induced disordering are not yet completely understood. New insights could come from field-theoretical treatments along lines similar to those used to study surface criticality at a continuous phase transition.[2] We hope that our work will lead to future studies in that direction.

ACKNOWLEDGMENTS

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