Boundary and Bulk Phase Transitions in the Two Dimensional $Q > 4$ State Potts Model

Ferenc Iglói
Research Institute for Solid State Physics and Optics, H-1525 Budapest, P.O.Box 49, Hungary
Institute for Theoretical Physics, Szeged University, H-6720 Szeged, Hungary

Enrico Carlon
Institute for Theoretical Physics, Katholieke Universiteit Leuven, Celestijnenlaan 200D, B-3001 Leuven, Belgium
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The surface and bulk properties of the two-dimensional $Q > 4$ state Potts model in the vicinity of the first order bulk transition point have been studied by exact calculations and by density matrix renormalization group techniques. For the surface transition the complete analytical solution of the problem is presented in the $Q \to \infty$ limit, including the critical and tricritical exponents, magnetization profiles and scaling functions. We have shown in an accurate numerical study that the universality class of the surface transition is independent of the value of $Q > 4$. For the bulk transition we have numerically calculated the latent heat and the magnetization discontinuity and we have shown that the correlation lengths in the ordered and disordered phases are identical at the transition point.

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I. INTRODUCTION

The two-dimensional $Q$-state Potts model is an important testing ground of statistical physics for different approximate theories and numerical methods. For $Q \leq 4$ the model has a second order phase transition and the critical exponent, both in the bulk and at the surface, are $Q$-dependent as they have been predicted by conformal invariance and by Coulomb-gas methods.

On the other hand in the first order regime (i.e. $Q > 4$) there are analytical results about the properties of the system at the transition point, such as the latent heat, $\Delta E$, the discontinuity of the magnetization, $\Delta m$, and the correlation length in the disordered phase, $\xi_d$, but still some issues are unsolved. One of these is the relation between the correlation lengths in the order ($\xi_o$) and in the disordered ($\xi_d$) phase for which different theoretical approaches which predict either $\xi_o/\xi_d = 1/2$ or $\xi_o/\xi_d = 1$, where the latter is supported by recent Monte Carlo simulations.

Another unclarified problem of the $Q > 4$ model concerns the behavior of the surface phase transition. In studies of surface critical behavior most of the theoretical investigations have been focused on the so-called ordinary transition which occurs at a bulk continuous transition in absence of enhanced surface couplings and/or surface fields. In this case scaling ideas and, in two dimensions, conformal invariance are often used to predict surface critical exponents and scaling functions.

A completely different approach is necessary for systems with a discontinuous bulk phase transition, like the $Q > 4$ state Potts model, where bulk scaling and conformal invariance do not hold. It was Lipowsky who first showed, in a mean-field calculation, that one can have a first order transition in the bulk and a second order one at the surface. This phenomenon, known as surface induced disorder (SID) and closely related to the wetting phenomena, has been studied at the mean field level by means of Monte Carlo simulations and in some experimental systems, but no exact results are available on microscopic models so far.

In this paper we present exact and numerical results on surface phase transitions in the two-dimensional $Q > 4$ state Potts model. Our study is based on two complementary approaches. First, we show that there exists a systematic large $Q$ expansion of the problem, which is exactly solvable in the $Q \to \infty$ limit. We show that in this limit there is SID with a surface magnetization which vanishes continuously by approaching the bulk transition temperature and we find the exact values of the whole sets of surface exponents. At a sufficiently large value of a surface field applied to the spins at the free boundary, the surface transition becomes first order. The continuous and first order regimes are separated by a tricritical transition whose exponents are also found exactly.

The analytical results are complemented by numerical investigations based on density matrix renormalization group techniques (DMRG) through which we calculate magnetization and energy density profiles in $L \times \infty$ strips for $5 \leq Q \leq 9$. Following the approach of Ref. we restricted ourselves to moderately large values of $L$; typically we considered $L \leq 40$ and occasionally also larger systems (up to $L = 80$). We analyzed the numerically accurate data by efficient extrapolation techniques and using information of scaling functions obtained in the exact solution at $Q \to \infty$. We found again SID and strong indications that the surface exponents do not depend on the value of $Q$.

The same type of DMRG technique is used also to cal-
culate properties of the bulk transition. Here we note that for weak first-order transitions, when $Q$ is close to four, it is a challenge for numerical methods (Monte Carlo simulation, renormalization group (RG) methods, finite-size scaling, series expansion, etc.) to detect the correct order of the transition and to estimate the corresponding discontinuities. In all cases studied we found good agreement between the numerically extrapolated values and the exact results, which once again proves the powerfulness and reliability of the DMRG algorithm. The numerical calculation of the bulk correlation length in the ordered phase ($\xi_d$) for $Q = 9$ confirms with good accuracy the conjectured relation $\xi_d = \xi_o$.

The paper is organized as follows. In Section II we introduce the model, define the basic quantities and outline the use of the DMRG method for the problem. In Section III we present some numerical results concerning bulk quantities and analyze the behavior of the bulk correlation length. The surface transition of the model is studied in Section IV by analytical and numerical methods. Section V concludes the paper with some discussion.

II. FORMALISM

We consider the $Q$-state Potts model in a $L \times \infty$ square lattice defined by the Hamiltonian

$$-\beta H = K_1 \sum_{k=-\infty}^{\infty} \sum_{l=1}^{L-1} \delta(s_{l,k} - s_{l+1,k}) + K_2 \sum_{k=-\infty}^{\infty} \sum_{l=1}^{L} \delta(s_{l,k} - s_{l,k+1}),$$

in terms of a $Q$ component spin variable $s_{l,k} = 1, 2, \ldots, Q$. We use for the inverse temperature $\beta = 1$ and consider the ferromagnetic model $K_1, K_2 > 0$, where the transition temperature is given from a duality relation as:

$$(e^{K_1} - 1) (e^{K_2} - 1) = Q.$$  

We work in the transfer matrix formalism, with the transfer matrix along the strip given by

$$T = \exp \left[ \frac{K_1}{Q} \sum_{l=1}^{L} \sum_{q=1}^{Q-1} M_l^q \right] \times \exp \left[ K_2 \sum_{l=1}^{L-1} \left( \delta(s_l - s_{l+1}) - \frac{1}{Q} \right) \right],$$

where $M_l$ is a spin-flip operator: $M_l |s_l\rangle = |s_l + 1, \mod Q\rangle$ and $K_1^*$ is the dual coupling defined as $(e^{K_1} - 1)(e^{K_1^*} - 1) = Q$, thus at the critical point $K_1^* = K_2$.

Different physical quantities of the model can be expressed by the leading and next to leading eigenvalues of $T$, $\Lambda_0$ and $\Lambda_1$, respectively, and by the corresponding dominant eigenvector $|v_0\rangle$. For example one obtains for the magnetization profile

$$m_l = Q \langle v_0 | \delta(s_l - 1) | v_0 \rangle - 1, \quad Q - 1,$$

and for the energy density

$$\epsilon_l = \langle v_0 | \delta(s_{l,k} - s_{l+1,k}) | v_0 \rangle.$$  

The correlation length along the strip is given by

$$\xi_{||} = \log^{-1}(\Lambda_0/\Lambda_1).$$

In what follows we use symmetry breaking boundary conditions (BC) and fix spins along one of the surfaces to the same state $s_{1,k} = 1$, $k = 0, \pm 1, \ldots$ and at the other surface of the strip we apply a surface field of the form $-\beta H \sum_{k} \delta(s_{L,k} - 1) - 1/Q$.

In the transfer matrix approach one needs to diagonalize the transfer matrix, which is technically very demanding, since the dimension of the matrix being $Q^{L-1} \times Q^{L-1}$ grows very rapidly with the width of the strip. With the traditional finite size scaling methods based on the use of the Lánçzos algorithm one can only treat very limited range of the values of $L$, especially for not too small $Q$-s. This limitation is the reason why density profiles and surface quantities have not been studied following this method. Another possibility is the representation of the Potts variables in terms of Temperly-Lieb (TL) operators. This has the advantage that the transfer matrix dimension does not depend on $Q$, which enters in the calculation as a parameter, therefore this representation could be suitable for studying large $Q$. However quantities as density profiles cannot be directly expressed by the TL operators. For the study of these quantities one should then use the DMRG in the original Potts representation.

In a previous paper hereafter referred to as Paper I, we have used the DMRG method for the $Q \leq 4$ Potts models to study the critical properties, such as density profiles, Casimir amplitudes and critical exponents. Here we extend the investigations to the first order transition regime with $Q > 4$.

The principle and the technical details of the DMRG method are well documented in the literature and its application to the $Q$-state Potts model is described in I. Here we just mention that in the DMRG method a strip of large width $L$ is described by an approximated transfer matrix as represented in Fig. 1(a), where the rectangles denotes blocks containing a large number of spins, but described by only $m$ states. For the Potts model the total dimension of the matrix would be $m^2 Q^2 \times m^2 Q^2$. Although $m$, the number of states kept, can be small (typically $m \sim 100$) the algorithm provides accurate results even for large $L$. For a strip of given width, as $Q$ increases, one needs to increase $m$ in order to have sufficient accuracy. This limits the range of values of $Q$ that can be investigated with this method. Therefore
for the $Q = 9$ model we have implemented a method, which in principle can be used for $Q = 2^2, 3^2, 4^2, \ldots$, and which considerably speeds up the numerical computation. It consists in rewriting the original Hamiltonian for the $Q = q^2$-Potts model as a $q$-Potts model with plaquette and further neighbor interactions as illustrated in Fig. 1(b). Two neighboring $q$-spins (or pseudospins) in a row form a $Q$-spin; in terms of these new variables which we indicate as $\hat{s}_{i,j}$ the Hamiltonian takes the following form:

$$-\beta H = K_1 \sum_{k=\infty}^{L-1} \sum_{l=1}^{L-1} \delta(\hat{s}_{2l-1,k} - \hat{s}_{2l+2,k})\delta(\hat{s}_{2l,k} - \hat{s}_{2l+1,k})$$

$$+ K_2 \sum_{k=\infty}^{L} \sum_{l=1}^{L} \delta(\hat{s}_{l,k} - \hat{s}_{l,k+1})\delta(\hat{s}_{2l,k} - \hat{s}_{2l+1,k}) . \quad (7)$$

When the DMRG algorithm is applied to this Hamiltonian one deals with matrices of dimension $m^2Q \times m^2Q$, and the number of states kept in the blocks can be enlarged, with respects of the original representation. Comparisons of the standard and pseudo-spin version for the $Q = 9$ case indicate that the latter provides a remarkable increase in computational speed and accuracy. We also point out that a similar idea has been applied recently to study of quantum systems with a large number of states per site.

![Figure 1](image1.png)

**FIG. 1.** (a) Schematic view of a transfer matrix element as generated by the DMRG algorithm; the blocks describe approximately a large number of spins using $m$ states only. (b) Pseudospin version of the $Q = q^2$ Potts model as described in the text; two $q$ spins grouped by the dashed ellipses form a $Q$ spin and interactions are defined on plaquettes and between further neighbors along the row as indicated in the figure.

Before closing this section we turn back to the transfer matrix in (3), which in the vicinity of the critical point can be simplified in the anisotropic or Hamiltonian limit of strong vertical and weak horizontal couplings where both $K_1$ and $K_2$ are small. Then one can combine the exponentials to obtain $T = \exp(-K_2\mathcal{H})$ with a Hamilton operator

$$\mathcal{H} = -\sum_{l=1}^{L-1} \delta(s_l - s_{l+1}) - h \sum_{l=1}^{L} \sum_{q=1}^{Q-1} M^q_l , \quad (8)$$

up to a constant term and $h = K_1^2/K_2Q$. Thus at the critical point $h_c = 1/Q$.

In this Hamiltonian version of the model quantities of physical interest are derived from the ground state wavefunction $|\Psi_0\rangle$ and from the ground state and first excited state energies $E_0$ and $E_1$. In the anisotropic limit the transfer matrix and the Hamilton operator commute, $[T, \mathcal{H}] = 0$; the corresponding eigenvectors are the same, $|\Psi_0\rangle = |v_0\rangle$, consequently the density profiles in Eqs. (4) and (5) stay in the same form. On the other hand the correlation length along the strip is now expressed by the inverse gap

$$\xi_\parallel = 1/(E_1 - E_0) , \quad (9)$$

instead of Eq. (4). In the Hamiltonian version the symmetry breaking BC are equivalent to fix one of the surface spins to the state $|s_1\rangle = |1\rangle$ and to add a term $-H_s|\delta(s_{L-1} - 1)/Q\rangle$ to $\mathcal{H}$ in (8) in order to study the effect of a surface field $H_s$ on the system. This Hamiltonian version of the model will be used to solve the surface properties of the model in the $Q \to \infty$ limit.

### III. BULK TRANSITION

In this Section we consider the isotropic model, $K_1 = K_2$, and present numerical results about the bulk transition obtained by the DMRG method for $5 \leq Q \leq 9$. Our aim in calculating the latent heat and the magnetization discontinuity is to demonstrate the accuracy of the DMRG approach. On the other hand we used the numerical results about the correlation length in the ordered phase at the transition point to analyze the ratio $\xi_o/\xi_d$.

We start with the calculation of the latent heat, $\Delta E$, which is just the difference in the energy densities in the ordered and the disordered phases at the transition point $\Delta E = \epsilon_o - \epsilon_d$. The arithmetic average of the above two energy densities is the energy per bond, $\epsilon = (\epsilon_o + \epsilon_d)/2$, which is known from self-duality at the transition point

$$\epsilon = \frac{1}{2} \left( 1 + \frac{1}{\sqrt{Q}} \right) . \quad (10)$$

Consequently it is enough to calculate the energy density in the ordered phase and the latent heat then follows as:

$$\Delta E = 2(\epsilon_o - \epsilon) . \quad (11)$$

To estimate $\epsilon_o$ we have considered $L \times \infty$ systems with fixed spin BC at both edge of the strip and calculated by the DMRG method the energy density in (1) at the
middle of the strip, \( \epsilon_{L/2} \), for a series of the lengths \( L = 8, 12, 16, \ldots, L_{\text{max}} \). We selected moderately large finite systems, \( L_{\text{max}} \sim 40 - 80 \), so that the DMRG data are still accurate enough (with a relative accuracy of \( 10^{-5} - 10^{-6} \)) to use sophisticated series extrapolation procedures, such as the BST algorithm. As we have shown in paper I, this type of combination of the DMRG method and the finite-size extrapolation methods results in accurate data in the thermodynamic limit. (In a very recent corner transfer matrix DMRG calculation of the latent heat of the \( Q = 5 \) Potts model Nishino and Okunishi[26] used another strategy and performed the calculation for several thousand of layers without using series extrapolation algorithms.) To demonstrate the accuracy of our approach we show in Table I the BST extrapolants for the latent heat of the \( Q = 8 \) model. As seen in this Table the extrapolants seem to converge to a value of \( \Delta L(Q = 8) = 0.242(2) \), which is fairly close to the exact value 0.2432. Results of the extrapolated latent heats for \( Q = 5, 6, 8 \) and 9, together with the exact values are presented in Table III. It is seen that the DMRG method combined with series extrapolation techniques predicts the right order of the transition and the estimated latent heats are in good agreement with the exact results, even for \( Q = 5 \). As expected, the accuracy of the numerical results is lower for weakly first order transitions, i.e. which are characterized by a small latent heat.

Next we turn to calculate the magnetization discontinuity, \( \Delta m \), at the transition point. Since the magnetization in the disordered phase is zero \( \Delta m \) is just the bulk magnetization in the ordered phase. This can be estimated from the magnetization profile in \( \epsilon_{L} \) in the middle of the strip, \( m_{L/2} \), with fixed spin BC at both edges of the strip. As for the latent heat we have calculated \( m_{L/2} \) for a series of moderately large \( L \)-s by the DMRG method and then performed an extrapolation with the BST procedure. The estimated values of \( \Delta m \) in the ordered phase which is characterised by the Hamiltonian in (8) and use the analytical results obtained for the critical singularities and scaling functions, as a help for the \( Q \rightarrow \infty \) limit.

Finally, at the bulk transition point we have calculated the correlation length in the ordered phase, \( \xi_{o} \), for \( Q = 9 \), since for smaller \( Q \)-s the correlation length exceeds the available size of the strip.

Figure 2 shows a plot of the correlation length \( \xi_{o}(L) \) for \( Q = 2, 3, 5 \) and 9, calculated from the ratio of the largest and the second largest eigenvalues of the transfer matrix in Eq. (1). The \( Q = 2 \) and 3 cases follow the expected behavior derived from conformal invariance for a strip with fixed and equal spins at the boundary, i.e. \( \xi_{o}(L) \sim L/(2\pi) \). Notice that also in the \( Q = 5 \) case \( \xi_{o}(L) \) follows a straight line with the same slope as for the \( Q = 2 \) and 3. The transition, as pointed out above, is only weakly first order in the case \( Q = 5 \) with a correlation length much larger than the largest system size available here. The data for \( Q = 9 \) show a clear sign of saturation for large \( L \). The extrapolation to \( L \rightarrow \infty \) has been performed by the BST method and yields \( \xi_{o} = 15.0(4) \). This quantity is in good agreement with the exactly known correlation length of the disordered phase which is \( \xi_{d} = 14.94 \). These results corroborate the recent conjecture of Ref. 3, namely that \( \xi_{o} = \xi_{d} \), based on results from Monte Carlo simulations.

**IV. SURFACE TRANSITION**

The surface transition of the model is studied by two complementary methods. First, we present the analytical solution of the problem in the \( Q \rightarrow \infty \) limit, then the transition for finite \( Q \)-s are studied numerically by the DMRG method. Also in this numerical part of the work we use the analytical results obtained for \( Q \rightarrow \infty \) about the critical singularities and scaling functions, as a help in analyzing the DMRG data.

**A. Analytical solution in the \( Q \rightarrow \infty \) limit**

Here we work with the anisotropic version of the model, which is characterised by the Hamiltonian in (8) and use the BC described below (9), i.e. fixed spin at \( i = 1 \) and a surface field of strength \( H_{s} \) in the other end, \( i = L \). (For a free surface we have \( H_{s} = 0 \).)

The Hamiltonian \( \mathcal{H} \) is represented by a matrix of dimensions \( Q^{L-1} \times Q^{L-1} \), which can be further reduced in
a block-diagonal form by making use of the symmetries of the problem. The dimension of the block which contains the ground state (and also the first excited state) is independent of the value of $Q$. For small systems, $L = 2$ and $L = 3$, this block, which has the highest symmetry, has been explicitly constructed in the Appendix. Analyzing the structure of this ground-state block one can notice further simplifications in the vicinity of the critical point, where one can perform a large $Q$ expansion, such that the corrections to the leading behaviour are of $O(Q^{-1/2})$. As shown in the Appendix in the limit $Q \to \infty$ the ground-state block has a dimension of $L$ with an eigenvalue matrix $\tilde{H}$ given by

$$\tilde{H} = -(L-1) - h\sqrt{Q} \begin{pmatrix} h_s & 1 & 0 \\ 1 & t & 1 \\ 0 & 1 & (L-1)t \end{pmatrix}.$$ \tag{12}

Here $t = (hQ - 1)/h\sqrt{Q}$ measures the distance from the bulk transition point and $h_s = \tilde{H}_s/h\sqrt{Q}$. Denoting the components of the eigenvectors of $\tilde{H}$ as $\psi_i(n)$ with $n = 1, \ldots, L$ one can express the magnetization profile in terms of the ground state wavefunction as follows:

$$m_l = \sum_{n=1}^{L+1-l} |\psi_0(n)|^2. \tag{13}$$

At the transition point $t = 0$ the matrix (12) is exactly diagonalizable with eigenvectors

$$\psi_i(n) = A_i \sin[k_i(L+1-n)], \tag{14}$$

and eigenvalues

$$E_i = -(L-1) - 2h\sqrt{Q}\cos k_i, \tag{15}$$

where $i = 0, 1, \ldots, L-1$ and the wavenumbers $k_i$ are determined by the equation:

$$h_s \sin(Lk_i) = \sin[(L+1)k_i]. \tag{16}$$

As known by standard analysis the spectrum and the ground state of $\tilde{H}$ have different properties for $h_s < 1$ and $h_s > 1$, respectively. In the following we treat the different regions of surface transition separately.

1. Critical surface transition regime - $h_s < 1$

For $h_s < 1$ there are $L$ real solutions of Eq. (16) and the spectrum of $\tilde{H}$ is quasi-continuous. The qualitative behaviour of the surface transition is the same in the whole region, therefore we consider here the free surface case, $h_s = 0$, when the the solution of (16) is given explicitly as:

$$k_i = \frac{\pi(i+1)}{L+1}, \quad h_s = 0, \tag{17}$$

and the normalization in (14) is $A_i = [2/(L+1)]^{1/2}$.

The boundary magnetization from (13) is given by:

$$m_s = m_L = \frac{2}{L+1} \sin^2 \left( \frac{\pi}{L+1} \right) \sim L^{-3}, \tag{18}$$

thus it goes zero at the bulk transition point, $t = 0$. Consequently the surface phase transition is of second order, furthermore the anomalous dimension of the surface magnetization operator is

$$x_{s}^{cr} = 3, \tag{19}$$

as obtained from the finite size dependence in (18).

The magnetization profile from (13) can also be evaluated, which in the continuum approximation $L, l \gg 1$ and as a function of the distance from the free surface, $\Delta l = L + 1 - l$, is given by

$$m_{\Delta l} = \frac{\Delta l}{L} - \frac{1}{2\pi} \sin \left( \frac{2\pi \Delta l}{L} \right) \sim \left( \frac{\Delta l}{L} \right)^3 + O \left( \left( \frac{\Delta l}{L} \right)^5 \right), \quad h_s = 0.$$ 

This profile is shown as a solid line in Fig. 3.

FIG. 3. Magnetization profiles of the $Q \to \infty$ Potts model at the bulk transition point with fixed spin BC at $l = 1$ and with different values of the surface field, $h_s$, at $l = L$. Solid line - critical surface transition, $h_s = 0$; dotted line - tricritical surface transition, $h_s = 1$; dashed line - first order surface transition, $h_s > 1$. 


In a strip of width $L$ the correlation length parallel with the free surface is given from (8):

$$\xi^{-1}_\parallel = 2h\sqrt{Q} \left[ \cos \left( \frac{\pi}{L+1} \right) - \cos \left( \frac{2\pi}{L+1} \right) \right] \sim L^{-2}. \quad (21)$$

Since the correlation length perpendicular to the strip is just $\xi_\perp \sim L$, we have the asymptotic relation $\xi_\parallel \sim \xi_\perp^{\nu_s}$, with an anisotropy exponent

$$z^{\nu_s} = 2. \quad (22)$$

Away from the bulk transition point for $0 < -t < 1$ the boundary magnetization can be studied by a perturbation expansion, when the diagonal term of $\tilde{H}$ in (8), $\tilde{H}_{i,j} = -t(i-1)\delta_{i,j}$, is considered as a perturbation. From this calculation the first order correction to the magnetization is given for $L \to \infty$ and $0 < -t < 1$ as:

$$m_s = \frac{2\pi^2}{L^3} + \frac{1}{2} \sqrt{Q} t + \ldots. \quad (23)$$

Thus the surface magnetization exponent, defined in the thermodynamic limit ($L \to \infty$) as $m_s \sim (-t)^{\beta_s^{\nu_s}}$ is given by:

$$\beta_s^{\nu_s} = 1. \quad (24)$$

The small $t$-behavior of the system can also be investigated in the frame of a continuum approximation, when the eigenvalue problem of $\tilde{H}$ in (8), which is a second-order difference equation, is transformed into a differential equation of the continuous variable $x = i$:

$$\frac{\partial^2 \psi}{\partial x^2} + (\epsilon + i\lambda)\psi(x) = 0, \quad (25)$$

with $\epsilon = 2 + E/(h\sqrt{Q})$ and $\lambda = t/h\sqrt{Q}$, whereas the boundary conditions are $\psi(x = 0) = \psi(x = L) = 0$. From the properties of the solution of (25) one obtains for the temperature dependence of the correlation lengths as:

$$\xi_\parallel \sim |t|^{-2/3}, \quad \xi_\perp \sim |t|^{-1/3}, \quad (26)$$

thus the corresponding critical exponents are $\nu_\parallel^{\nu_s} = 2/3$ and $\nu_\perp^{\nu_s} = 1/3$ and the scaling relation $\nu_\parallel/\nu_\perp = z^{\nu_s}$ is satisfied with $z^{\nu_s}$ from (22). The exponents of the surface critical transition are collected in Table III.

2. First-order surface transition regime - $h_s > 1$

The qualitative behavior of the solution of $\tilde{H}$ is changing when the strength of the surface field, $h_s$, grows over $h_s = 1$. For $h_s > 1$ the ground state of $\tilde{H}$ has the form of a localised mode and the corresponding wavenumber in (16) is complex, $k_0 = i\kappa$. In the limit $L \to \infty$ the wavefunction of this localised mode is given by

$$\psi^{loc}(n) = (h_s^2 - 1)^{1/2}h_s^{-n}, \quad (27)$$

with the energy

$$E^{loc} = -(L-1) - h\sqrt{Q}(h_s + h_s^{-1}), \quad (28)$$

which is separated from the continuum part of the spectrum given in the form of (15).

The surface magnetization at the bulk transition point, $t = 0$, from (14)

$$m_s = 1 - \frac{1}{h_s^2} \quad (29)$$

is finite, thus the surface transition is of first-order for $h_s > 1$. The $\delta_{1,1}$ exponent defined as $m_s \sim (\delta h_s)^{1/\delta_{1,1}}$ with $\delta h_s = h_s - 1$ is given by:

$$\delta_{1,1}^{\nu_s} = 1, \quad (30)$$

where the superscript “$^{\nu_s}$” refers to the tricritical point, which is approached as $h_s \to 1^+$. The surface correlation length parallel with the surface is finite in the $L \to \infty$ limit

$$\xi^{-1}_s = E_1 - E^{loc} = h\sqrt{Q}(h_s + h_s^{-1} - 2) \sim (\delta h_s)^2, \quad (31)$$

as expected for a discontinuous surface transition. In (11) for $E_1$ the edge of the continuum spectrum in (15) is used. The magnetization profile as a function of the distance from the free surface, $\Delta l = L + 1 - l$, is given by:

$$m_{\Delta l} = 1 - h_s^{-2\Delta l} \quad h_s > 1, \quad L \to \infty. \quad (32)$$

As seen from the dashed line of Fig. 3 there is a surface region of the profile having a size of

$$\xi_\perp(h_s) = \frac{1}{2\ln h_s} \sim (\delta h_s)^{-1}, \quad (33)$$

which defines the perpendicular correlation length at the surface. As the tricritical point is approached, $h_s \to 1^+$, the two correlation lengths are related as $\xi_\perp^{tr} \sim \xi_\parallel$, thus the anisotropy exponent in the tricritical point

$$z^{tr} = 2, \quad (34)$$

is the same as in the critical region Eq. (22).
3. Tricritical surface transition - $h_s = 1$

As we mentioned before the tricritical point with $h_s = 1$ separates the continuous and first-order surface transition regimes. At the bulk transition point, $t = 0$, the solution of (34) for the wavenumbers is given by

$$k_i = \frac{\pi}{2L + 1}(2i + 1), \quad h_s = 1,$$

(35)

and the normalization in (14) is $A_i = 2/\sqrt{2L + 1}$.

The surface magnetization

$$m_s = \frac{4}{2L + 1} \cos^2 \left( \frac{\pi}{2(2L + 1)} \right) \sim L^{-1},$$

(36)

goes to zero as $L \to \infty$, however the tricritical surface magnetization scaling dimension

$$x_s^{tr} = 1,$$

(37)

is different from its value in the critical region (15).

The tricritical magnetization profile can be evaluated from (6), which in the continuum approximation is given by

$$m_{\Delta l} = \frac{\Delta l}{L} + \frac{1}{\pi} \sin \left( \frac{\Delta l}{L} \right) \sim \frac{\Delta l}{L} + O \left[ \left( \frac{\Delta l}{L} \right)^3 \right], \quad h_s = 1.$$

(38)

as a function of the distance from the free surface, $\Delta l$. This profile is also shown in Fig. 3 as a dotted line where one can notice the different behavior close to the free surface for the critical and tricritical cases. This is due to the fact that the profiles grow with the respective $x_s$ scaling dimensions, which are different in the two fixed points. The correlation length parallel with the surface can be calculated as in (22) with the asymptotic behavior $\xi_s = L^2$. Thus the anisotropy exponent is $z_s^{tr} = 2$ in accordance with the previous derivation in (15).

Away from the bulk transition point for $|t| \ll 1$ one can repeat the calculations as described for the critical surface transition. In the continuum approximation the differential equation in (25) remains the same and just the boundary condition at $x = 0$ will be changed to $\partial\psi/\partial x|_{x=0} = 0$. The tricritical exponents obtained from the solution of the differential equation are presented in Table II, together with their critical counterparts. We stress that scaling in the surface region is anisotropic, both in the critical and tricritical fixed points the correlation lengths are related as $\xi_\parallel \sim \xi_\perp^{z_s}$, with the same anisotropy exponent $z = 2$. On the other hand the $x_s$ and $\beta_s$ exponents are different in the two cases, but the scaling relation $\beta_s = \nu_\perp x_s$ is satisfied in both fixed points. Notice also that the exponents in Table II are the same as for the restricted solid-on-solid model of the interface localization-delocalization transition [4].

4. Crossover regime

It is interesting to study the behavior of the surface magnetization in the vicinity of the tricritical point when $0 < 1 - h_s < 0$. This is a crossover region where the surface critical behavior for finite $L$ is strongly influenced by the presence of the tricritical transition occurring at $h_s = 1$.

Analyzing the exact relations in (13-16) one can define a length scale $\xi_s = \sqrt{1/2 \ln h_s}$ which is identical to $\xi_\perp$ defined above in the first order case $h_s > 1$ in (15). Then one can show that the finite size surface magnetization at the transition point, $t = 0$, satisfies the scaling relation:

$$m_s(L, \ln h_s) = L^{-x_s^{tr}} \tilde{m}_s(L/\xi_s)$$

(39)

with $\xi_s$ defined above and where the scaling function $\tilde{m}_s(y)$ goes to a constant for $y \to 0$ and behaves as $\tilde{m}_s(y) \sim 1/y^2$ for $y \to \infty$. This scaling function is expected to be universal, provided the surface critical behavior of the model is independent of $Q > 4$. We shall study this point numerically in the next Section.

B. DMRG study

Having the complete analytical solution for $Q \to \infty$ at hand, we are interested in the surface critical behavior for finite values of $Q$. The expected surface phase diagram of the model is schematically drawn in Fig. 4.

![FIG. 4. Schematic phase diagram for the surface critical behavior of the Q-state Potts model as function of the applied surface field $h_s$. The thick solid line departing from $Q = 4$ denotes a tricritical line, which separates a continuous from a first order surface transition. For $Q \leq 4$ (along the thick dashed line) the surface critical exponents depend continuously on $Q.

\begin{table}
\centering
\begin{tabular}{|c|c|c|c|}
\hline
$Q$ & $x_s$ & $\beta_s$ & \\
\hline
4 & 2 & 2 & \\
\hline
5 & 3/2 & 3/2 & \\
\hline
6 & 2 & 2 & \\
\hline
\end{tabular}
\caption{Critical exponents for the surface critical behavior of the Q-state Potts model.}
\end{table}
In the second-order bulk transition regime, \( Q \leq 4 \), the critical and tricritical surface transition lines merge and are characterized by \( Q \)-dependent exponents. For \( Q > 4 \), in the first-order bulk transition regime, the second- and first-order surface transition regions are separated by a tricritical line, which is expected to depart from \( Q = 4 \). It should also be noticed that some of the tricritical exponents obtained from the exact solution at \( Q \to \infty \) are the same as for the \( Q = 4 \) Potts model: \( x_s^c = x_s(Q = 4) \) and \( \nu_s^c = \nu_{\text{bulk}}(Q = 4) \), whereas other are different. Then one can expect two scenarios about the surface (critical and tricritical) exponents of the \( Q > 4 \) model: i) the exponents vary with \( Q \), like for \( Q \leq 4 \); or ii) the exponents are universal and their fixed-point values are those calculated at \( Q \to \infty \).

To decide between the two possibilities we have investigated the problem numerically using the density matrix renormalization group. As for the bulk transition in Section III we have considered the isotropic model for \( 5 \leq Q \leq 9 \) on moderately large finite strips \((L \leq 40)\) where we have calculated the magnetization profiles with fixed-free boundary conditions, using the finite system algorithm described in Ref. 17. Comparing the numerical data for a different number of states kept in the DMRG procedure we could estimate the accuracy for the finite surface magnetization as about \( 5 - 6 \) digits.

Figures 5 and 6 show plots of magnetization profiles for the \( Q = 7 \) and \( Q = 9 \) cases, for different values of the strip width \( L \). From the surface magnetization \( m_s(L) \) at the bulk transition point and at \( h_s = 0 \) we first formed finite-size extrapolants: \( x_s(L) = \ln(m_s(L - 4)/m_s(L))/\ln(1 - 4/L) \) from the data for \( L = 8, 12, 16, \ldots, 40 \). For \( L \to \infty \) one has \( x_s(L) \to x_s \). Table IV shows the values of \( x_s(L) \) for the cases \( Q = 8 \) and \( Q = 9 \). All the finite size data are above the value \( x_s = 1 \) (the surface critical dimension for the \( Q = 4 \) model) and tend to increase at larger \( Q \). Extrapolations from the BST sequence extrapolation method yield \( x_s = 2.7(4) \) for \( Q = 8 \) and \( x_s = 2.9(3) \) for \( Q = 9 \), both compatible with the value of \( x_s = \frac{3}{4} \) found in the \( Q \to \infty \) limit. These estimates have quite large error bars (from this reason we could not get a sensitive estimate for \( Q \leq 7 \)) and we did not find nice convergence of the BST extrapolants for \( x_s(L) \) as was found in the cases \( Q = 2 \) and \( Q = 3 \) in Ref. 17. This is typically due to strong finite size corrections, which in the present case are essentially caused by two effects. First of all the bulk correlation length \( \xi_b(Q) \), which remains finite at a first-order transition is still very large for the values of \( Q \) analyzed. As seen in the values of the bulk correlation lengths in Table II only the highest values of \( Q \) are reliable for extrapolations of finite size data with \( L \leq 40 \). A second point is that in the range \( 5 \leq Q \leq 9 \) we expect that the tricritical surface transition is at small surface fields, so that even at \( h_s = 0 \) strong influence from the tricritical fixed-point can be observed.

To clarify this point we have reanalyzed our numerical data using the analytical scaling relation in (33) for the \( Q \to \infty \) limit, which describes the behavior of the surface magnetization at and in the vicinity of the tricritical point. As already mentioned the scaling function in (33) is expected to be universal, provided the surface critical behavior of the model is independent of \( Q > 4 \). In the analysis of numerical results we have compared the ratio of surface magnetizations for a finite \( Q \) and \( h_s = 0 \), with the corresponding analytical results at \( Q \to \infty \) and at finite \( h_s \). We found the value of \( h_s \) such that the equality: \( m_s^Q(L)/m_s^Q(L - 4) = m_s^\infty(L, h_s)/m_s^\infty(L - 4, h_s) \) is satisfied. The universality hypothesis about the scaling
function is connected with the convergence of the finite size estimates \( h_s(L) \) to a finite limit. Moreover, the difference, \( \Delta h_s = 1 - h_s \), gives an estimate on the position of the tricritical line at a given \( Q > 4 \).

As seen in Table IV the \( \Delta h_s(L) \) finite size extrapolants for the \( Q = 7 \) model are nicely converging to a limiting value and the same observation has been found for the other \( Q \)-s, as well. The extrapolated position of the tricritical line is found as \( \Delta h_s = 0.0125, 0.0215, 0.0310 \) and 0.040, for \( Q = 6, 7, 8 \) and 9, respectively. This is a strong numerical indication that the surface critical phenomena of the \( Q > 4 \) state Potts model is universal and the corresponding exponents are those given in Table III.

The influence of the tricritical point is also visible in the profiles for \( Q = 7 \) of Fig. 3 where the magnetization has an approximately linear behavior as function of the distance from the free surface as found for the tricritical profile in the limit \( Q \to \infty \) (see dotted line of Fig. 3). In the case \( Q = 9 \) instead, the curvature of the profile is clearly noticeable for the largest systems analyzed.

Finally, we turn to compare the two finite length scales appearing in the problem: the \( \xi_s \approx 1/2\Delta h_s \) surface length scale and the \( \xi_\ell \) bulk correlation length. Assuming anisotropic scaling as \( \xi_\ell \sim \xi_\ell^q \), we obtain \( \theta = 1.15, 1.24 \) and 1.4 for \( Q = 8, 7 \) and 6, respectively. In the \( Q \to 4^+ \) limit, when the correlation lengths are divergent, it is natural to assume that the anisotropy exponent will approach \( \theta = 2 \), so that the perpendicular and parallel correlation lengths are related as in the critical and tricritical surface transitions (see Table III). With this assumption we can conjecture the position of the tricritical line as

\[
\lim_{Q\to 4^+} \Delta h_s(Q) \approx [\xi_s(Q)]^{-1/2} \sim \exp \left[ -\frac{\pi^2}{2\sqrt{Q - 4}} \right], \tag{40}
\]

where the limiting form of \( \xi_s(Q) \) can be found in II.

V. DISCUSSION

In this paper the two-dimensional \( Q \)-state Potts model has been studied by analytical and numerical methods in the first-order bulk transition regime, \( Q > 4 \). In the bulk transition point we have used the DMRG method and sequence extrapolation techniques to accurately estimate the latent heat and the magnetization discontinuity at the transition point. Calculating the correlation lengths at the transition point we have shown with good numerical accuracy that they are identical in the ordered and in the disordered phases.

For the surface transition we have demonstrated the existence of surface induced disorder, for the first time for a microscopic model. We have calculated the complete set of critical and tricritical surface exponents and showed that the surface transition of the model is universal for \( Q > 4 \), thus do not depend on the value of the discontinuities at the bulk transition point. Based on this observation we conjecture that the surface exponents in Table III are universal for all two dimensional systems with a first-order bulk transition. This statement is in accordance with the prediction of the restricted solid-on-solid model of the interface localization-delocalization transition [25]. It is interesting to note that the transfer matrix of the restricted solid-on-solid model is formally equivalent to the Hamiltonian \( \tilde{H} \) in (12), which represents the ground-state block of the anisotropic version of the \( Q \to \infty \) Potts model. The physical interpretation of the same operator in the two problems is, however, completely different.

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APPENDIX: SOLUTION OF THE GROUND-STATE SECTOR OF \( \mathcal{H} \)

Here we show how to construct the ground-state sector of \( \mathcal{H} \) for the smallest systems, \( L = 2 \) and \( L = 3 \) and then use these results to define a systematic \( 1/Q \)-expansion in the vicinity of the bulk transition point.

The ground-state sector for the \( L = 2 \) system is spanned by two vectors:

\[
\psi_1 = 11,
\psi_2 = \frac{1}{\sqrt{Q - 1}} (12 + 13 + \ldots + 1q)
\]

and the eigenvalue matrix with zero surface field, \( H_s = 0 \), is given by:

\[
\tilde{H}^2 = \begin{pmatrix}
-1 & -h\sqrt{Q - 1} \\
-h\sqrt{Q - 1} & -h(Q - 2)
\end{pmatrix}.
\]

For \( L = 3 \) the ground-state sector is spanned by five vectors:

\[
\psi_1 = 111,
\psi_2 = \frac{1}{\sqrt{Q - 1}} (121 + 131 + \ldots + 1q)
\]

\[
\psi_3 = \frac{1}{\sqrt{(Q - 1)(Q - 2)}} (123 + 124 + \ldots + 12q + 132 + \ldots + 1q(q - 1))
\]

and the eigenvalue matrix for \( H_s = 0 \) is given by:
whereas the off-diagonal matrix-elements are now degenerate with the same diagonal matrix-elements, \( Q \) the \( Q h L \) point depends on leading order of \( 1/Q \). There are three asymptotically degenerate states \( H = 11 \ldots 1 Q \).

It is remarkable that the dimension of the ground-state sector is independent of the value of \( Q \) and only depends on \( L \). In the vicinity of the bulk transition point \( h_c = 1/Q \) further simplifications take place in the \( Q \to \infty \) limit. To see this, first, we consider the \( L = 2 \) problem, where the two vectors \( \psi_1 \) and \( \psi_2 \) are now degenerate with the same diagonal matrix-elements, whereas the off-diagonal matrix-elements are \( -h\sqrt{Q} \) in leading order of \( 1/Q \). Similarly, in the \( L = 3 \) system there are three asymptotically degenerate states \( \psi_1, \psi_2 \) and \( \psi_3 \) in (A3) with diagonal matrix-elements \( \tilde{H}_{11}^3 = \tilde{H}_{22}^3 = \tilde{H}_{33}^3 = -2 \) and these states are separated from the others by an amount of \( O(1) \). Since the off-diagonal matrix-elements between the relevant states are \( \tilde{H}_{12}^3 = \tilde{H}_{21}^3 = \tilde{H}_{35}^3 = -h\sqrt{Q} \approx 1/\sqrt{Q} \) the two non-relevant states do not influence the behavior of the ground state (and the first excited state) in the large \( Q \) limit.

Generalizing the observation found in the \( L = 2 \) and \( L = 3 \) systems one can show that in the vicinity of the bulk transition point in the \( Q \to \infty \) limit for general \( L \) the ground state sector is spanned by \( L \) asymptotically degenerate vectors:

\[
\psi_1 = 11 \ldots 1
\]

\[
\psi_2 = \frac{1}{Q^{1/2}} (11 \ldots 12 + 11 \ldots 13 + \ldots + 11 \ldots 1 Q)
\]

\[
\psi_3 = \frac{1}{Q} (11 \ldots 123 + 11 \ldots 24 + \ldots + 11 \ldots Q(Q - 1))
\]

\[
\psi_4 = \frac{1}{Q^{3/2}} (11 \ldots 1234 + 11 \ldots 1235 + \ldots + 11 \ldots 1 Q(Q - 1)(Q - 2))
\]

\[
\vdots
\]

\[
\psi_L = \frac{1}{Q^{(L-1)/2}} (1234 \ldots L + \ldots + Q(Q - 1) \ldots (Q - L))
\]

and the corresponding eigenvalue matrix is given in (12).

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TABLE I. Table of the BST extrapolants for the latent heat for the $Q = 8$ Potts model. In the first column are the DMRG data for finite systems with $L = 8, 12, 16, \ldots, 40$. (The parameter of the BST algorithm is $\epsilon = 2$.)

| $Q$ | $\Delta E$ | $\Delta E^{(*)}$ | $\Delta m$ | $\Delta m^{(*)}$ | $\xi_o$ | $\xi_d^{(*)}$ |
|-----|-------------|------------------|-------------|------------------|--------|--------------|
| 5   | 0.028(3)    | 0.0265           | 0.49(1)     | 0.4921           | –      | 2512         |
| 6   | 0.102(3)    | 0.1007           | 0.66(1)     | 0.6652           | –      | 158.9        |
| 8   | 0.242(2)    | 0.2432           | 0.798(3)    | 0.7998           | –      | 23.9         |
| 9   | 0.299(2)    | 0.2998           | 0.833(2)    | 0.8333           | 15.0(4)| 14.9         |

TABLE II. Physical quantities at the bulk transition point of the $Q$ state Potts model as found from finite size BST extrapolation of DMRG data (* denotes the exact values).

| $Q$ | $\Delta E$ | $\Delta E^{(*)}$ | $\Delta m$ | $\Delta m^{(*)}$ | $\xi_o$ | $\xi_d^{(*)}$ |
|-----|-------------|------------------|-------------|------------------|--------|--------------|
| 5   | 0.028(3)    | 0.0265           | 0.49(1)     | 0.4921           | –      | 2512         |
| 6   | 0.102(3)    | 0.1007           | 0.66(1)     | 0.6652           | –      | 158.9        |
| 8   | 0.242(2)    | 0.2432           | 0.798(3)    | 0.7998           | –      | 23.9         |
| 9   | 0.299(2)    | 0.2998           | 0.833(2)    | 0.8333           | 15.0(4)| 14.9         |

TABLE III. Surface critical and tricritical exponents of the $Q$ state Potts model calculated in the $Q \to \infty$ limit.

|          | critical | tricritical |
|----------|----------|-------------|
| $x_s$    | 3        | 1           |
| $\beta_s$| 1        | 1/3         |
| $\nu_\perp$| 1/3     | 1/3         |
| $\nu_\parallel$| 2/3 | 2/3        |
| $z$      | 2        | 2           |

TABLE IV. Finite size extrapolants for the surface magnetization scaling dimension, $x_s^Q(L)$, and for the position of the tricritical line, $\Delta h^Q_s(L)$, as a function of the width of the strip for various values of $Q$. The last row shows the BST extrapolations at $L \to \infty$.

| $L$  | $x_s^Q=8(L)$ | $x_s^Q=9(L)$ | $\Delta h^Q_s=7(L)$ |
|------|--------------|--------------|----------------------|
| 20   | 1.15892328   | 1.25272509   | 0.013300             |
| 24   | 1.22149616   | 1.32785249   | 0.017501             |
| 28   | 1.27464891   | 1.39259493   | 0.019548             |
| 32   | 1.32114750   | 1.44961396   | 0.020599             |
| 36   | 1.36226612   | 1.50098953   | 0.021121             |
| 40   | 1.39920082   | 1.54783012   | 0.021344             |
| $\infty$ | 2.7(4)$   | 2.9(3)$       | 0.0215(1)$           |