

# Interfacial Adsorption in Two-Dimensional Potts Models

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The interfacial adsorption  $W$  at the first-order transition in two-dimensional  $q$ -state Potts models is studied. In particular, findings of Monte Carlo simulations and of density-matrix renormalization group calculations at  $q=16$  are consistent with the analytic result, obtained in the Hamiltonian limit at large values of  $q$ , that  $W \propto t^{-1/3}$  on approach to the bulk critical temperature  $T_c$ ,  $t = |T_c - T|/T_c$ . In addition, the numerical findings allow to estimate corrections to scaling. Our study supports and quantifies a previous conclusion by Bricmont and Lebowitz based on low temperature expansions.

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**KEY WORDS:** Potts model; interfacial adsorption; Monte Carlo simulations; density-matrix renormalization group; Hamiltonian limit.

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## 1. INTRODUCTION

The interface between two phases may become unstable against the appearance of a third phase. This wetting phenomenon has been studied in various circumstances, considering different materials and geometries, both experimentally and theoretically.<sup>(1)</sup>

Good candidates for modelling wetting are  $q$ -state Potts models,<sup>(2,3)</sup> where the two phases correspond to distinct boundary states, say, 1 and  $q$ , at opposite sides of the system. In that case one observes an excess adsorption of the non-boundary states at the interface between “1” rich and “ $q$ ” rich domains.

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In particular, in two dimensions, the interfacial adsorption,  $W$ , is found to diverge on approach to the critical temperature  $T_c$  like  $W \propto t^{-\omega}$ , where  $t = |T_c - T|/T_c$ . For  $q = 3$  and 4, the bulk transition is continuous and  $\omega$  can be expressed in terms of canonical bulk critical exponents,  $\omega = \nu - \beta$ .<sup>(2)</sup> For larger values of  $q$ , the transition is of first order. On general, phenomenological grounds,<sup>(4)</sup> one may expect then  $\omega = 1/3$ , as observed in Monte Carlo (MC) simulations on the two-dimensional Blume–Capel model.<sup>(5)</sup> However, previous simulations on the two-dimensional 20-state Potts model suggested that  $\omega$  may be significantly larger than  $1/3$ , albeit a pronounced curvature in the corresponding log–log plots for  $W(t)$  was noticed indicating that the asymptotic behavior may not have been reached.<sup>(3)</sup> A reasonable explanation of the numerical findings was then offered by Bricmont and Lebowitz.<sup>(6)</sup> Based on low-temperature expansions, the critical region is argued to be extremely narrow in the Potts case, in contrast to the Blume–Capel case.<sup>(6)</sup> However, a numerical confirmation remained to be done.

Motivated by a recent intriguing analysis of the interfacial tension of the  $q$ -state Potts model in two dimensions employing a field-theoretic representation for configurations of the interface<sup>(7)</sup> (extending prior considerations)<sup>(2)</sup>, we decided to reconsider the somewhat irritating problem on the value of  $\omega$  for  $q > 4$ . Indeed, advances in methods and computer facilities allow now to explore numerically the critical region more deeply than some years ago. In addition, we dealt with the issue analytically by studying the Hamiltonian limit of the Potts model for large values of  $q$  exactly.

The outline of the article is as follows. In the next Section, the model is defined, and the numerical methods of our choice, MC simulations and density-matrix renormalization group (DMRG) calculations, are introduced. Then, we discuss the results obtained from those methods. In Section 4, the analytical findings in the Hamiltonian limit are presented. A summary concludes the paper.

## 2. MODEL AND NUMERICAL METHODS

The two-dimensional  $q$ -state Potts model is described by the Hamiltonian

$$\mathcal{H} = -J \sum_{(ij), (i'j')} \delta_{n_{ij}, n_{i'j'}} \quad (1)$$

summing over neighboring sites  $(ij)$ ,  $(i'j')$  on a  $L \times M$  rectangular lattice, with the Potts variable  $n_{ij} = 1, 2, \dots, q$ . In the thermodynamic limit,

$L, M \rightarrow \infty$ , the model displays a bulk phase transition at the critical temperature  $k_B T_c / J = 1 / \ln(\sqrt{q} + 1)$ ,<sup>(8)</sup> where  $k_B$  is the Boltzmann constant. The transition is of continuous type at  $q \leq 4$ , while it is of first order at larger values of  $q$ .

To introduce an interface, we add a column of  $M$  sites on the left side boundary, fixing the Potts variable to be in the state  $n_L = 1$ , and another column on the right side boundary with  $n_R = q$ . The Potts variables on the top and at the bottom of the lattice may be connected by periodic boundary conditions ("periodic case"). Alternatively, the interface may be pinned at the lower and upper boundaries by inserting there additional boundary rows with fixed states being "1" on the left half and "q" on the right half (pinned case).

By examining typical Monte Carlo equilibrium configurations below  $T_c$ , it is seen that an excess of non-boundary states is adsorbed at the interface, as illustrated in Fig. 1. This wetting phenomenon may be described quantitatively by the net interfacial adsorption  $W$  per unit length

$$W = 1/M \sum_{(ij), nb} (\langle \delta_{nb, n_{ij}} \rangle_{1:q} - \langle \delta_{nb, n_{ij}} \rangle_{1:1}) \quad (2)$$

summing over all  $L \times M$  sites in the inner part of the system; the  $\langle \rangle$  brackets refer to thermal averages; the index  $nb$  denotes the non-boundary states,  $nb = 2, \dots, q - 1$ ; the subscripts  $1:q$  and  $1:1$  refer to systems with corresponding fixed states at the boundaries, i.e., with and without interface. The net adsorption  $W$  is closely related to the density profiles

$$n_{b_1:b_2}(s, i) = 1/M \sum_j \langle \delta_{s, n_{ij}} \rangle_{b_1:b_2} \quad (3)$$

describing the variation of the density of state  $s$  by going from the left side, fixed in state  $b_1$ , to the right side, fixed in state  $b_2$ , of the lattice, summing over each column,  $j = 1, \dots, M$ , with  $i$  running from 1 to  $L$ . Obviously,

$$W = \sum_{i, nb} (n_{1:q}(nb, i) - n_{1:1}(nb, i)) \quad (4)$$

We computed profiles and net adsorption numerically, using Monte Carlo techniques<sup>(9)</sup> and the density-matrix renormalization group method.<sup>(10)</sup> In the MC simulations, the standard single-variable flip algorithm was applied, for system sizes  $L \leq 256$  and  $M \leq 2000$ , studying mostly the periodic case, augmented by a few runs for the pinned case. To obtain accurate equilibrium data, we typically averaged over several realizations (using different random numbers), each consisting of  $10^6$  Monte Carlo steps per site,

including at least  $10^5$  steps for equilibration. Error bars resulted from averaging over the ensemble of realizations. Usually, we set  $q = 16$ , where the bulk phase transition is strongly first order with a bulk correlation length of a few lattice spacings at  $T_c$ .<sup>(11)</sup> To search for possible  $q$ -dependencies, we also simulated models with  $q = 20$  and  $40$ . Furthermore, because clusters, formed by neighboring sites in the same state, seem to play an interesting role in the wetting phenomenon, see Fig. 1, we also computed cluster properties in the MC study.

In the DMRG method, one considers strip-like lattices, i.e.,  $M \rightarrow \infty$ , while  $L$  is finite. The algorithm, introduced by White in 1992<sup>(12)</sup> for the study of the low-lying spectrum of quantum spin chains, has been extended in several directions.<sup>(10)</sup> In the present study we follow Nishino's<sup>(13)</sup> formulation of the method adapted to treat classical two-dimensional systems, where the approach is used for constructing iteratively approximate transfer matrices, starting from strips of small width (say,  $L = 8$ ) which can be also handled numerically exactly. At each DMRG step the strip width is increased, and the configurational space is truncated efficiently through the projection into smaller subspaces with the help of appropriate density matrices.

We do not need to describe details of the widely used DMRG procedure here: a good introduction, together with recent developments, can be

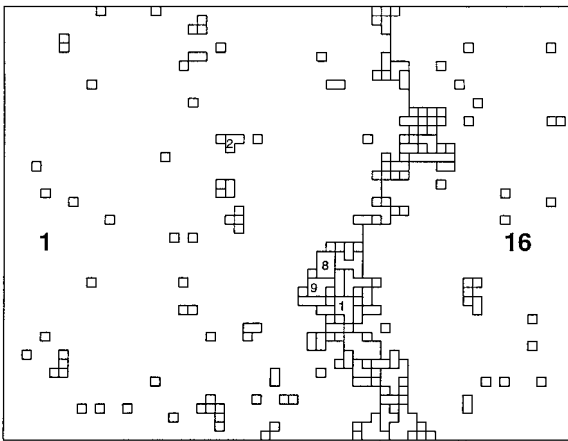


Fig. 1. Typical Monte Carlo equilibrium configuration of the two-dimensional 16-state Potts model with an interface, at  $T = 0.99T_c$ : On the left (right) hand side there is a large “1” (“16”) cluster. The boundaries of the other clusters of distinct Potts states at and away from the interface are indicated by closed lines; a few of those clusters are labeled by their states. A MC system of size  $L = 60$  and  $M = 60$ , periodic case, was simulated, but only 48 (out of  $M = 60$ ) successive rows are depicted.

found in ref. 10. The DMRG technique has already been applied to the two-dimensional Potts model, both at continuous,  $q \leq 4$ ,<sup>(14,15)</sup> and first-order transitions,  $q > 4$ .<sup>(16)</sup> In the former case, bulk and surface critical exponents have been calculated with a high degree of accuracy.<sup>(15)</sup> In the present study we are interested in rather large values of  $q$ , where the standard DMRG method is less suitable. An appropriate, powerful variant, the “pseudo-spin” version, has been introduced in ref. 16. It enables one to treat systems with special values of  $q$ , namely  $q = p^2$ ,  $p = 2, 3, \dots$ . We used that algorithm in the current work. Most calculations were performed at  $q = 16$ , augmented by some calculations at  $q = 9$ , for strips of widths up to  $L = 80$ . We kept up to  $m = 60$  states per block with a typical truncation error of  $\varepsilon \approx 10^{-6}$ . From the dominant eigenvector of the transfer matrix the profiles<sup>(15)</sup> and the interfacial adsorption  $W$  were calculated.

### 3. NUMERICAL RESULTS

The crucial quantity, which we computed numerically, is the net adsorption  $W$  as a function of the system size,  $L, M$ , and temperature  $t$ ,  $W(L, M, t)$ . The main aim is to analyze its critical behavior as  $t \rightarrow 0$  or  $T \rightarrow T_c$ , in the thermodynamic limit  $L, M \rightarrow \infty$ . For that, one may extrapolate the numerical data for  $W$  to that limit, or one may study systems for which finite-size effects can be neglected. We also tried to perform a finite-size scaling analysis on  $W(L, M, t)$ ,<sup>(5)</sup> see below.

In any event, accurate data are needed. Their quality can be conveniently tested by comparing results obtained from the MC simulations and the DMRG calculations, as illustrated in Figs. 2 and 3.

In Fig. 2, profiles, Eq. (3), are shown for the 16-state Potts model with and without interface, demonstrating again the excess adsorption of non-boundary states at the interface. In Fig. 3, the increase of the net adsorption  $W$  with increasing width  $L$  of the Potts model, at various temperatures, is displayed. In both figures, the finite-size effect arising from the length  $M$  of the system can be disregarded. In fact,  $M$  is infinite in the DMRG approach. In the simulations (periodic case),  $M$  was checked to be sufficiently large so that  $W$  approached closely  $W(L, M = \infty, t)$ , with the characteristic crossover value depending, of course, on the width  $L$  and the distance from criticality  $t = |T_c - T|/T_c$ .

As exemplified in Figs. 2 and 3, data from both methods do, indeed, agree nicely, being obviously accurate and reliable. Slight systematic deviations seem to become significant only for quite wide systems, say,  $L > 60$ . A reasonable extrapolation of our data for  $W$  to the thermodynamic limit is feasible for temperatures  $T \leq 0.998T_c$ , see Fig. 3. Closer to  $T_c$ , both

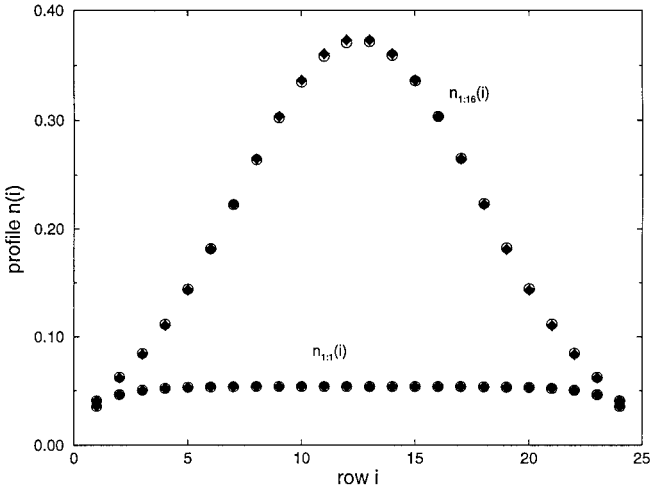


Fig. 2. Profiles, summed over the non-boundary ( $nb$ ) states,  $n_{1:b}(i) = \sum_{nb} n_{1:b}(nb, i)$  for systems with interface,  $b = 16$ , and without interface,  $b = 1$ , at  $T = 0.99T_c$  and  $L = 24$ , as obtained from the DMRG method (open circles) and MC simulations (periodic case with  $M = 400$ ; full diamonds).

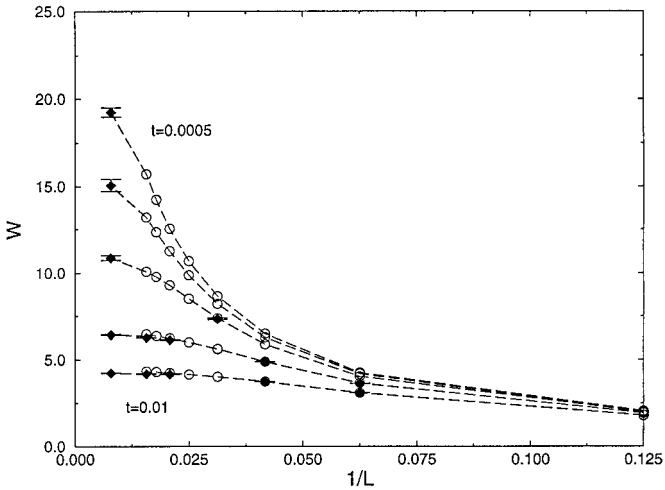


Fig. 3. Net adsorption,  $W$ , vs. inverse width,  $1/L$ , of the lattice at (from bottom to top)  $t = 0.01, 0.005, 0.002, 0.001$ , and  $0.0005$ , depicting DMRG (open circles) and MC (periodic case with  $M \leq 1000$ ; full diamonds) data.

numerical methods would require much larger system sizes demanding extremely large storage and/or computing time.

In the thermodynamic limit, one expects  $W \propto t^{-\omega}$  as  $t \rightarrow 0$ . To monitor the approach to the asymptotic behavior, one may consider the effective exponent

$$\omega_{\text{eff}}(t) = -d \ln W / d \ln t \quad (5)$$

with  $\omega = \omega_{\text{eff}}(t=0)$ . In Fig. 4, numerical estimates of the effective exponent are shown. At  $t \geq 0.02$ , we determined  $\omega_{\text{eff}}$  from MC data for systems being large enough to disregard finite-size effects. Actually, finite-size effects are much stronger in the pinned case than in the periodic case, and only MC data for the latter case are included, with  $L = 64$  and  $M \geq 400$ . At  $t \leq 0.01$ , estimates are based on extrapolating MC and DMRG results for  $W$  to the thermodynamic limit, see Fig. 3. Note that the net adsorption is calculated at discrete temperatures,  $t_i$ , and the effective exponent may be approximated by  $\omega_{\text{eff}}(t) = -\ln(W(t_i)/W(t_{i+1}))/\ln(t_i/t_{i+1})$ , with  $t = \sqrt{t_i t_{i+1}}$ . Error bars in Fig. 4 stem from a proliferation of the error in the net adsorption  $W$ . Evidently,  $\omega_{\text{eff}}$  depends strongly on the distance from criticality  $t$ .

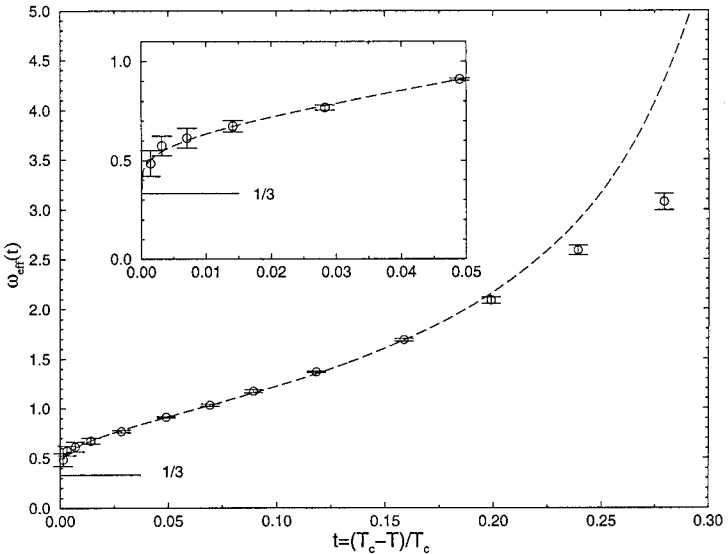


Fig. 4. Temperature,  $t$ , dependence of the effective exponent of the net adsorption  $W$ ,  $\omega_{\text{eff}}(t)$ , for numerical data “free of finite-size effects,” see text. The dashed curve corresponds to the fit to Eq. (6), with  $W_0 = 3.280$ ,  $a = -1.977$ ,  $b = 0.939$ , and  $x = 0.165$ , quantifying the corrections to scaling.

For instance, in the range  $0.1 > t > 0.002$ , it changes from about 1.2 to about 0.5 when moving towards  $T_c$ . Accordingly, an average critical exponent in that interval would be supposedly significantly larger than the true asymptotic critical exponent  $\omega$ , as observed before.<sup>(3)</sup> Presuming  $\omega = 1/3$ , see refs. 4 and 6 as well as Section 4, it follows from Fig. 4 that the asymptotic regime is very narrow, and corrections to scaling are quite pronounced. To quantify these corrections, one may postulate the standard ansatz

$$W(t) = W_0 t^{-1/3} (1 + at^x + bt^{2x} + \dots) \quad (6)$$

The coefficients can be calculated from chi-square fits to the numerical data near  $T_c$ . Using, for instance, a fit to the points in the interval  $0.02 \leq t \leq 0.1$  (shown in Fig. 4), leads to a net adsorption  $W$  reproducing very well the numerical findings both closer to  $T_c$  and further away from  $T_c$ . Eventually, systematic deviations show up when further lowering the temperature, reflecting the need for additional correction terms in Eq. (6) in that region, see Fig. 4. The exponent  $x$  characterizing the corrections to scaling is found to be rather small,  $x = 0.14 \pm 0.06$ . Because of its smallness, we included the leading, with the exponent  $x$ , and subleading,  $2x$ , terms in the ansatz (6). The error bars arise from using a variety of plausible fitting intervals and points.

From MC simulations of Potts models with larger number of states,  $q = 20$  and  $40$ , one may conclude that the corrections to scaling, at  $t > 0.01$ , are rather insensitive to the concrete value of  $q$ .

From general considerations,<sup>(4,5)</sup> one expects two diverging lengths at the interface, in the direction parallel to the interface,  $\xi_{\parallel}$ , and perpendicular to it,  $\xi_{\perp}$ , with  $\xi_{\perp} \propto t^{-\omega}$  and  $\xi_{\parallel} \propto t^{-2\omega}$ , as  $t \rightarrow 0$ , see also Section 4. For strip-like systems,  $M \rightarrow \infty$ , the following finite size scaling expressions can be then motivated<sup>(5)</sup>

$$W(L, M = \infty, t) = t^{-\omega} w_1(Lt^{\omega}) \quad (7)$$

in the limit of  $Lt^{\omega} \gg 1$ , and

$$W(L, M = \infty, t = 0) \propto L \quad (8)$$

for  $L \gg 1$ . Indeed, the DMRG results indicate that Eq. (8) seems to be satisfied rather well already for strips of moderate width, say,  $L \geq 16$ , see also ref. 3. On the other hand, the numerical data do not suffice to establish the scaling form (7) with  $\omega = 1/3$ . In fact, a “reasonable” collapse of our



data on an apparent scaling function  $w_1$  might be achieved with a somewhat larger value,  $\omega \approx 1/2$ . Careful inspection, however, reveals that systematic deviations from a unique scaling curve  $w_1$  set in for large arguments  $Lt^\omega$ . Thence, larger systems close to  $T_c$  had to be studied (which are, at present, out of reach, because of limitations in storage and computing time). Indeed,  $\omega \approx 1/2$  is merely an upper bound of the true value of  $\omega$ . This observation corroborates the above mentioned finding on  $\omega_{\text{eff}}$ : One has to include corrections to scaling to demonstrate consistency of the numerical data with the theoretically expected asymptotic behavior, due to the narrowness of the critical region.

In closing the Section on the MC and DMRG results, we remark that the thermally averaged largest cluster of non-boundary states, as computed in the simulations, seems to diverge by approaching  $T_c$  from below. A detailed analysis would be desirable, but it is beyond the scope of the present study.

#### 4. THE HAMILTONIAN LIMIT FOR LARGE VALUES OF $q$

In the following we consider the Hamiltonian limit of the Potts model with strong vertical and weak horizontal couplings.<sup>(17)</sup> The transfer matrix in the vertical direction has the form  $\mathcal{T} = \exp(-\hat{H})$ , with the one-dimensional Hamiltonian  $\hat{H}$ <sup>(18)</sup>

$$\hat{H} = - \sum_{i=1}^{L-1} \delta_{n_i, n_{i+1}} - h \sum_{i=1}^L \sum_{k=1}^{q-1} M_i^k \tag{9}$$

$n_i$  is the Potts variable on site  $i$  and  $M_i^k$  denotes the flip operation  $M_i^k |n_i\rangle = |n_i + k, \text{ mod } q\rangle$ . The strength of the transverse field,  $h$ , at the transition point is  $h_c = 1/q$ . Quantities of physical interest are derived from the ground state,  $|\Psi_0\rangle$ , and from the energies of the ground state and the first excited state,  $E_0$  and  $E_1$ , of (9).

The Hamiltonian limit of the Potts model has been treated recently<sup>(16)</sup> for free boundary conditions. In that case, the solution has a remarkably simple form in the vicinity of the transition point for large values of  $q$ . Repeating the same type of considerations for models with an interface, fixing the variables at the boundaries in the states “1” and “ $q$ ” ( $1:q$ ) (as before), one finds that the ground state sector of the Hamiltonian (9) is spanned by the vectors

$$|\psi_{i,j}\rangle = |11 \dots 1(nb)(nb) \dots (nb) qq \dots q\rangle \tag{10}$$

where a non-boundary state is given by  $|(nb)\rangle = 1/\sqrt{q} (|2\rangle + |3\rangle + \dots + |q-1\rangle)$ , and the positions of the domain walls separating the boundary and non-boundary states are denoted by  $i (= 1, 2, \dots, L)$  and  $j (= i, i+1, \dots, L)$ . The diagonal matrix-elements of these states,  $\langle \psi_{i,j} | \hat{H} | \psi_{i,j} \rangle = -L - (j-i)t$ , with  $t (= hq-1, |t| \ll 1)$  being the distance from the critical point, are smaller by an amount of  $O(1)$  compared to any other states, like those containing boundary states in the domain of non-boundary ( $nb$ ) states. The Hamiltonian in the ground state sector, spanned by the vectors (10), can be written as

$$\hat{H}_g = -(j-i)t - h\sqrt{q} [(a^+ + a^-) + (b^+ + b^-)] \quad (11)$$

up to a constant; the operators,  $a^\pm$  and  $b^\pm$  which move the positions of the domain walls in (10), are defined as

$$\begin{aligned} a^\pm |\psi_{i,j}\rangle &= |\psi_{i\pm 1,j}\rangle, & 1 < i < j; & & a^+ |\psi_{i,i}\rangle &= a^- |\psi_{1,j}\rangle = 0 \\ b^\pm |\psi_{i,j}\rangle &= |\psi_{i,j\pm 1}\rangle, & i < j < L; & & b^- |\psi_{i,i}\rangle &= b^+ |\psi_{i,L}\rangle = 0 \end{aligned} \quad (12)$$

In the continuum limit, when  $L \gg 1$ ,  $i \gg 1$  and  $j \gg 1$ , but  $x = i/L = O(1)$  and  $y = j/L = O(1)$ , the Hamiltonian (11) can be written in the form of a differential operator

$$\hat{H}_g \psi(x, y) = - \left[ \frac{h\sqrt{q}}{L^2} \left( \frac{\partial^2}{\partial x^2} + \frac{\partial^2}{\partial y^2} \right) + tL(y-x) \right] \psi(x, y) = E\psi(x, y) \quad (13)$$

with the boundary condition  $0 \leq x \leq y \leq 1$ .

At the critical point,  $t=0$ , the solution of the eigenvalue problem (13) reads

$$\psi(x, y) = 2[\sin(\pi k_1 x) \sin(\pi k_2 y) - \sin(\pi k_2 x) \sin(\pi k_1 y)] \quad (14)$$

with  $k_1 = 1, 2, \dots$  and  $k_2 = k_1 + 1, k_1 + 2, \dots$ . For the ground state,  $\psi_0(x, y)$ , one has  $k_1 = 1$  and  $k_2 = 2$ , whereas for the first excited state  $k_1 = 1$  and  $k_2 = 3$ . Thus the energy gap is  $\Delta E = E_1 - E_0 = 5\pi^2 h \sqrt{q} L^{-2}$ , and the correlation length parallel to the interface behaves as  $\xi_{||} \sim (\Delta E)^{-1} \sim L^2$ . Since the correlation length perpendicular to the interface is, at the critical point, limited by the width of the system,  $\xi_{\perp} \sim L$ , one arrives at  $\xi_{||} \sim \xi_{\perp}^2$ , in agreement with the relation mentioned above.

The density profiles satisfy the relations  $n_{1:q}(1, x) = n_{1:q}(q, 1 - x)$  and  $n_{1:q}(x) = \sum_{nb} n_{1:q}(nb, x) = 1 - n_{1:q}(1, x) - n_{1:q}(q, x)$ . From the ground state, one obtains

$$\begin{aligned}
 n_{1:q}(1, x) &= \int_x^1 dx' \int_{x'}^1 dy [\psi_0(x, y)]^2 \\
 &= \frac{4}{\pi^2} \left\{ \left[ \frac{\pi}{2} (1 - x) + \frac{1}{4} \sin 2\pi x \right] \left[ \frac{\pi}{2} (1 - x) + \frac{1}{8} \sin 4\pi x \right] - \frac{4}{9} \sin^6 \pi x \right\}
 \end{aligned}
 \tag{15}$$

For small  $x$ , one finds  $n_{1:q}(1, x) = 1 - (10\pi^2/3) x^3 + O(x^6)$ , whereas for  $x$  close to one, the profile behaves like  $n_{1:q}(1, x) \sim (1 - x)^{10}$ . The profile of non-boundary states is symmetric and its maximal value is given by  $n_{1:q}(1/2) = 1/2 + 32/(9\pi^2) = 0.86025$ .

For the (1:1) boundary condition, the profile of non-boundary states tends to zero for large values of  $q$ . Therefore the interfacial adsorption  $W$ , Eq. (2), at the transition point may be approximated by

$$\frac{W}{L} = \int_0^1 n_{1:q}(x) dx = \frac{1}{3} + \frac{35}{72\pi^2} = 0.3826
 \tag{16}$$

Thus, at the transition point,  $W$  is, indeed, proportional to  $L$ , see Eq. (8). Note that the prefactor seems to depend on  $q$ , being, at  $q = 16$ , about 0.3, according to the DMRG calculations.

Below the critical point,  $t \neq 0$ , we consider the eigenvalue equation (13) in terms of the new variables  $x_+ = (y + x)/\sqrt{2}$  and  $x_- = (y - x)/\sqrt{2}$ . Then

$$- \left[ \frac{h \sqrt{q} 2}{L^2} \left( \frac{\partial^2}{\partial x_+^2} + \frac{\partial^2}{\partial x_-^2} \right) + tL \sqrt{2} x_- \right] \psi(x_+, x_-) = E \psi(x_+, x_-)
 \tag{17}$$

with the boundary condition  $0 \leq x_- \leq x_+ \leq 1/\sqrt{2}$  and  $0 \leq x_- \leq \sqrt{2} - x_+ \leq 1/\sqrt{2}$ . Now the eigenfunction  $\psi$  can be written as  $\psi(x_+, x_-) = \phi_+(x_+) \phi_-(x_-)$ .  $\phi_+(x_+)$  satisfies the freeparticle equation  $-d^2 \phi_+/dx_+^2 = L^2 E_+ / (2h \sqrt{q}) \phi_+$ ;  $\phi_-(x_-)$  is the solution of the Schrödinger equation of a particle in a linear potential

$$- \left[ \frac{h \sqrt{q} 2}{L^2} \frac{\partial^2}{\partial x_-^2} + tL \sqrt{2} x_- \right] \phi_-(x_-) = E_- \phi_-(x_-)
 \tag{18}$$

Equation (18) leads to bound states, and the energy scale (both for the ground state and the excited states) is set by  $\varepsilon \sim t^{2/3}$ . Hence the temperature dependence of the parallel correlation length is given by  $\xi_{\parallel} \sim (\Delta E)^{-1} \sim t^{-2/3}$ , in accordance with the phenomenological considerations.<sup>(4)</sup> On the other hand, the extent of the bound states sets the length scale  $\xi_{\perp} \sim t^{-1/3}$ , which is then proportional to the interfacial adsorption,  $W$ . Thence, in the Hamiltonian limit for large values of  $q$ , one has  $\omega = 1/3$ .

## 5. SUMMARY

In this article, critical interfacial properties of two-dimensional  $q$ -state Potts models at the bulk first-order phase transition have been studied. We applied two numerical methods, Monte Carlo simulations and the density-matrix renormalization group approach, mainly at  $q = 16$ . Furthermore, we considered analytically the model in its Hamiltonian limit at large values of  $q$ .

The different methods lead to a consistent description of the critical behavior. The interfacial adsorption  $W$  diverges on approach to the phase transition temperature as  $W \propto t^{-\omega}$ ,  $\omega = 1/3$ , with a very narrow asymptotic region. The strong corrections to scaling are characterized by a small exponent,  $x = 0.14 \pm 0.06$ , which seems to depend (if at all) only weakly on the number of Potts states,  $q$ . At the critical point,  $W$  diverges linearly with the width of the system (being indefinitely long in the direction parallel to the interface). The proportionality factor has been calculated in the Hamiltonian limit.

The value of the critical exponent  $\omega$ ,  $\omega = 1/3$ , is typical for wetting phenomena at bulk transitions of first order in two dimensions. It follows from general, phenomenological considerations, based on an effective interface Hamiltonian,<sup>(4)</sup> as well as from calculations on various microscopic multi-state models, such as Potts and the Blume–Capel models. The strong corrections to scaling and the narrowness of the critical region are, on the other hand, features which are specific for Potts models. They have been predicted before<sup>(6)</sup> by using low-temperature arguments, and they have been quantified in this study.

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