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Interfacial adsorption in Potts models on the square lattice

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Abstract. We study the effect of interfacial phenomena in two-dimensional perfect and random (or disordered) q -state Potts models with continuous phase transitions, using, mainly, Monte Carlo techniques. In particular, for the total interfacial adsorption, the critical behavior, including corrections to scaling, are analyzed. The role of randomness is scrutinized. Results are discussed applying scaling arguments and invoking findings for bulk critical properties. In all studied cases, i.e., $q = 3, 4$, and $q = 8$, the spread of the interfacial adsorption profiles is observed to increase linearly with the lattice size at the bulk transition point.

PACS. 75.10.Hk Classical spin models – 05.50+q Lattice theory and statistics (Ising, Potts. etc.) – 05.10.Ln Monte Carlo method, statistical theory

1 Introduction

At the interface between coexisting phases various intriguing phenomena may occur, like roughening and wetting [1, 2]. An interesting complication arises when one considers the possibility of more than two phases. A third phase may be formed at the interface between the two other phases. An experimental realization is the two-component fluid system in equilibrium with its vapor phase [2]. The situation may be mimicked in a simplified fashion via multi-state models by fixing distinct boundary states at the opposite sides of the system. The formation of the third phase, with an excess of the non-boundary states, in such models has been called “interfacial adsorption” [3, 4].

Various aspects of interfacial adsorption, including its novel critical behavior at the bulk phase transition and the interplay with wetting, have been investigated quite extensively. In particular, specific models, like Potts and Blume-Capel models, have been studied using numerical techniques, especially, Monte Carlo (MC) methods and density renormalization-group calculations [3, 5–12]. Furthermore, scaling and analytic arguments have been presented [3, 6, 8, 13–16]. In particular, critical exponents and scaling properties of the temperature and lattice size dependencies have been determined. The fundamental role of the type of the bulk transition has been clarified, with isotropic scaling holding at continuous and tricritical bulk transitions, while interfacial adsorption is described by anisotropic scaling at a bulk transition of first-order type.

Despite the resulting interesting insights, open questions still exist. In this article, we shall mainly consider two aspects which have been largely neglected before, the

adsorption profiles and the effect of randomness on the interfacial adsorption in two-dimensional (2D) Potts models [17]. Concretely, we shall consider the q -state Potts model on the square lattice, where the ferromagnetic nearest neighbor couplings may take the values J_1 or J_2 , occurring with the same probability and being distributed randomly. Of course, when the ratio $r = J_2/J_1$ takes the value 1, one deals with the pure (or perfect) case. In the dilute (or random) case, the position of the interface, as well as the extent of the intervening third phase of non-boundary states, may be strongly affected by the spatial distribution of the couplings. Because of the inhomogeneity of a given bond realization, it seems, obviously, worthwhile to monitor not only the total excess adsorption of the non-boundary states but also the local structure of the interfacial adsorption, especially the adsorption profiles.

The bulk transition temperatures of these Potts models are known exactly from self-duality for arbitrary values of the internal states q and disorder-strength ratios r [18]. Accordingly, analyses on the critical behavior of the interfacial adsorption, based on extensive MC simulation data, as it is also done in the present paper, are significantly simplified.

Bulk criticality of such random Potts models on the square lattice has attracted much interest, partly, because the transition is of continuous type for all values of q , while being, in the perfect case, of first order for $q > 4$ [17, 19]. Then, the analysis of the interfacial adsorption in these models may be simplified by the fact, that isotropic finite-size scaling is expected to hold at continuous transitions [3, 6, 7]. Static and dynamic bulk critical properties of the random Potts models have been estimated, suppos-

edly, rather accurately, using a variety of, predominantly, numerical methods [19]. Some of these results will turn out to be very useful in our study on the interfacial adsorption.

Attention should be drawn to related previous work on interfacial phenomena in dilute ferromagnetic Potts models, in particular, considering hierarchical lattices, i.e. applying the Migdal-Kadanoff real space renormalization to the square lattice [20], or performing a preliminary MC study for the square lattice model [21].

The outline of the article is as follows: In the next Section 2, the model and the methods, especially, MC simulations of Metropolis and Wolff type, will be introduced, followed by the discussion of our main results in Section 3. The summary, Section 4, will conclude the article.

2 Model and methods

We shall study the nearest-neighbor random-bond q -state Potts model on the square lattice described by the Hamiltonian

$$\mathcal{H} = - \sum_{\langle(i,j)\rangle} J_{i,j} \delta_{s_i, s_j}, \quad (1)$$

where the Potts variable at site i , s_i , takes the values $1, 2, \dots, q$ [17]. The ferromagnetic random couplings $J_{i,j} > 0$ between nearest neighbor sites i and j are either, with probability p , J_1 or, with probability $1-p$, J_2 . In the case $J_1 > J_2$, one has either strong or weak bonds. Of course, $r = J_2/J_1 = 1$ denotes the pure (or perfect) q -state Potts model. In our study, we shall consider Potts models with $q = 3, 4$, and $q = 8$.

In this article, we shall consider the system at its self-dual point, where both couplings occur with the same probability, $p = 1/2$. Then the phase transition temperature, $k_B T_c / J_1$, between the ordered ferromagnetic phase and the high-temperature disordered phase is known to follow from [18]

$$\left(e^{(J_1/k_B T_c)} - 1 \right) \left(e^{(r J_1/k_B T_c)} - 1 \right) = q. \quad (2)$$

In the random case, the phase transition is of continuous type for all values of q , while, in the perfect case, the transition is continuous only for $q \leq 4$, being of first order at larger number of Potts states q . Exact values of the critical exponents are, so far, only known in the perfect case [17]. Numerical analyzes, in the dilute case suggest that the bulk critical exponents depend rather mildly on q [19].

The degeneracy between the q equivalent Potts states may be lifted by appropriate boundary conditions. Here, to study interfacial adsorption, we shall employ special boundary conditions, distinguishing the cases $[1 : 1]$ and $[1 : 2]$. For the case $[1 : 1]$, the Potts variable is set, at all boundary sites, equal to $q = 1$, while for the case $[1 : 2]$, the variable is set equal to 1 at one half of the boundary sites, and to 2 at the opposite half of the boundary sites. Then, the boundary condition $[1 : 2]$ introduces an interface between the 1-rich domain (or phase) and the 2-rich

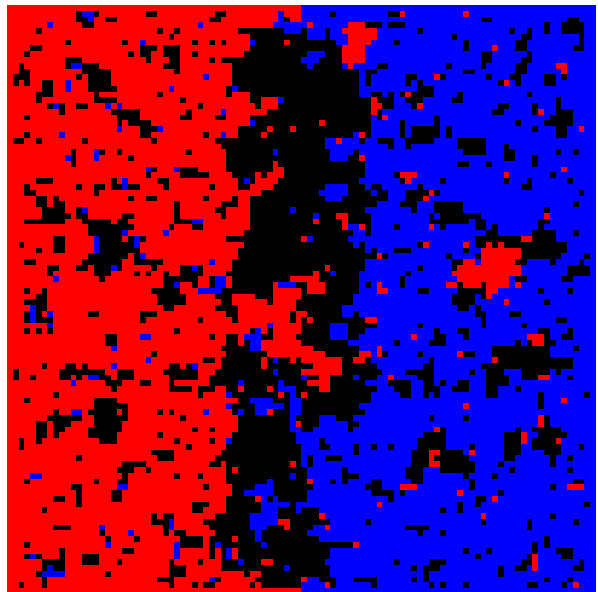


Fig. 1. (color online) Typical equilibrium MC configuration of the $L = 100$ $q = 8$ random-bond ($r = 1/10$) Potts model at temperature $T = 0.98T_c$ showing an interface for a particular bond-disorder realization. Red color depicts the $q = 1$ states, blue color the $q = 2$ states, whereas the non-boundary states ($q \geq 3$) adsorbed at the interface are shown blackened. Note that the fixed boundaries $[1 : 2]$ are also included in this illustration.

domain (or phase). By examining typical MC equilibrium configurations, as shown in Figure 1, it is seen that at the interface between the 1- and 2-rich domains an excess of the non-boundary states is generated compared to the case in the absence of an interface.

Then, the interfacial adsorption, W , measuring the surplus of non-boundary states induced by the interface between the 1-rich and 2-rich regions, is defined, for lattices with L^2 non-boundary sites, with L being the linear dimension of the lattice, by [3]

$$W = \frac{1}{L} \sum_n \sum_{\langle(i,j)\rangle} [(\delta_{s_{(i,j)},n})_{[1:2]} - (\delta_{s_{(i,j)},n})_{[1:1]}], \quad (3)$$

summing over all non-boundary sites i, j and all non-boundary states $n = 3, 4, \dots, q$. Obviously, W may be interpreted as the effective width of the domain of non-boundary states between the 1- and 2-rich domains.

Another useful quantity we shall consider is the profile, w_l , of the interfacial adsorption, measuring the surplus of the non-boundary states in line, l , parallel to the ideal, straight interface. Then,

$$W = \sum_l w_l. \quad (4)$$

One may expect w_l to fall off as one moves away from the interface. Its maximum indicates the location of the interface, which is, for a single realization of the Potts

Table 1. Numerical details used in the Wolff simulations of the 8-state ($r = 1/10$) random-bond Potts model on the square lattice. In particular, the first column marks the linear size of the lattice, the second column the number of clusters \mathcal{R}_{cl} (created during averaging) and the third the number of the independent disorder realizations \mathcal{N} .

L	Number of clusters \mathcal{R}_{cl}	Disorder samples \mathcal{N}
10	2×10^7	20000
20	2×10^7	5000
30	2×10^7	4000
40	2×10^7	5000
50	30×10^7	4200
60	40×10^7	3200
70	50×10^7	1000
80	70×10^7	1000
90	200×10^7	1000
100	300×10^7	1000

model with random couplings, not necessarily in the center of lattice. The spread, d_w , of the adsorption profile may be measured by the distance, at which w_l decreases to half of its maximal value, using a linear interpolation for the adsorption between successive lines, as will be discussed below.

Using MC techniques, we recorded, in addition to the interfacial properties, standard thermodynamic quantities, for both types of boundary conditions. In particular, we measured the thermally averaged energy, $E_{1:1}$ and $E_{1:2}$, the specific heat given by the energy fluctuations, $C_{1:1}$ and $C_{1:2}$, and the order parameter given by the majority fraction of the Potts states [17,19], $m_{1:1}$ and $m_{1:2}$.

In our simulations of the Potts models on square lattices with L^2 sites, we applied the Metropolis and the cluster-flip Wolff algorithm [22]. Of course, cluster flips violating the boundary conditions are not allowed [23]. As usual, small lattices may be simulated using the Metropolis algorithm, while the Wolff algorithm is more efficient and is preferred for larger, say $L > 30$, system sizes. Overall, we studied lattices with up to 100^2 sites for the random Potts model and 200^2 sites for its pure counterpart.

Certainly, equilibration and averaging times depend on the lattice size. Moreover, for random models, we observed that the given bond realization may affect these times. In case of the Metropolis algorithm, eventually, simulations with 10^7 Monte Carlo steps per site for $L = 10$ were performed, increasing the length of the runs, roughly, with L^2 . In case of the Wolff algorithm, the number of clusters \mathcal{R}_{cl} used in our simulations varied from 2×10^7 for the smaller systems sizes up to 3×10^9 for the larger sizes considered (see also Table 1).

The main source of error is, for random systems, the fact that the simulation data may vary quite drastically from bond configuration to bond configuration. The corresponding histograms or distributions have been recorded, especially, for the 8-state Potts model with $r = 1/10$. Bulk properties of this model have been studied quite extensively before [19,24–28]. Indeed, in the present study,

we focused much attention on this case as well. The histograms at the critical point, for the various quantities discussed above, show nearly Gaussian shapes, but being weakly tailed, in accordance with previous observations and discussions for dilute Potts models on hierarchical lattices [20]. The standard errors resulting from an ensemble average over bond realizations decrease with the number of configurations, \mathcal{N} , approximately, proportionally to $1/\sqrt{\mathcal{N}}$. The proportionality factor seems to become somewhat smaller for larger lattices. To obtain reasonable accuracy, as will be elucidated below, we averaged over a large number of different bond configurations, as given explicitly in Table 1. For pure Potts models ($r = 1$) error bars follow from averaging over a few MC runs employing different random numbers, as usual. Typically, somewhat shorter runs are needed compared to those for the random models. Usually, the error bars are not depicted in the figures, because they are smaller than the sizes of the symbols.

To determine critical properties from the MC data, we use finite-size scaling arguments. For example, for the interfacial adsorption, W , one expects [3]

$$W \approx L^a \Omega(tL^{1/\nu}), \quad (5)$$

with $a = 1 - \beta/\nu$ and the reduced critical temperature $t = |T - T_c|/T_c$. Ω is the scaling function; β and ν are the usual bulk critical exponents for the order parameter and the correlation length. A more refined ansatz invokes corrections to the asymptotic scaling behavior, as will be discussed in the following Section.

3 Results

3.1 Interfacial properties

In the perfect 2D q -state Potts models the total interfacial adsorption W is known to vanish at zero and infinite temperature, with a maximum, for finite lattices, near the critical temperature T_c . In the thermodynamic limit, $W(T, L)$ diverges with characteristic critical exponents [3, 8,13]. In the present article, we shall take a closer look at the interfacial adsorption by analyzing the corresponding profile, w_l , as well. Moreover, the impact of randomness on the interfacial properties will be studied.

Indeed, due to randomness in the couplings, the geometry of the interface between the 1- and 2-domains may be rather complicated. Straightforward considerations on the ground-state energy show readily that, in contrast to the perfect case, the interface for a given random-bond configuration is at sufficiently small values of r , not necessarily straight or in the center of the lattice. Depending on that configuration, there may be even overhangs, i.e., interfaces may not satisfy the SOS criterion. As a consequence, the adsorption profile w_l , for a fixed bond configuration, may, at non-zero temperatures, display a maximum away from the center of the lattice, as illustrated in Figure 2. As shown in that figure as well, after averaging

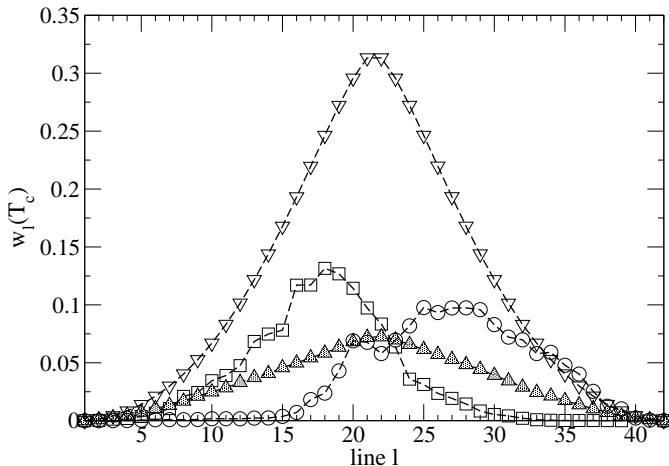


Fig. 2. Critical adsorption profiles w_l in the dilute 8-state Potts model, $r = 1/10$, for a single random-bond configuration (circles and squares) and for an average over $\mathcal{N} = 120$ realizations (triangles up). For comparison, the critical adsorption profile in the pure 8-state Potts model is depicted (triangles down).

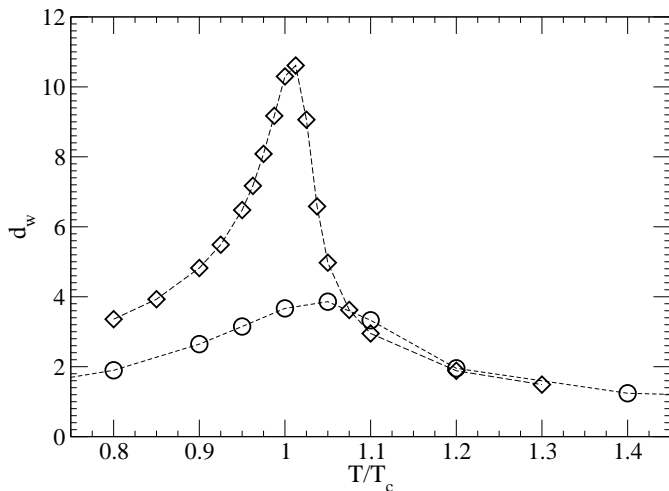


Fig. 3. Temperature dependence of the spread of the adsorption profiles $d_w(T)$ in the perfect 3-state Potts model, as observed in simulations of lattices with 20^2 (circles) and 60^2 (diamonds) sites.

over the ensemble of bond realizations, w_l is expected to be symmetric about the center of the lattice.

The total interfacial adsorption W , at the critical point, for lattices of small and moderate sizes, tends to increase with the number of non-boundary states, $q - 2$, and it is smaller in the random case compared to the perfect model. This latter observation may be explained by the fact that in the random case the system is, both for predominantly strong and weak bonds, locally effectively below or above criticality, while the interfacial adsorption is expected to be maximal close to T_c [3, 8].

Figure 2 indicates that the spread in the adsorption profiles, d_w , as defined in the previous Section, seems to increase fairly weakly due to randomness. It is found to

depend rather mildly on q . Note that the temperature dependent spread $d_w(T)$ displays a maximum close to the critical point, as illustrated in Figure 3, similar to the behavior of W [3, 8]. Its critical behavior, in the thermodynamic limit $L \rightarrow \infty$, will be analyzed in the following subsection.

3.2 Critical phenomena

Following the finite-size scaling ansatz for continuous phase transitions, equation (5), the leading critical behavior of the interfacial adsorption, W , is given by [3]

$$W(T_c) \propto L^a \quad (6)$$

and

$$W(L \rightarrow \infty, t) \propto t^b, \quad (7)$$

with the critical exponents a and b being determined by the bulk critical exponents β and ν [3]

$$a = 1 - \beta/\nu ; \quad b = \beta - \nu. \quad (8)$$

As stated before, the critical temperature, T_c , is known exactly for perfect and random Potts models on the square lattice, equation (2).

These predictions have been confirmed quite reasonably in previous Monte Carlo simulations for perfect Potts models with $q = 3$ and 4. In the present study, we extend and refine the comparison by considering randomness as well and by including corrections to scaling. The (leading or effective) corrections may be cast in the form, as usual,

$$W(T_c) = W_0 L^a (1 + c_0 L^{-x}) \quad (9)$$

and

$$W(L \rightarrow \infty, t) = W_1 t^b (1 + c_1 t^y) \quad (10)$$

with $t = |T_c - T|/T_c$. In fact, the correction terms play an important role when fitting the MC data for the lattice sizes we simulated.

Let us first discuss results for the perfect 3-state Potts model. Compared to previous simulations [3], the statistics has been improved significantly and larger lattice sizes have been studied. The size dependence of the critical adsorption, $W(T_c)$, is depicted in Figure 4. The simulation data for the complete lattice-size spectrum $L = 10 - 200$ have been analyzed by fitting them to equation (9). We have also performed a fitting for the temperature dependence of the critical adsorption of the form (10) for the largest linear size studied, i.e., $L = 200$. The resulting estimates for the critical exponents, obtained from good quality fittings with $\chi^2/\text{dof} \in \{0.6 - 1\}$, $a = 0.867(2)$ and $b = -0.728(6)$ agree nicely within errors with the predicted exact values $a = 13/15 = 0.866\cdots$ (we remind the reader that $\beta/\nu = 2/15$) and $b = -13/18 = -0.722\cdots$ [17]. Note that we fixed the leading correction-to-scaling exponents, x and y , to the predicted exact values, $x = 3/5$ and $y = 4/3$ [29–31]. Likewise, the estimates for the exponents, x and y , are observed to agree with the predicted values, when fixing the critical exponents a and b in the

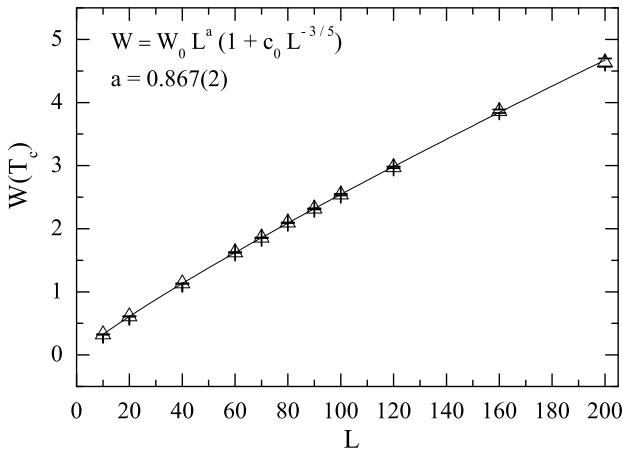


Fig. 4. Finite-size scaling of the critical interfacial adsorption of the pure 3-states Potts model, showing the simulation data and the fitting curve.

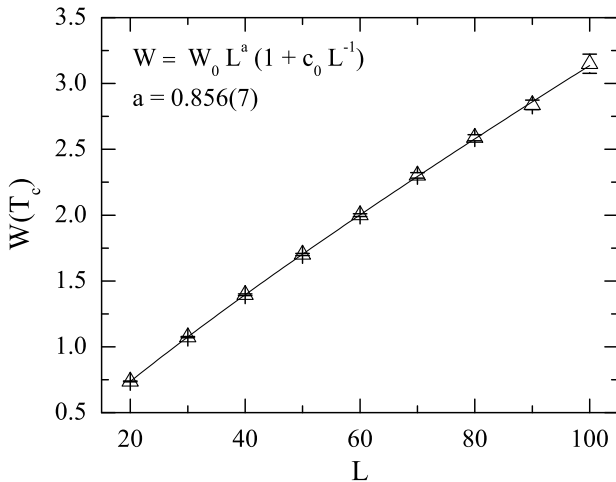


Fig. 5. Finite-size scaling of the critical interfacial adsorption data for the $q = 8$ and $r = 1/10$ diluted Potts model, showing the simulation data and the fitting curve.

fittings. Accordingly, the findings on the perfect 3-state Potts model strongly support the correctness of the finite-size scaling description (5).

The main focus of the current study is on the dilute 8-state Potts model. Following previous considerations on its bulk critical properties, we set $r = J_2/J_1 = 1/10$, where the randomness dominated behavior is expected to show up already for moderate lattice sizes [19,24–28]. In particular, we monitored, in our simulations, the size dependence of the critical interfacial adsorption $W(T_c)$. As discussed above, the standard errors stem from averaging over many bond realizations. Numerical results are depicted in Figure 5. Fitting the MC data to equation (9) with a correction-to-scaling exponent set to the value $x = -1$ which optimizes the fit, one obtains the value $a = 0.856(7)$.

For the above random case ($q = 8$ and $r = 1/10$) and from previous MC simulations and transfer-matrix calcu-

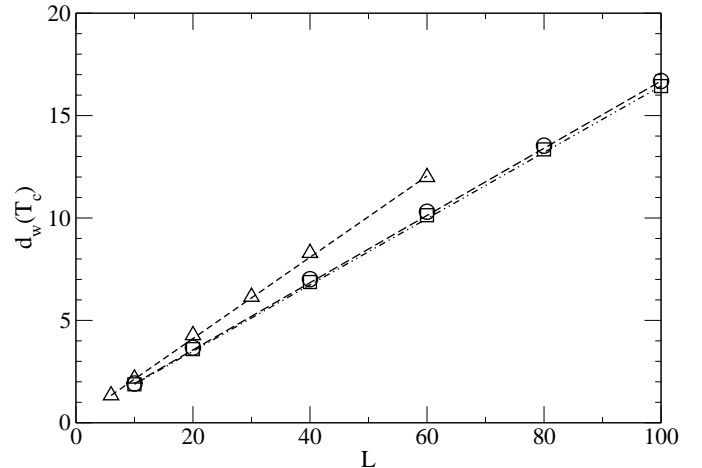


Fig. 6. Size dependence of the critical spread of the adsorption profiles $d_w(T_c)$ in the perfect 3- (circles) and 4- (squares) state as well as in the random, $r = 1/10$, 8- (triangles) state Potts models on square lattices with L^2 sites. Lines are simple guides to the eye.

lations [19,24–28], β/ν has been determined to be, approximately, 0.145 ± 0.005 . Actually, in the present simulations, we also recorded the size dependence of the order parameter, for both types of fixed boundary conditions, $m_{1:1}$ and $m_{1:2}$, vanishing, at T_c , as $\sim L^{-\beta/\nu}$. The resulting estimate for the exponent, based on simple power-law fits to the magnetization with systematically increasing the smallest lattice size, confirms the previous findings. Actually, a linear extrapolation of the fit exponent leads to the value $\beta/\nu = 0.145 \pm 0.003$ for $m_{1:1}$ as well as for $m_{1:2}$. Accordingly, we may safely conclude for the random case as well $a = 1 - \beta/\nu$, in accordance with the finite-size scaling ansatz, equation (5).

We note in passing that our Monte Carlo data on the specific heat demonstrate that the absolute value of the corresponding critical exponent α/ν is very small [19]. However, its more accurate determination is beyond the scope of the present study.

Finally, critical properties of the adsorption profile, w_l , and its spread, d_w , will be reported. As indicated by Figure 3, the spread d_w at T_c grows when increasing the lattice size. We monitored the growth for the perfect 3- and 4-state as well as for the dilute, with $r = 1/10$, 3-, 4-, and 8-state Potts models on the square lattice. The lattice size ranged from $L = 6$ up to $L = 100$. All data could be fitted well to the ansatz

$$d_w(T_c, L) = d_0 + d_1 L, \quad (11)$$

with the slope, d_1 , depending rather strongly on the randomness, but only weakly on q , as illustrated in Figure 6.

4 Summary

We performed extensive Monte Carlo simulations to study critical interfacial properties in perfect and random ferromagnetic q -state Potts models on the square lattice. In the

dilute case, there are two distinct, strong and weak, bonds connecting neighboring sites. Both bonds are assumed to occur with the same probability, leading to self-duality. Interfaces have been introduced, by fixing the Potts variables at opposite sites in two different states. The local Metropolis and the cluster-flip Wolff algorithms have been used.

Randomness is found to affect, especially, the position of the interface, the excess or interfacial adsorption, and the form of the histograms resulting from the bond realizations.

Nevertheless, predictions of the isotropic finite-size scaling description for the interfacial adsorption at continuous phase transitions are observed to hold both for the perfect and random cases, as has been exemplified for the pure 3-state and the dilute 8-state Potts models. In particular, critical exponents of the interfacial adsorption are, indeed, determined by the bulk critical exponents for the order parameter and the correlation length. These bulk exponents depend on the number of Potts states, q .

Moreover, we analyzed the adsorption profiles, describing the spatial structure of the total interfacial adsorption. The spread of the profiles seems to diverge at the phase transition in the thermodynamic limit. For lattices with L^2 sites, we find a linear increase with the linear dimension of the lattice for perfect and random models, simulating the cases $q = 3, 4$, and 8.

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