ELSEVIER

Nuclear Physics B 562 (3) [FS] (1999) 549–566

NUCLEAR PHYSICS B

www.elsevier.nl/locate/npe

Universal amplitude ratios in the 2D four-state Potts model

Michele Caselle [a], Roberto Tateo [b], Stefano Vinti [c]

[a] *Dipartimento di Fisica Teorica dell'Università di Torino and Istituto Nazionale di Fisica Nucleare, Sezione di Torino via P. Giuria 1, I-10125 Turin, Italy*

[b] *Universiteit van Amsterdam, Instituut voor Theoretische Fysica, 1018 XE Amsterdam, The Netherlands*

[c] *Institut für Theoretische Physik I, Universität Münster, Wilhelm-Klemm-Strasse 9, D-48149 Münster, Germany*

Received 1 March 1999; received in revised form 22 April 1999; accepted 16 August 1999

Abstract

We present a Monte Carlo study of various universal amplitude ratios of the two-dimensional $q = 4$ Potts model. We simulated the model close to criticality in both phases taking care to keep the systematic errors, due to finite size effects and logarithmic corrections in the scaling functions, under control. Our results are compatible with those recently obtained using the form-factor approach and with the existing low temperature series for the model.

PACS: 75.10.H; 11.10.J
Keywords: Four-state Potts; Monte Carlo; Universal amplitude ratios

1. Introduction

One of the peculiar features of the two-dimensional four-state Potts model is the presence of a marginal field which leads to universal multiplicative logarithmic corrections to the scaling laws.

These corrections can be exactly evaluated [1,2] but, as often happens when dealing with marginal fields, they are accompanied by still large subleading non-universal contributions which completely mask the scaling behaviour of the system (at least for those values of the correlation length which can be reached in standard simulations).

This is different from the behaviour, for instance, of the 3d Ising model where even at moderate values of the correlation length, the non-universal corrections [3] give very small contributions; thus they can be safely taken into account by adding to the scaling functions only the first non-universal term.

In the present case, instead, these corrections are so large that the reliability of the fits, in which only the first subleading term is taken into account, becomes questionable.

0550-3213/99/$ - see front matter
PII: S0550-3213(99)00521-0

Table 1
Results in the high temperature phase

β	L	ξ_{2nd}	E	C	χ
1.06722	120	6.44(5)	0.64604(6)	1.571(12)	11.83(2)
1.07722	120	8.46(4)	0.66318(6)	1.892(13)	18.78(3)
1.07972	120	9.25(3)	0.66808(6)	2.018(14)	21.80(4)
1.08222	120	10.26(3)	0.67337(6)	2.189(15)	25.90(5)
1.08472	120	11.60(3)	0.67909(6)	2.405(15)	31.69(6)
1.08722	180	13.37(5)	0.68544(6)	2.614(22)	40.31(9)
1.08972	180	15.94(5)	0.69232(6)	3.033(24)	54.05(13)
1.09222	240	20.33(7)	0.70056(6)	3.574(35)	80.88(24)

On the other hand, with current numerical precision, it is almost impossible to add further corrections without losing any predictive power in the fits.

This makes the numerical study of the four-state Potts model one of the most difficult tasks in the context of Monte Carlo simulations of two-dimensional spin models.

This problem was recently addressed by Salas and Sokal in [4] by extending the RG analysis of [1,2] up to third order in the fields. They succeeded in obtaining the universal leading corrections to the scaling, which turn out to be additive terms of the generic form $\log\log/\log$. The improved scaling functions were then tested by looking at the critical finite size properties of the model, and an improvement of the scaling behaviour of the data was observed which however turned out to be still affected by large non-universal $1/\log$ terms.

In this paper we return to this problem by looking at various universal amplitude combinations of the model (for a comprehensive review on amplitude ratios, see for instance, Ref. [5]). We find an improvement in the scaling behaviour of our data if the universal contributions evaluated in Ref. [4] are taken into account.

However, as in Ref. [4], this is not enough to describe the data; non-universal corrections must be considered and final results crucially depend on the type of terms included in the scaling functions. We consider this one of the most delicate aspects of this paper. For this reason we described, as precisely as possible, the procedure used to construct the scaling functions (see Section 7) and included in the paper, besides final estimates for the amplitude ratios, also the direct results of the Monte Carlo simulation (see Tables 1, 2 and 3) so that the reader can use the data to study alternative scaling

Table 2
Results in the low temperature phase: thermal observables and correlation lengths

β	L	ξ_{2nd}	E	C
1.130500	120	2.85(5)	0.850888(5)	1.3718(10)
1.120231	120	3.69(5)	0.835061(7)	1.7474(16)
1.117684	120	4.00(4)	0.830453(8)	1.8851(17)
1.115135	120	4.45(4)	0.825436(8)	2.0516(20)
1.112597	120	5.01(4)	0.820001(9)	2.2604(24)
1.110065	120	5.77(4)	0.813951(10)	2.5274(28)
1.107540	120	6.98(4)	0.807100(12)	2.9048(40)
1.105020	180	8.89(7)	0.799095(9)	3.4872(49)

Table 3
Results in the low temperature phase: magnetic observables

β	L	m	χ_l
1.130500	120	0.633288(7)	1.2180(9)
1.120231	120	0.612874(11)	2.1072(23)
1.117684	120	0.606331(13)	2.5080(26)
1.115135	120	0.598834(14)	3.0572(36)
1.112597	120	0.590219(16)	3.8447(51)
1.110065	120	0.579950(19)	5.0315(72)
1.107540	120	0.567272(26)	7.053(14)
1.105020	180	0.550686(23)	10.987(19)

functions and possibly find a clever way to control the systematic errors involved in the truncation that we suggest.

Fortunately for the present problem we have an independent way to test our results. In fact, thanks to a recent work by Cardy and Delfino [6], precise estimates for amplitude combinations are now available in the continuum limit. The relatively good agreement found between our estimates and those of [6] make us confident of the reliability of our results and at the same time strongly supports the correctness of the form-factor derivation of Ref. [6].

This paper is organized as follows. In Section 2 we give a general introduction to the q-state Potts model and we summarize a few known facts concerning the phase diagram and its scaling limit description in the framework of conformal and perturbed conformal field theory. In Sections 3 and 4 we introduce and discuss the observables and the amplitude ratios in which we are interested. In Sections 5 and 6 we describe the Monte Carlo simulation and test the results by comparing them with existing low temperature series and by imposing the duality relations on the internal energy and the specific heat. Section 7 is devoted to the study of the scaling behaviour of the observables and to extract the best estimates for the amplitude combinations. Section 8 is devoted to a comparison of the results with those of Ref. [6] while in Section 9 we have collected some concluding remarks.

2. The model

We study the four-state Potts model in two dimensions on a simple square lattice. The action is given by

$$S_{\text{Potts}} = -\beta \sum_{\langle x,y \rangle} \delta_{s(x),s(y)}, \tag{1}$$

where the field variable $s(x)$ takes the values 0,1,2,3; $x \equiv (x_0, x_1)$ labels the sites of the lattice and the notation $\langle x,y \rangle$ indicates that the sum is taken on nearest neighbor sites only. The δ function is defined as usual: $\delta_{a,b} = 1$ if $a = b$ and 0 otherwise. The coupling β is related to the temperature in the standard way $\beta \equiv 1/kT$. In the following we shall always consider lattices of equal extension L and periodic boundary conditions in both directions.

Several results are known exactly for this model. The action (1) is invariant under the permutation group S_4. However, in the low temperature phase this symmetry is spontaneously broken to S_3. The two phases are related by duality and separated by a second-order phase transition located at $\beta_c \equiv 1/kT_c = \log(3) = 1.098612$. The dual coupling $\tilde{\beta}$ is related to the original coupling β by

$$\tilde{\beta} = -\log\left(\frac{1-e^{-\beta}}{1+3e^{-\beta}}\right), \tag{2}$$

and the fixed point of this relation is the critical coupling β_c.

It is useful to introduce the variables

$$\sigma_\alpha(x) = \delta_{s(x),\alpha} - \frac{1}{4}, \quad \alpha = 0,1,2,3. \tag{3}$$

It is easy to see that $\langle \sigma_\alpha \rangle = 0 \ \forall\alpha$ in the high temperature phase and that they all become different from zero in the low temperature phase. In particular for one of the four values of the spin (which we shall call in the following ''majority spin'') $\langle \sigma_\alpha \rangle > 0$, while for the three other values we have $\langle \sigma_\alpha \rangle < 0$.

It has been shown (cf. Ref. [7]) that the partition function $Z(T,q)$ for the q-state Potts models (q integer) on a square lattice Λ can be written as

$$Z(T,q) = \sum_{\{G\}} (e^\beta - 1)^N q^\nu. \tag{4}$$

The sum in Eq. (4) runs over all the graphs G on Λ, C is the number of connected components (including isolated sites) in G, and N is the number of bounds on the lattice edges. For a better understanding of some of the peculiar features of the four-state Potts model it is convenient to consider the phase diagram of the whole family of models, defined for arbitrary $q > 0$. Eq. (4) provides an expression suitable for extending the definition of $Z(T,q)$ to non-integer values of q. The q-state Potts model undergoes a phase transition at

$$\beta_c = \log\left(\sqrt{q} + 1\right). \tag{5}$$

Below this temperature the system is in its S_q-broken symmetry phase whereas above it the system is fully disordered. The transition at $T = T_c$ is first-order for $q > 4$ but becomes second-order for $q \leqslant 4$, in the latter case the model gets renormalized into a conformal field theory with central charge [8]

$$c = 1 - \frac{6}{(l-1)l}, \tag{6}$$

where l is related to q by

$$\frac{2\pi}{l} = \arctan\left(\frac{\sqrt{4q-q^2}}{(q-2)}\right). \tag{7}$$

In the scaling limit, at rational points $l = p/(p' - p)$, the thermal field ε rescales with scaling dimension [9]

$$\Delta_\varepsilon = \frac{1}{2}\left(1 + \frac{3}{l-1}\right), \tag{8}$$

hence it can be identified with the operator ϕ_{21} in the $M_{p,p'}$ minimal conformal model. Notice also that Eq. (7) shows that two square-root branch points at $q = 0$ and $q = 4$ are present. At $q = 0$ the thermal operator is marginal, in the analytically continued second branch it becomes irrelevant and the critical point has moved into the antiferromagnetic region. The physics in this sector is certainly very interesting but it is slightly less relevant for our current interests. More related to the subject of this paper is, instead, the physical meaning of the second branch point at $q = 4$. Let us consider a further variant of the model in which vacancies are allowed, and correspondingly a chemical potential μ is introduced. In the sector $0 < q < 4$ with μ negative or sufficiently small, the additional dilution field turns out to be irrelevant and the system still undergoes a second-order phase transition in the same universal class of the pure Potts model. Near the transition point the dilution field scales with a conformal dimension

$$\Delta_\mu = 2 + \frac{4}{l-1}, \tag{9}$$

and it can be identified with the primary conformal operator ϕ_{31}.

At $q = 4$, the dilution field ϕ_μ becomes marginal; along the critical RG flow its slow rate of disappearance causes now multiplicative logarithm corrections to the critical behaviour. From Eq. (7) we also see that the net result of the entrance in the second branch consists of a turning negative of l. Hence at the same value of q, but on the second branch, we now have a conformal field theory (CFT) with central charge

$$c = 1 - \frac{6}{l(l+1)}, \tag{10}$$

with thermal and dilution fields with dimensions

$$\Delta_\varepsilon = \frac{1}{2}\left(1 - \frac{3}{l+1}\right), \qquad \Delta_\mu = 2 - \frac{4}{l+1}. \tag{11}$$

These two fields can now be respectively identified with the relevant conformal operators ϕ_{12} and ϕ_{13}. In conclusion, at fixed $q < 4$, the phase diagram in the plane (μ, T) is as follows: if μ is negative or sufficiently small, then at $T = T_c(\mu)$ the system undergoes a second-order phase transition in the universal class of the pure Potts model, whereas when μ is large the transition becomes of first order. On the critical line $(\mu, T_c(\mu))$ the point marking the change of critical behavior is the tricritical point. From the scaling quantum field theory point of view, the picture looks also consistent with the one described above. First notice that perturbation of the conformal field theory with either the thermal or the dilution field is integrable [10] and that the associated quantum field theories have been the subject of very deep studies (see for example Refs. [11–16]). The thermal operator ε drives the system into a massive ordered or disordered phase depending on the sign of the perturbing parameter [14–16]. The operator ϕ_μ instead moves the tricritical model either into a massive phase (a line of first-order

transitions) or into a critical massless phase. The IR fixed point of the latter is the Potts-model CFT and the two less irrelevant attracting operators are the fields ϕ_{31} and $T\bar{T}$ [14–16].

Quantum reductions of the Izergin–Korepin model at rational points, giving the S-matrix elements for the ϕ_{12}/ϕ_{21} perturbations, were first obtained by Smirnov [11]. Subsequently, using a somehow different kink basis, Chim and Zamolodchikov [17] defined alternative scattering elements for the model. The latter formulation, being more suitable for analytic continuation at arbitrary values of q, has been used by Cardy and Delfino [6] to make predictions about the values of some universal amplitudes. The method used is a variant of the form-factor approach to the correlation functions proposed in [18].

3. The observables

3.1. Magnetization

The magnetization of a given configuration is defined as

$$m = \frac{1}{V} \sum_x \sigma_{\alpha_m}(x), \tag{12}$$

where $V \equiv L^2$ is the volume of the lattice and α_m is the value of the spin corresponding to the majority of the spins. However, in a finite volume at arbitrary finite low temperature the S_4 symmetry of the model is not spontaneously broken. Practically this means that, in the simulation sample, configurations with all the four possible values of α_m appear with equal probability. In order to obtain a low temperature non-vanishing magnetization a magnetic field h that explicitly breaks the symmetry, must be coupled to the system. The thermodynamic limit at non-zero h should be taken first, then the limit of vanishing magnetic field could be performed. However, it is difficult to follow this route in a numerical study. An alternative, commonly adopted, approach is to identify α_m in each configuration by counting the spins belonging to the four possible values of α and then extracting the majority one. This procedure works in a satisfactory way if the lattice size and coupling constants are such that the probability of finding interfaces among different vacua is negligible. We carefully chose our lattice sizes so as to satisfy this bound.[1]

In the following we shall assume for simplicity that $\alpha_m = 0$ is the value of the majority spin and shall denote the remaining three values with Latin indices $i, j, k, \ldots = 1,2,3$.

[1] Let us note, as a side remark, that this procedure in the Ising case is equivalent to the choice

$$\langle m \rangle \equiv \lim_{L \to \infty} \langle |m| \rangle \quad \left(m = \frac{1}{V} \sum_i s_i \right),$$

where the s_i's are in this case Ising spins. The finite size behaviour of this observable was carefully studied in [19]. It was shown that this choice converges to the infinite volume value better than any other existing proposal and that the asymptotic, infinite volume, value is reached for lattices of size $L > \sim 8\xi$, where ξ denotes the correlation length. In our simulations we always used lattice sizes much larger than this threshold.

Close to criticality and at $t \equiv \frac{\beta_c - \beta}{\beta_c} < 0$, the magnetization scales as [4]

$$\langle m \rangle \sim B(-t)^{1/12}(-\log(-t))^{-1/8} \times \left[1 - \frac{3}{16}\frac{\log(-\log(-t))}{-\log(-t)} + O\left(\frac{1}{\log(-t)}\right)\right]. \tag{13}$$

3.2. Magnetic susceptibility

The susceptibility

$$\chi = \frac{\partial \langle m \rangle}{\partial H} \tag{14}$$

gives the response of the magnetization to an external magnetic field and it can be expressed in terms of moments of the magnetization

$$\chi = V\left(\langle m^2 \rangle - \langle m \rangle^2\right). \tag{15}$$

In the high temperature phase this means

$$\chi = V\langle m^2 \rangle = V\langle \sigma_\alpha{}^2 \rangle, \tag{16}$$

where α is any one of the four values (0,1,2,3).[2]

In the broken symmetric phase, depending on the choice of coupling the external magnetic field to the majority spin or to one (or more) of the other values, two kinds of susceptibilities can be defined [21]

$$\chi_l = \langle \sigma_0^2 \rangle \quad \text{longitudinal}, \tag{17}$$

$$\chi_t = \langle (\sigma_i - \sigma_j)^2 \rangle \quad (i \neq j) \quad \text{transverse}. \tag{18}$$

In this paper we concentrate on the longitudinal susceptibility χ_l.

Close to the critical temperature χ and χ_l scale as[3]

$$\chi \sim \Gamma_+ (t)^{-7/6}(-\log|t|)^{3/4}\left[1 + \frac{9}{8}\frac{\log(-\log|t|)}{-\log|t|} + O\left(\frac{1}{\log|t|}\right)\right] \quad (t > 0),$$

$$\chi_l \sim \Gamma_- (-t)^{-7/6}(-\log|t|)^{3/4}\left[1 + \frac{9}{8}\frac{\log(-\log|t|)}{-\log|t|} + O\left(\frac{1}{\log|t|}\right)\right] \quad (t < 0). \tag{19}$$

[2] Notice however that, inspired by the analogy with the Ising model or by the embedding in the AT model, different definitions of the order parameter (hence of the mean magnetization in the symmetric phase) are possible. For instance

$\langle m_1 \rangle = \langle \sigma_\alpha - \sigma_\beta \rangle$

with $\alpha \neq \beta$ or

$\langle m_2 \rangle = \langle \sigma_\alpha - \sigma_\beta + \sigma_\gamma - \sigma_\delta \rangle$

with $\alpha \neq \beta \neq \gamma \neq \delta$. The corresponding susceptibilities are related to χ by simple multiplicative constants. In comparing our results with those of Refs. [4,20] one must take into account this different normalization.

[3] Notice that there is a misprint in the analogue of this equation in Ref. [4].

3.3. Internal energy and specific heat

The internal energy is defined as

$$E = \frac{1}{2V} \sum_{\langle x,y \rangle} \delta_{s(x),s(y)}, \tag{20}$$

and the specific heat as

$$C \equiv \frac{d\langle E \rangle}{d\beta} = 2V\big(\langle E^2 \rangle - \langle E \rangle^2\big). \tag{21}$$

Duality relates both internal energy and specific heat in the low temperature phase to those in the high temperature phase. The relations are

$$(1 - e^{-\beta})\, E(\beta) = 1 - \big(1 - e^{-\tilde{\beta}}\big) E\big(\tilde{\beta}\big), \tag{22}$$

$$C(\beta)(1 - e^{-\beta})^2 + e^{-\beta}(1 - e^{-\beta})\, E(\beta) = C\big(\tilde{\beta}\big)\big(1 - e^{-\tilde{\beta}}\big)^2 + e^{-\tilde{\beta}}\big(1 - e^{-\tilde{\beta}}\big) E\big(\tilde{\beta}\big). \tag{23}$$

Close to the critical temperature we have

$$C \sim A_+ (t)^{-2/3} (-\log|t|)^{-1} \left[1 - \frac{3}{2} \frac{\log(-\log|t|)}{-\log|t|} + O\left(\frac{1}{\log|t|}\right)\right] \quad (t > 0),$$

$$C \sim A_- (-t)^{-2/3} (-\log|t|)^{-1} \left[1 - \frac{3}{2} \frac{\log(-\log|t|)}{-\log|t|} + O\left(\frac{1}{\log|t|}\right)\right] \quad (t < 0). \tag{24}$$

3.4. Second moment correlation length

We consider the decay of so-called time-slice correlation functions. The magnetization of a time slice is given by

$$S_\alpha(x_0) = \frac{1}{L} \sum_{x_1} \sigma_\alpha(x_0, x_1). \tag{25}$$

Let us define the correlation function

$$G_{\alpha\beta}(\tau) = \sum_{x_0} \big\{\langle S_\alpha(x_0) S_\beta(x_0 + \tau)\rangle - \langle S_\alpha(x_0)\rangle \langle S_\beta(x_0)\rangle\big\}. \tag{26}$$

For any choice of the indices α and β in (26), the dominant large distance behaviour of $G(\tau)$ is dominated by the lowest mass of the model,

$$G(\tau) \propto \exp(-\tau/\xi), \tag{27}$$

where ξ is the exponential correlation length and coincides with the inverse of the lowest mass of the model. However, at low temperature, the rich structure of the spectrum (cf. Ref. [6]) can mask this asymptotic behaviour. For this reason, in the following, we shall concentrate on G_{00} which has the ''neatest'' asymptotic behaviour.

This will also allow us to directly compare our results with those of Ref. [6]. In the high temperature phase the lowest mass is well separated from all other excitations in the spectrum and extracting the exponential correlation length is much simpler.

Close to criticality the behaviour of the correlation length is governed by the scaling laws

$$\xi \sim f_+(t)^{-2/3}(-\log|t|)^{1/2}\left[1+\frac{3}{4}\frac{\log(-\log|t|)}{-\log|t|}+O\left(\frac{1}{\log|t|}\right)\right] \quad (t>0),$$

$$\xi \sim f_-(-t)^{-2/3}(-\log|t|)^{1/2}\left[1+\frac{3}{4}\frac{\log(-\log|t|)}{-\log|t|}+O\left(\frac{1}{\log|t|}\right)\right] \quad (t<0). \tag{28}$$

We are also interested in the second moment correlation length ξ_2, to evaluate ξ_2 we used the estimator [4,20]

$$\xi^{(2)} \equiv \frac{\left(\frac{\chi}{F}-1\right)^{1/2}}{2\sin(\pi/L)}, \tag{29}$$

where χ is the susceptibility and F is the Fourier transform of the correlation function at the smallest non-zero momentum $(2\pi/L,0)$.

Notice that the susceptibility can be rewritten as the zero momentum Fourier transform of the correlation function, hence, in order to have a consistent definition, the same correlation function must be chosen in both χ and F. In the low temperature regime we are interested in setting the longitudinal susceptibility

$$\chi_l \equiv \sum_x G_{0,0}(x) \tag{30}$$

in Eq. (29), hence, we shall study

$$F \equiv \sum_x e^{2i\pi x_1/L} G_{0,0}(x). \tag{31}$$

ξ_2 is a very popular approximation for the exponential correlation length since, in Monte Carlo simulations, its numerical evaluation is much simpler than that of ξ.

Moreover, it is the length scale which is directly observed in scattering experiments. It is important to stress that ξ_2 and ξ are not fully equivalent (cf. Ref. [3]), even though their critical behaviours are the same up to a multiplicative factor. In particular, the ratio ξ/ξ_2 gives an idea of the density of the lowest states of the spectrum. If the lower excited states are well separated the ratio is almost one, whereas a significantly bigger ratio indicate a denser distribution of states. Furthermore, different choices of the correlation function in Eqs. (30), (31) lead to different values of ξ_2, while the exponential correlation length is always the same. A careful study of these differences can give several information on the spectrum of the theory. We shall call the critical amplitudes $f_{2,\pm}$ for ξ_2 to distinguish them from $f_\pm$.

4. Amplitude ratios

We are interested in the following amplitude ratios

$$R_\chi = \frac{\Gamma_+}{\Gamma_-}, \qquad R_{\xi,2} = \frac{f_{2,+}}{f_{2,-}}, \tag{32}$$

and the following amplitude combinations:

$$R_1 = \frac{\Gamma_-}{f_{2,-}^2 B^2} \qquad R_2 = \frac{\Gamma_+}{f_{2,+}^2 B^2}, \tag{33}$$

which are scale invariant thanks to the (hyper)scaling relations among the critical exponents

$$\alpha + 2\beta + \gamma = 2, \qquad d\nu = 2 - \alpha. \tag{34}$$

We are also interested in the combinations

$$R_c^+ = \frac{A_+ \Gamma_+}{B^2}, \qquad R_\xi^+ = \sqrt{A_+}\, f_{2,+}, \tag{35}$$

$$R_c^- = \frac{A_- \Gamma_-}{B^2}, \qquad R_\xi^- = \sqrt{A_-}\, f_{2,-}. \tag{36}$$

which have particularly interesting behaviours in the four-state Potts model (see below). We shall neglect the amplitude ratio A_+/A_- which is trivially 1 due to duality.[4]

5. The simulations

We produced a standard cluster algorithm using both the Wolff single cluster update and the Swendson–Wang cluster update. After preliminary tests, we used the latter algorithm for our high statistic simulations.

To check our program we made comparisons of the MC results with the exact solution on a 3^2 lattice and with the Salas and Sokal [4,20] results at the critical point on a 16^2 lattice, with a comparable statistics.

We simulated the four-state Potts model in the high and low temperature phases for 16 values of the couplings which were chosen exactly as dual pairs. This choice allowed us, first, to perform a very stringent test on our estimates for the thermal observables which must be related by duality and, second, to obtain a direct estimate of some amplitude ratios. The results for the observables in which we are interested are reported in Tables 1, 2 and 3.

[4] In principle this result could be used to test our simulation. But such a test is completely equivalent to the test of the duality relation (23) that we perform in Tables 4 and 5.

Table 4
Comparison between the internal energy measured in the simulation at high temperature (second column) and the values obtained, from the internal energy measured at low temperature, using the duality relation (22) (third column)

β	HT	LT + Eq. (22)
1.06722	0.64604(6)	0.646061(5)
1.07722	0.66318(6)	0.663179(7)
1.07972	0.66808(6)	0.668074(8)
1.08222	0.67337(6)	0.673365(8)
1.08472	0.67909(6)	0.679055(9)
1.08722	0.68544(6)	0.685341(10)
1.08972	0.69232(6)	0.69240(1)
1.09222	0.70056(6)	0.70060(1)

Lattice sizes were chosen large enough to make finite size effects negligible within our statistical errors. After a preliminary test on the finite size behaviour of our observables we chose $L > 10\xi$ in the high temperature phase and $L > 20\xi$ in the low temperature phase, a default size $L = 120$ was taken for small values of ξ. In each simulation the number of measurements was 2×10^7. Each measurement was separated from the next one by two Swendsen–Wang updates. A standard jacknife procedure has been used to analyze statistical errors.

6. Analysis of the results

6.1. Energy and specific heat

By using Eq. (22) we have a non-trivial test of our estimates both for the energy and for the specific heat. In Table 4 we compare the results for the internal energy in the high temperature phase with those obtained using Eq. (22) and the values measured with

Table 5
Comparison between the specific heat measured in the simulation at high temperature (second column) and the values obtained, from the internal energy and the specific heat measured at low temperature, using the duality relations (22), (23) (third column)

β	HT	LT + Eq. (23)
1.06722	1.571(12)	1.555(1)
1.07722	1.892(13)	1.903(2)
1.07972	2.018(14)	2.032(2)
1.08222	2.189(15)	2.191(2)
1.08472	2.405(15)	2.391(3)
1.08722	2.614(22)	2.646(3)
1.08972	3.033(24)	3.011(4)
1.09222	3.574(35)	3.579(5)

Table 6
Comparison of our Monte Carlo results for the magnetization with a Padé resummation of the series of Ref. [22]

β	Our MC	Series
1.130500	0.633288(7)	0.633275
1.120231	0.612874(11)	0.612863
1.117684	0.606331(13)	0.606310
1.115135	0.598834(14)	0.598853
1.112597	0.590219(16)	0.590268
1.110065	0.579950(19)	0.580154
1.107540	0.567272(26)	0.567899
1.105020	0.550686(23)	0.552456

the dual coupling, at low temperature as input. A similar comparison for the specific heat can be found in Table 5.

6.2. Magnetization and susceptibility

In Tables 6 and 7 we compare our results for the magnetization and the low temperature longitudinal susceptibility with the series of Ref. [22]. Both for the magnetization and for the susceptibility we used the diagonal Padé approximant. As expected, the agreement, which is rather good far from the critical point becomes worse and worse as β_c is approached. Notice however that we used the simplest possible resummation technique, more sophisticated approaches like the double biased IDA of Ref. [23] could give better results and could also give a way to estimate the systematic errors involved in the truncation and resummation of the series (for an attempt in this direction in the case of the 3d Ising model see for instance Ref. [3]).[5] In the case of the susceptibility the discrepancy between the results from the series expansion and our Monte Carlo are larger and only the first value of beta agree within the errors. It is clear however that we are pushing the series to their limit of validity and in fact, looking at non-diagonal Padé approximants, one sees very large fluctuations (much larger than in the case of magnetization) in the series estimates.

7. Scaling behaviour

Let us now address the problem of extracting the continuum limit values of the quantities discussed in the previous section. As mentioned in Section 1, due to the presence of large corrections to scaling terms, this requires a rather non-trivial analysis. We followed a three step procedure.

(1) As first test we tried to fit the data using only the dominant multiplicative log correction keeping into account for C and χ the possible existence of bulk constant terms. Hence a one-parameter fit for ξ_2 and m and a two-parameter fit for C and χ. In all cases we found very high χ_r^2 and, even eliminating all the data except the two

[5] In comparing our values of the magnetization with those of Ref. [22] one must notice that there is a factor $4/3$ between the two definitions of magnetization. On the contrary, there is complete agreement between the two definitions for the longitudinal susceptibility.

Table 7
Comparison of our Monte Carlo results for χ_l with a Padé resummation of the series of Ref. [22]

β	Our MC	Series
1.130500	1.2180(9)	1.2187
1.120231	2.1072(23)	2.1241
1.117684	2.5080(26)	2.5395
1.115135	3.0572(36)	3.1179
1.112597	3.8447(51)	3.9661
1.110065	5.0315(72)	5.3242
1.107540	7.053(14)	7.795
1.105020	10.987(19)	13.647

couplings nearest to β_c, it was impossible to reach a reasonable confidence level. This clearly indicates that additive corrections to the scaling cannot be neglected.

(2) The second step was to add the first non-universal correction, (that of the form $1/\log$). At the same time we also included the universal corrections evaluated by Salas and Sokal, which are of the same order of magnitude and do not add degrees of freedom in the fit. The resulting fitting functions are (see Section 3)

$$\chi(t) = a_0 + \Gamma_{\pm}|t|^{-7/6}(-\log|t|)^{3/4}\left[1 + \frac{9}{8}\frac{\log(-\log|t|)}{-\log|t|} + \frac{a_1}{-\log|t|}\right], \tag{37}$$

$$\xi_2(t) = f_{2,\pm}|t|^{-\frac{2}{3}}(-\log|t|)^{1/2}\left[1 + \frac{3}{4}\frac{\log(-\log|t|)}{-\log|t|} + \frac{a_1}{-\log|t|}\right], \tag{38}$$

$$m(t) = B|t|^{1/12}(-\log|t|)^{-1/8}\left[1 - \frac{3}{16}\frac{\log(-\log|t|)}{-\log|t|} + \frac{a_1}{-\log|t|}\right]. \tag{39}$$

$$C(t) = a_0 + A_{\pm}|t|^{-2/3}(-\log|t|)^{-1}\left[1 - \frac{3}{2}\frac{\log(-\log|t|)}{-\log|t|} + \frac{a_1}{-\log|t|}\right], \tag{40}$$

We performed these two- (or three-) parameter linear fits, first taking into account all the data and then systematically eliminating those farthest from the critical point until an acceptable reduced χ^2 (namely a χ^2 lower than 1) was reached. In all cases, except for the magnetization, with this second step we reached an acceptable C.L. and stopped. Notice that in most of the cases such acceptable C.L. could be reached keeping all the data (see the second column of Table 8). We also realized at this stage that the critical

Table 8
Results of the fits for susceptibility, magnetization and correlation length. In the second column we report the number of data taken into account in the fit, in the third column the reduced chi squared and in the fourth column the confidence level of the fit. The last four columns contain the best fit estimates of the parameters of the fit. For the magnetization we also have the contribution of a next to leading magnetization operator (see text) a_2

Obs.	N	χ^2_r	C.L.	Amplitude	a_0	a_1	a_2
χ_+	8	0.93	46%	$\Gamma_+ = 0.0223(14)$	0.05(14)	6.5(4)	
χ_-	8	0.44	81%	$\Gamma_- = 0.00711(10)$	0.02(1)	−1.24(10)	
$\xi_{2,+}$	8	0.48	82%	$f_{2,+} = 0.192(4)$		1.35(11)	
$\xi_{2,-}$	7	0.44	82%	$f_{2,-} = 0.088(4)$		1.06(27)	
m	8	0.80	54%	$B = 1.1621(11)$		−0.220(6)	−0.144(9)

amplitudes $A_\pm$ could be obtained in a much more efficient way by looking at the internal energy data. We shall discuss this point in detail in Subsection 7.1.

(3) In the next step we added a next-to-leading non-universal correction. Among the various possible terms we chose the one giving, in the range of values of β of our simulations, the largest contribution. We had to resort to this last step only for the magnetization. In this case there are two competing corrections. The first one is the $1/\log^2$ term: certainly expected due to the presence of the marginal field. But there is also second possibility: thanks to the CFT solution of the model we know that in the spectrum there is a subleading magnetic operator to which corresponds a new critical index $\beta' = 3/4$.

The two terms have comparable magnitude, but it turns out that the subleading magnetic correction gives a slightly larger contribution in the range of interest. So, according to our strategy, we kept only this contribution and neglected the $1/\log^2$ one. The resulting scaling function is

$$m(t) = B|t|^{1/12}(-\log|t|)^{-1/8}\left[1 - \frac{3}{16}\frac{\log(-\log|t|)}{-\log|t|} + \frac{a_1}{-\log|t|} + a_2|t|^{2/3}\right]. \tag{41}$$

Adding also the subleading magnetic term in the fit we found an impressive lowering of the χ^2.

The results of these fits are summarized in Table 8. It is important to stress that all the quoted errors are *statistical*. Apart from them we also expect *systematic* errors due to the truncation of the scaling functions to $O(\log|t|)$ or, in the case of the magnetization, to the choice of the next-to-leading non-universal correction. In Subsection 7.2 we shall discuss this problem in more detail.

7.1. The critical amplitudes $A_\pm$

The most efficient way to obtain the critical amplitudes $A_\pm$ is to fit the internal energy (for which we have very precise data) instead of the specific heat. The bulk value of the energy is known (from duality) to be $E(\beta_c) = \frac{3}{4}$ however, due to the finite size of the lattice that we simulated we must account for possible small deviations from this asymptotic result. We end up with the following fitting function:

$$E(t) = \frac{3}{4} + a_{-1} + a_0|t| + 3A_\pm|t|^{1/3}(-\log|t|)^{-1} \times\left[1 - \frac{3}{2}\frac{\log(-\log|t|)}{-\log|t|} + \frac{a_1}{-\log|t|}\right]. \tag{42}$$

A severe constraint on the results of this fit is represented by duality which implies $A_+ = A_-$. The result of the fits in the low and high T phases are reported in Table 9,

Table 9
Results of the fits for the internal energy

Obs.	N	χ^2_r	C.L.	Amplitude	a_{-1}	a_0	a_1
E_+	7	0.67	57%	$A_+ = 1.29(5)$	−0.0001(29)	3.0(1.3)	−1.47(48)
E_-	7	0.87	45%	$A_- = 1.316(9)$	−0.0056(5)	1.30(18)	−0.93(6)

where it can be seen that the values of a_0, and $A_\pm$ extracted in the two phases are indeed compatible within the errors and that a_{-1} is, as expected, very small. Combining the two estimates of A_+ and A_- we extract as our final estimate: $A_\pm = 1.30(6)$.

7.2. Non-universal corrections

A crucial ingredient to test the reliability of the above fits is given by the magnitude of the non-universal corrections. In the range of β values that we studied the log of the reduced temperature t takes values which range from -4 up to -5. The non-linear contributions listed in Tables 8 and 9 must be compared with this reference scale. One easily realizes that for all quantities these corrections are rather large (they are more or less of the same order of magnitude of the universal corrections evaluated in Ref. [4]) and in the particular case of the high temperature susceptibility they are very large. This suggests that, even if the fits have a very good confidence level, caution is needed in assuming the best fit estimates for the amplitudes which could be affected by systematic deviations. Notice that there is no hope to control such large non-universal contributions by tuning β towards the critical temperature. In fact it would be necessary to gain at least a factor 10 in $\log(t)$ which, as can easily be seen, would imply a huge enhancement of ξ.

We tried to estimate the systematic errors which affect our estimates of the critical amplitude with the following method. We repeated the analysis discussed above adding in the fitting functions a term of the form $1/(\log(t))^2$ (which in the range of values of t that we study is the largest among the corrections to scaling terms that we neglect) with amplitude equal in modulus to the a_1 amplitudes listed in Tables 8 and 9 and with plus and minus sign. The two resulting values for the critical amplitude give an (admittedly rough) idea of the systematic deviations that we may expect in our estimates. The results are collected in Table 10. By comparing with the statistical errors listed in Tables 8 and 9, one can see that the in all cases the systematic deviations are larger than the statistical errors.

7.3. Universal amplitude ratios

Plugging the values of the critical amplitudes quoted in Table 10 in the definitions (32), (33), (35), (36) we find the values for the amplitude ratios reported in the second

Table 10
Critical amplitudes with a tentative estimate of the systematic errors

Amplitude
$\Gamma_+ = 0.0223(40)$
$\Gamma_- = 0.00711(30)$
$f_{2,+} = 0.192(10)$
$f_{2,-} = 0.088(6)$
$B = 1.1621(25)$
$A_\pm = 1.30(10)$

Table 11
Comparison between our estimates for the universal amplitude ratios and those of Ref. [6]

Ratio	This work	Ref. [6]
R_χ	3.14(70)	4.013
R_ξ	2.19(26)	1.935
R_1	0.68(13)	0.4539
R_2	0.44(13)	0.4845
R_c^+	0.021(5)	0.0204
R_c^-	0.0068(9)	0.0051
R_ξ^+	0.220(20)	0.2052
R_ξ^-	0.100(10)	0.1060

column of Table 11. The errors quoted in Table 11 have been obtained by using the systematic errors quoted in Table 10 and discussed in Subsection 7.2.

8. Comparison with field theory predictions

It is very interesting to compare our results with the R_χ, R_ξ, R_c^+, and R_ξ^+ estimates obtained, using the S-matrix form-factor approach to the correlation functions, in Ref. [6]. It easy to obtain the remaining four ratios by using the following relations:

$$R_c^- = \frac{R_c^+}{R_\chi}, \qquad R_\xi^- = \frac{R_\xi^+}{R_\xi}, \qquad R_1 = \frac{R_c^-}{\left(R_\xi^-\right)^2}, \qquad R_2 = \frac{R_c^+}{\left(R_\xi^+\right)^2}. \tag{43}$$

We compare our final estimates and those of Ref. [6] in Table 11. We immediately observe a good overall agreement. This agreement is highly non-trivial since, as discussed above, in our estimates we had to face large non-universal corrections, while in the predictions of [6] only the lowest states of the spectrum were taken into account and some small discrepancies with the exact results were expected. If we trust the overall agreement that we have found we immediately see that the major discrepancies between the two sets of data are in the two ratios R_χ and R_1, which could both be consequences of a biased estimate of Γ_-. It would be important to understand the reason of this discrepancy. In this respect it is worthwhile to notice that χ_l is the only observable for which the non-universal correction has the opposite sign with respect to the universal additive one.

9. Concluding remarks

The aim of this paper was to test the recent predictions of Ref. [6] for various amplitude ratios in the four-state Potts model, with the results of a high precision Monte Carlo simulation.

We made four tests on the results of our simulations:

- Comparison with exact results for small lattices.
- Comparison with the results of Refs. [4,20] at the critical point.
- Comparison with low temperature series.
- Agreement with the duality relations.

All these tests were successfully passed.

In looking at the scaling behaviour of our observables, we had to face a major problem, due to the presence of a marginal field in the spectrum. In performing the analysis we used the recent results of Salas and Sokal on the universal additive $\log\log/\log$ correction terms, and found in our fits the same behaviour and the same features that they reported in Ref. [4] where they looked at the finite size corrections at the critical point.

We found a relatively good overall agreement with the predictions of Cardy and Delfino with the exception of two ratios involving the low temperature susceptibility. It remains an open problem to find a more efficient way of dealing, in the analysis of Monte Carlo data, with corrections originated by the presence of marginal operators. These contributions are the probable main cause of these discrepancies.

Acknowledgements

We thank J.L. Cardy, G. Delfino, P. Dorey, F. Gliozzi and B. Nienhuis for helpful discussions. This work was partially supported by the European Commission TMR programme ERBFMRX-CT96-0045.

References

[1] M. Nauenberg, D.J. Scalapino, Phys. Rev. Lett. 44 (1980) 837.
[2] J.L. Cardy, M. Nauenberg, D.J. Scalapino, Phys. Rev. B 22 (1980) 2560.
[3] M. Caselle, M. Hasenbusch, J. Phys. A 30 (1997) 4963.
[4] J. Salas, A.D. Sokal, J. Stat. Phys 88 (1997) 567.
[5] A. Aharony, P.C. Hohenberg, V. Privman, Universal critical point amplitude relations in: Phase Transitions and Critical Phenomena, Vol. 14, ed. C. Domb, J.L. Lebowitz (Academic Press, New York, 1991).
[6] J.L. Cardy, G. Delfino, Nucl. Phys. B 519 (1998) 551.
[7] C.M. Fortuin, P.W. Kasteleyn, Physica 57 (1972) 36.
[8] V.S. Dotsenko, V.A. Fateev, Nucl. Phys. B 240 (1984) 312.
[9] B. Nienhuis, J. Stat. Phys 34 (1984) 731.
[10] A.B. Zamolodchikov, Integrable Field Theory from Conformal Field Theory, Proc. of Taniguchi Symposium, Kyoto (1988).
[11] F.A. Smirnov, Int. J. Mod. Phys. A 6 (1991) 1407.
[12] F.A. Smirnov, Nucl. Phys. B 337 (1990) 156.
[13] D. Bernard, A. Leclair, Nucl. Phys. B 340 (1990) 721.
[14] A.B. Zamolodchikov, Nucl. Phys. B 358 (1991) 497.
[15] A.B. Zamolodchikov, Nucl. Phys. B 358 (1991) 524.
[16] A.B. Zamolodchikov, Nucl. Phys. B 366 (1991) 122.

[17] L. Chim, A.B. Zamolodchikov, Int. J. Mod. Phys. A 7 (1992) 5317.
[18] M. Karowski, P. Weisz, Nucl. Phys. B 139 (1978) 445.
[19] A.L. Talapov, H.W.J. Blöte, J. Phys. A 29 (1996) 5727.
[20] J. Salas, A.D. Sokal, J. Stat. Phys. 85 (1996) 297.
[21] J.P. Straley, M.E. Fisher, J. Phys. A 6 (1973) 1310.
[22] K.M. Briggs, I.G. Enting, A.J. Guttmann, J. Phys. A 27 (1994) 1503.
[23] A.J. Liu, M.E. Fisher, Physica A 156 (1989) 35.