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Numerical revision of the universal amplitude ratios for the two-dimensional 4-state Potts model

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Abstract

Monte Carlo (MC) simulations and series expansion (SE) data for the energy, specific heat, magnetization and susceptibility of the ferromagnetic 4-state Potts model on the square lattice are analyzed in a vicinity of the critical point in order to estimate universal combinations of critical amplitudes. The quality of the fits is improved using predictions of the renormalization group (RG) approach and of conformal invariance, and restricting the data within an appropriate temperature window.

The RG predictions on the cancelation of the logarithmic corrections in the universal amplitude ratios are tested. A direct calculation of the effective ratio of the energy amplitudes using duality relations explicitly demonstrates this cancelation of logarithms, thus supporting the predictions of RG.

We emphasize the role of corrections *and* of background terms on the determination of the amplitudes. The ratios of the critical amplitudes of the susceptibilities obtained in our analysis differ significantly from those predicted theoretically and supported by earlier SE and MC analysis. This disagreement might signal that the two-kink approximation used in the analytical estimates is not sufficient to describe with fair accuracy the amplitudes of the 4-state model.

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1. Introduction

In a first paper [1], we studied the universal combinations of critical amplitudes of the 3-state Potts model. The present paper is devoted to a similar analysis in the 4-state case, which is much more involved due to the presence of logarithmic corrections strongly influencing the critical behavior.

We analyze numerical data obtained in Monte Carlo (MC) simulations using the Wolff [2] single-cluster algorithm and also the series expansion (SE) data available in the literature. In the following, we refer to the data type as MC and SE data, respectively. For comparison with our own results, we shall also reconsider the data obtained in MC simulations using the Swendsen–Wang cluster algorithm [3] by Caselle, Tateo, and Vinci [4] and indicated as CTV data.

Our motivation in using different data sets is to achieve a better control of the critical behavior, since one may expect, for the three sources, some differences in the critical region due to the different interplay of the finite size effects. In addition, one can apply different techniques to the data analysis: the fits in the case of the MC data and the approximant technique in the case of the SE data. The consistency of the final results will increase our confidence. We care so much because the presence of logarithmic corrections makes the numerical determination of the critical behavior of the 4-state Potts model a rather delicate task.

To be even safer, two different approaches are used, which were successfully applied also to the $q = 3$ state Potts model in [1]. First we estimate the critical amplitudes, which are then used to compute universal ratios. Second, besides the direct determination of the amplitudes themselves, we estimate *ratios* of critical amplitudes, constructing effective ratio functions, and computing their limiting values at the critical point. This provides a direct estimate of universal ratios. Analyzing the renormalization group equations, we have shown in Appendix A (see also [5,6]) that, in the absence of any regular background term, the logarithmic corrections cancel in the effective ratio functions.

The Hamiltonian of the ferromagnetic Potts model [7] reads as

$$H = -\sum_{\langle ij\rangle} \delta_{s_i s_j}, \tag{1}$$

where s_i is a "spin" variable taking integer values between 0 and $q-1$, and the sum is restricted to the nearest neighbor sites $\langle ij\rangle$ on a lattice of N sites with periodic boundary conditions. The partition function Z is defined by

$$Z = \sum_{\text{conf}} \mathrm{e}^{-\beta H} \tag{2}$$

with $\beta = 1/k_B T$,[1] and k_B the Boltzmann constant (fixed to unity). On the square lattice in zero magnetic field, the model is self-dual. Denoting by β^* the dual of the inverse temperature β, the duality relation

$$\left(e^{\beta} - 1\right)\left(e^{\beta^*} - 1\right) = q \tag{3}$$

determines the critical value of the inverse temperature [7] $\beta_c = \ln(1 + \sqrt{q}\,) \approx 1.09861$. Dual reduced temperatures τ and τ^* can be defined by

$$\beta = \beta_c(1-\tau) \quad \text{and} \quad \beta^* = \beta_c(1+\tau^*). \tag{4}$$

[1] According to the usual terminology, the inverse temperature and the critical exponent of the magnetization are denoted by the same symbol β, since there is no risk of confusion in this context.

Close to the critical point, τ and τ^* coincide through first order, since $\tau^* = \tau + \frac{\ln(1+\sqrt{q})}{\sqrt{q}}\tau^2 + O(\tau^3)$.

The critical amplitudes and the critical exponents describe the singular behavior of the thermodynamic quantities close to the critical point. For example the magnetization M, the (reduced) susceptibility χ and the specific heat C of a spin system in zero external field[2] behave as[3]

$$M(\tau) = B(-\tau)^{\beta}(1 + \text{corr. terms}), \quad \tau < 0, \tag{5}$$

$$\chi(\tau)_{\pm} = \Gamma_{\pm}|\tau|^{-\gamma}(1 + \text{corr. terms}), \tag{6}$$

$$C(\tau)_{\pm} = \frac{A_{\pm}}{\alpha}|\tau|^{-\alpha}(1 + \text{corr. terms}). \tag{7}$$

Here τ is the reduced temperature $\tau = (T - T_c)/T$ and the labels $\pm$ refer to the high-temperature (HT) and low-temperature (LT) sides of the critical temperature T_c. In addition to the mentioned observables, for the Potts models with $q > 2$ a transverse susceptibility can be defined in the low-temperature phase[4]

$$\chi_T(\tau) = \Gamma_T(-\tau)^{-\gamma}(1 + \text{corr. terms}). \tag{8}$$

The critical exponents are known exactly for the 2D Potts model [8–12]:

$$x_\epsilon = \frac{1+y}{2-y}, \qquad x_\sigma = \frac{1-y^2}{4(2-y)}, \tag{9}$$

where y is related to the number of states q of the Potts variable by

$$\cos\frac{\pi y}{2} = \frac{1}{2}\sqrt{q}. \tag{10}$$

The standard exponents follow from $x_\epsilon = (1-\alpha)/\nu$ and $x_\sigma = \beta/\nu$. The central charge of the corresponding conformal field theory is also simply expressed [11,12] in terms of y

$$c = 1 - \frac{3y^2}{2-y}. \tag{11}$$

Analytical estimates of critical amplitude ratios for the q-state Potts models with $q = 1, 2, 3$, and 4 were recently obtained by Delfino and Cardy [13]. They used the exact 2D scattering field theory of Chim and Zamolodchikov [14] and estimated the ratios using a two-kink approximation for $1 < q \leqslant 3$. For $3 < q \leqslant 4$, they considered both the two-kink approximation and the contribution from the bound state. For $q = 4$ this approximation leads to the value $c = 0.985$ for the central charge, to be compared to the exact value $c = 1$. Using this approximate value, one can calculate the scaling dimensions from (11) and (9) obtaining the values $x_\sigma = 0.117$ and $x_\epsilon = 0.577$, to be compared with the exact values $1/8$ and $1/2$, respectively. So, the deviation from the exact values becomes as large as 6 and 15 per cent, emphasizing the difficulty of the $q = 4$ case. In the 3-state case the situation is much better (see [1]).

[2] In this paper we only deal with the physical properties in zero magnetic field.

[3] Note that for simplicity we have dropped for the moment the multiplicative logarithmic corrections and allowed only for additive corrections.

[4] In the following we shall use the notations Γ_L or Γ_T for the longitudinal or transverse susceptibility amplitudes in the low-temperature phase. When still used, Γ_- is identified with Γ_L.

Let us recall that the existence of logarithmic corrections to scaling in the 4-state Potts model was pointed out in the pioneering works of Cardy et al. [15,16], where a set of non-linear RG equations was solved. Their discussion was recently extended by Salas and Sokal [17].

The universal susceptibility amplitude ratio Γ_+/Γ_L was calculated by Delfino and Cardy in [13] for both the 3-state and 4-state Potts models. Later Delfino et al. [18] estimated analytically also the ratio of the transverse to the longitudinal susceptibility amplitudes Γ_T/Γ_L. The values obtained in the 4-state case are

$$\Gamma_+/\Gamma_L = 4.013, \qquad \Gamma_T/\Gamma_L = 0.129. \tag{12}$$

In this latter paper [18], the results of MC simulations were also reported, but they were considered inconclusive by the authors. More recently Delfino and Grinza report compatible values in the case of the Ashkin–Teller model, using the same technique at the same level of approximation [19].

Another contribution to the study of the amplitude ratios in the 2D 4-state Potts model was reported by Caselle et al. [4]. These authors presented a MC determination of various amplitudes. In particular, their estimate of the susceptibility amplitude ratio $\Gamma_+/\Gamma_L = 3.14(70)$ is in reasonable agreement with the theoretical estimate of Delfino and Cardy, in spite of a somewhat controversial [18] use of the logarithmic corrections in the fitting procedure.

Enting and Guttmann [20] also analyzed SE data for the 4-state Potts model and found

$$\Gamma_+/\Gamma_L = 3.5(4), \qquad \Gamma_T/\Gamma_L = 0.11(4), \tag{13}$$

results which are compatible with the predictions of [13] and [18]. Their series analysis does not rely on differential approximants, but, in the hope to achieve better control of the log-corrections of the $q = 4$ case, they address directly the asymptotic behavior of the series coefficients.

In the present paper we present more accurate MC data supplemented by a reanalysis of the extended series derived by Enting and Guttmann [20]. We address the following question: Is it possible to estimate the influence of the logarithmic corrections on the fit procedure? Is it possible to devise some procedure in which the role of the logarithmic corrections is properly taken into account?

In the rest of the paper, we shall be concerned with the following universal combinations of critical amplitudes

$$\frac{A_+}{A_-}, \quad \frac{\Gamma_+}{\Gamma_L}, \quad \frac{\Gamma_T}{\Gamma_L}, \quad R_C^+ = \frac{A_+\Gamma_+}{B^2}, \quad R_C^- = \frac{A_-\Gamma_L}{B^2} \tag{14}$$

where the last two are a consequence of the scaling relation[5] $\alpha = 2 - 2\beta - \gamma$. To the various critical amplitudes of interest, $A_\pm, \Gamma_\pm, \ldots$, we have associated appropriately defined "effective amplitudes", namely temperature-dependent quantities $A_\pm(\tau), \Gamma_\pm(\tau), \ldots$, which take as limiting values, when $\tau \to 0$, the critical amplitudes $A_\pm, \Gamma_\pm, \ldots$. In order to avoid any risk of confusion between the critical amplitude and the corresponding effective temperature-dependent amplitude, reference to these temperature-dependent quantities is always made with their explicit τ-dependence.

Also in this paper, we make use of the duality relation in order to improve the estimates of the ratios between effective amplitudes measured at *dual* temperatures. In the case of the 4-state Potts model, this procedure *would even eliminate all logarithmic corrections* from the fit

[5] We refer the reader to the review Ref. [21] for a detailed discussion of the universality of the critical amplitudes ratios.

in absence of background contributions, which unfortunately do exist for most quantities! We again use the duality relation to estimate the correction-to-scaling amplitudes in the behavior of the specific heat and of the susceptibility. For this purpose, we compute ratios also on the duality line, e.g. the susceptibility effective-amplitude ratio $\Gamma_+(\tau)/\Gamma_L(\tau^*) = \chi_+(\beta)/\chi_L(\beta^*)$ as the ratio of $\chi_+(\beta)$, the high-temperature susceptibility at inverse temperature β, and of $\chi_L(\beta^*)$, the low-temperature susceptibility at the dual inverse temperature β^*. Furthermore, we show analytically that the leading logarithmic corrections cancel on the duality line for the ratio of the specific-heat amplitudes as extracted from the energy at dual temperatures.

As a final result of our analysis,[6] we propose estimates of the susceptibility critical-amplitude ratios $\Gamma_+/\Gamma_L = 6.49(44)$ and $\Gamma_T/\Gamma_L = 0.154(12)$ which are significantly different both from the predictions (12) of [13,18], and from the numerical estimates of [4,20]. The deviation from the numerical estimates of other authors might be explained by the complicated logarithmic corrections used to fit the data in [4,20]. The difference from the theoretical predictions might be due to the limited accuracy of the approximation scheme used for $q > 3$.

In conclusion, obtaining an accurate (say, within a few per cent) and generally accepted approximation of the critical amplitude combinations for the four-state Potts model still remains an open issue both theoretically and numerically.

2. Computational procedures

2.1. Monte Carlo simulations

We use the single-cluster Wolff algorithm [2] for studying square lattices of linear size L with periodic boundary conditions. Starting from an ordered state, we let the system equilibrate in 10^5 steps measured by the number of flipped Wolff clusters. The averages are computed over 10^6–10^7 steps. The random numbers are produced by an exclusive-XOR combination of two shift-register generators with the taps (9689, 471) and (4423, 1393), which are known [22] to be safe for the Wolff algorithm.

The order parameter of a microstate $\mathtt{M(t)}$ is evaluated during the simulations as

$$\mathtt{M} = \frac{qN_m/N - 1}{q-1}, \tag{15}$$

where N_m is the number of sites i with $s_i = m$ at the time $\mathtt{t}$ of the simulation [23], and $m \in [0, 1, \ldots, (q-1)]$ is the spin value of the majority of the spins. $N = L^2$ is the total number of spins. The thermal average is denoted $M = \langle \mathtt{M} \rangle$.

Thus, the longitudinal susceptibility in the low-temperature phase is measured by the fluctuation of the majority spin orientation

$$k_B T \chi_L = \frac{1}{N}\left(\langle N_m^2\rangle - \langle N_m\rangle^2\right) \tag{16}$$

and the transverse susceptibility is defined in terms of the fluctuations of the minority of the spins

$$k_B T \chi_T = \frac{1}{(q-1)N} \sum_{\mu \neq m} \left(\langle N_\mu^2\rangle - \langle N_\mu\rangle^2\right), \tag{17}$$

[6] The figures given here are an average between the MC and the SE determinations [5].

while in the high-temperature phase χ_+ is given by the fluctuations in all q states,

$$k_B T \chi_+ = \frac{1}{qN} \sum_{\mu=0}^{q-1} \left(\langle N_\mu^2 \rangle - \langle N_\mu \rangle^2 \right), \tag{18}$$

where N_μ is the number of sites with the spin in the state μ. Properly allowing for the finite-size effects, this definition of the susceptibilities is, in both phases, completely consistent with the available SE data [24].

The internal energy density of a microstate is calculated as

$$\mathtt{E} = -\frac{1}{N} \sum_{\langle ij \rangle} \delta_{s_i s_j} \tag{19}$$

its ensemble average is denoted by $E = \langle \mathtt{E} \rangle$ and the reduced specific heat per spin measures the energy fluctuations,

$$(k_B T)^2 C = -\frac{\partial E}{\partial \beta} = \langle \mathtt{E}^2 \rangle - \langle \mathtt{E} \rangle^2. \tag{20}$$

We have simulated the model on square lattices with linear sizes $L = 20$, 40, 60, 80, 100 and 200. In each case, we have measured the physical quantities within a range of reduced temperatures called the "critical window" and defined as follows. Assuming a proportionality factor of order 1 in the definition of the correlation length, the relation $L < \xi \propto |\tau|^{-\nu}$ yields the value of the reduced temperature at which the correlation length becomes comparable with the system size L and thus below which the finite-size effects are not negligible. This value defines the lower end of the critical window and avoids finite size effects which would make our analysis more complex. The upper limit of the critical window is fixed for convenience at $\tau = 0.20$–0.25.

2.2. *Series expansions*

Our MC study of the critical amplitudes will be supplemented by an analysis of the high-temperature and low-temperature expansions for $q = 4$, recently extended through remarkably high orders by Briggs et al. [20,25]. In terms of these series, we can compute the effective critical amplitudes for the susceptibilities, the specific heat and the magnetization and extrapolate them by the standard resummation techniques, namely simple Padé approximants (PA) and differential approximants (DA), properly biased with the exactly known critical temperatures and critical exponents.

The LT expansions are expressed in terms of the variable $z = \exp(-\beta)$. In the $q = 4$ case, the expansion of the energy extends through z^{43}. For the longitudinal susceptibility the expansion extends through z^{59}, and for the transverse susceptibility through z^{47}. In the case of the magnetization, the expansion extends through z^{43}. The HT expansions are computed in terms of the variable $v = (1 - z)/(1 + (q - 1)z)$. They extend up to v^{43} in the case of the energy and up to v^{24} for the susceptibility.

It is useful to point out that, for convenience, in Ref. [20] the product of the susceptibility by the factor $q^2/(q - 1)$, rather than the susceptibility itself, is tabulated at HT, because it has integer expansion coefficients. For the same reason, at LT the magnetization times $q/(q - 1)$ is tabulated. Therefore the appropriate normalization should be restored in order that the series yield amplitudes consistent with the MC results.

As a general remark on our series analysis, we may point out that the accuracy of the amplitude estimates given in Ref. [1] for the $q = 3$ case is good due to the relatively harmless nature of the power-like corrections to scaling, while in the $q = 4$ case the mentioned resummation methods cannot reproduce the expected logarithmic corrections to scaling and therefore the extrapolations to the critical point are more uncertain. In this case we have tested also a somewhat unconventional use of DAs: in computing the effective amplitudes, we only retain DA estimates outside some small vicinity of the critical point, where they appear to be stable and reliable. Finally, we perform the extrapolations by fitting these data to an asymptotic form which includes logarithmic corrections. We shall add further comments on the specific analyses in the next sections.

3. Critical amplitudes of 4-state Potts model

3.1. Expected temperature-dependence of the observables

In the case of the 4-state Potts model, we have $y = 0$ from (10) and the second thermal exponent [11,12,26] $y_{\phi_2} = -4y/3(1 - y)$ vanishes. Accordingly, the leading power-behavior of the specific heat (and of other physical quantities) is modified [15] by a logarithmic factor

$$C(\tau) = \frac{A_\pm}{\alpha} |\tau|^{-\alpha} \big(-\ln|\tau|\big)^{-1} \mathcal{X}_{\mathrm{corr}}\big(-\ln|\tau|\big) + \mathcal{Y}_{\mathrm{bt}}\big(|\tau|\big). \tag{21}$$

The exponent α takes the value $2/3$ and $\mathcal{X}_{\mathrm{corr}}(-\ln|\tau|)$ contains correction terms with powers of $|\tau|$, $-\ln|\tau|$ and $\ln(-\ln|\tau|)$. It may also contain non-integer power corrections due to the higher thermal exponents [8–12] y_{ϕ_n} or to other irrelevant fields, as well as power corrections due to the identity field. $\mathcal{Y}_{\mathrm{bt}}(|\tau|)$ contains all regular contributions and is referred to as the background term.

Extending the pioneering work of Cardy et al. [15,16], Salas and Sokal [17] obtained a set of non-linear RG equations. In Appendix A (see also Refs. [5,6]), we derive from this set of equations a closed expression for the leading logarithmic corrections, which is more suitable to describe the temperature range accessible in a numerical study, than the asymptotic form given by Salas and Sokal,

$$C(\tau) = \frac{A_\pm}{\alpha} |\tau|^{-2/3} \big(-\ln|\tau|\big)^{-1} \left[1 - \frac{3}{2} \frac{\ln(-\ln|\tau|)}{-\ln|\tau|} + O\left(\frac{1}{\ln|\tau|}\right)\right], \tag{22}$$

which is the first term of a slowly convergent expansion of $\mathcal{X}_{\mathrm{corr}}(-\ln|\tau|)$ in logs. We have observed that the following expansion (see Appendix A) is better behaved in the temperature window near the critical point accessible by MC and SEs

$$C(\tau) = \frac{A_\pm}{\alpha} |\tau|^{-2/3} \mathcal{G}^{-1}\big(-\ln|\tau|\big), \tag{23}$$

$$\mathcal{G}\big(-\ln|\tau|\big) = \big(-\ln|\tau|\big) \times \mathcal{E}\big(-\ln|\tau|\big) \times \mathcal{F}\big(-\ln|\tau|\big), \tag{24}$$

$$\mathcal{E}\big(-\ln|\tau|\big) = \left(1 + \frac{3}{4} \frac{\ln(-\ln|\tau|)}{-\ln|\tau|}\right) \left(1 - \frac{3}{4} \frac{\ln(-\ln|\tau|)}{-\ln|\tau|}\right)^{-1} \left(1 + \frac{3}{4} \frac{1}{(-\ln|\tau|)}\right), \tag{25}$$

$$\mathcal{F}\big(-\ln|\tau|\big) \simeq \left(1 + \frac{C_1}{-\ln|\tau|} + \frac{C_2 \ln(-\ln|\tau|)}{(-\ln|\tau|)^2}\right)^{-1}. \tag{26}$$

The function $\mathcal{E}(-\ln|\tau|)$ contains the exact form of the leading terms with universal coefficients predicted by RG. The remaining part is made of log terms, whose coefficients involve the non-universal dilution field ψ_0. The multiplicative function $\mathcal{F}(-\ln|\tau|)$ mimics, in a given temperature range close to the critical point, the higher-order terms of this non-universal part, which is a slowly convergent series in powers of logs starting with an $O(\frac{1}{\ln|\tau|})$ term. The values of C_1 and C_2 in (26) should not be considered as "real" amplitudes of correction-to-scaling terms, but only as "effective" parameters. A "zeroth-order" analysis may be performed taking $C_1 = C_2 = 0$, i.e. $\mathcal{F}(-\ln|\tau|) = 1$. A more refined estimate follows from the analysis of the magnetization, as explained in Section 3.2 and in Appendix A. The absence of a constant background term is a simplifying feature in the analysis of the magnetization.[7] The difference in behavior between the two types of expressions (22) and (23) for the specific heat is illustrated by the fact that, for example, at a typical value of temperature numerically accessible without finite-size effects, $\tau = 0.10$, we have $1 - \frac{3}{2}\frac{\ln(-\ln|\tau|)}{-\ln|\tau|} \simeq 0.457$, while $(1 - \frac{3}{4}\frac{\ln(-\ln|\tau|)}{-\ln|\tau|}) \times (1 + \frac{3}{4}\frac{\ln(-\ln|\tau|)}{-\ln|\tau|})^{-1} \simeq 0.786$ and the two functions are not simply proportional to each other in the typical range $\tau = 0.02$–0.20. Fitting the numerical data with one or the other choice may thus spoil the outcome for the leading amplitude.

Similar expressions of the logarithmic corrections are obtained for the other physical quantities in Eqs. (A.28)–(A.34) of Appendix A.

Further corrections to scaling may also be present in Eq. (23). They are discussed in Appendix A and may be of the form $a_{2/3}|\tau|^{2/3}$, $a_{h_3}|\tau|^{\Delta_{h_3}}$ or $a_{\phi_3}|\tau|^{\Delta_{\phi_3}}$, as well as powers of these terms, where $\Delta_{h_3} = 3/4$ and $\Delta_{\phi_3} = 5/3$. Pure power corrections and background terms may also be needed. Here we also stress that the inclusion of a leading correction in $a|\tau|^{2/3}$ and of analytic terms seems to be necessary according to the papers by Joyce [27,28], where the magnetization of a model, expected to belong to the 4-state Potts model universality class, is shown to have an expression of the form

$$M\big(-|\tau|\big) = |\tau|^{1/12}\big(f_0(\tau) + |\tau|^{2/3} f_1(\tau) + |\tau|^{4/3} f_2(\tau)\big) \tag{27}$$

with $f_i(\tau)$ analytic functions when $\tau \to 0^-$. The correction exponents are obtained from the table of the conformal scaling dimensions by Dotsenko and Fateev [11,12], but not all of them are necessarily present. However, at least the presence of the exponents 2/3, and possibly of 4/3, seems to be needed in order to account for the numerical results. Caselle et al. [4] also considered an $a_{2/3}|\tau|^{2/3}$ term to fit the magnetization. The parameter a_{h_3} is a priori possibly needed only for magnetic quantities, while the corrections in a_{ϕ_3} will systematically be dropped in our fits, since they are sub-sub-dominant.

In conclusion, the most general expression that we will consider is the following:

$$\text{Obs.}\big(\pm|\tau|\big) \simeq \text{Ampl.} \times |\tau|^{\blacktriangleleft} \times \mathcal{G}^{\bigstar}\big(-\ln|\tau|\big) \times (1 + \text{corr. terms}) + \text{backgr. terms}, \tag{28}$$

$$\text{corr. terms} = a_{2/3}|\tau|^{2/3} + b_\pm|\tau| + a_{4/3}|\tau|^{4/3} + \cdots, \tag{29}$$

$$\text{backgr. terms} = D_0 + D_1|\tau| + \cdots \tag{30}$$

where $\mathcal{G}(-\ln|\tau|)$ is defined by Eqs. (24)–(26), while $\blacktriangleleft$ and $\bigstar$ stand for exponents which depend on the observable considered. They are all given in Appendix A.

[7] The effective amplitudes are constructed by dividing the corresponding physical quantity by the leading terms (main power dependence with known logarithmic corrections), and, therefore the background terms, if present, will be divided by the logarithmic terms. These terms may seriously complicate the analysis of the limiting behavior of the effective amplitudes.

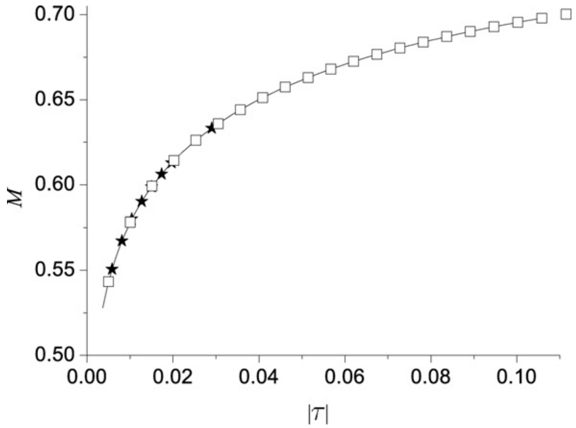

Fig. 1. The magnetization M in the critical window region. Our MC data are represented by boxes, the MC data from Ref. [4] by stars and the SE data by a solid line.

3.2. The magnetization amplitude

The amplitude B of the magnetization is defined by the asymptotic behavior (see Appendix A for details)

$$M(-|\tau|) = B|\tau|^{1/12}(-\ln|\tau|)^{-1/8}\left[\left(1+\frac{3}{4}\frac{\ln(-\ln|\tau|)}{(-\ln|\tau|)}\right)\left(1-\frac{3}{4}\frac{\ln(-\ln|\tau|)}{(-\ln|\tau|)}\right)^{-1}\right.$$
$$\left.\times\left(1+\frac{3}{4}\frac{1}{(-\ln|\tau|)}\right)\mathcal{F}(-\ln|\tau|)\right]^{-1/8}\left(1+a|\tau|^{2/3}+b|\tau|+\cdots\right). \tag{31}$$

We can extract an effective function $\mathcal{F}_{\text{eff}}(-\ln|\tau|)$ which mimics the real one $\mathcal{F}(-\ln|\tau|)$ in the convenient temperature range $|\tau| \simeq 0.01$–0.10. This is done by plotting an effective magnetization amplitude

$$B_{\text{eff}}(-|\tau|) = M(-|\tau|)|\tau|^{-1/12}(-\ln|\tau|)^{1/8}\left[\left(1+\frac{3}{4}\frac{\ln(-\ln|\tau|)}{(-\ln|\tau|)}\right)\right.$$
$$\left.\times\left(1-\frac{3}{4}\frac{\ln(-\ln|\tau|)}{(-\ln|\tau|)}\right)^{-1}\left(1+\frac{3}{4}\frac{1}{(-\ln|\tau|)}\right)\right]^{1/8} \tag{32}$$

which is then fitted to the expression

$$B_{\text{eff}}(-|\tau|) = B\left(1+\frac{C_1}{-\ln|\tau|}+\frac{C_2\ln(-\ln|\tau|)}{(-\ln|\tau|)^2}\right)^{1/8}\left(1+a|\tau|^{2/3}+b|\tau|+\cdots\right) \tag{33}$$

in which we have also included corrections to scaling. As we have already noticed, the coefficients appearing in the function $\mathcal{F}$ are effective parameters adapted to the temperature window considered, therefore the values of C_1 and C_2 have no special meaning.

In order to analyze the numerical data and to extract the different coefficients, one needs very accurate data. As an illustration, in Fig. 1 we compare MC and SE data, and MC data from Caselle et al. [4].

The behavior of $B_{\text{eff}}(-|\tau|)$ is shown in Fig. 2. In Table 1, we present a selection of our fits of MC data to Eq. (33). The first column of the table indicates the different choices of the function

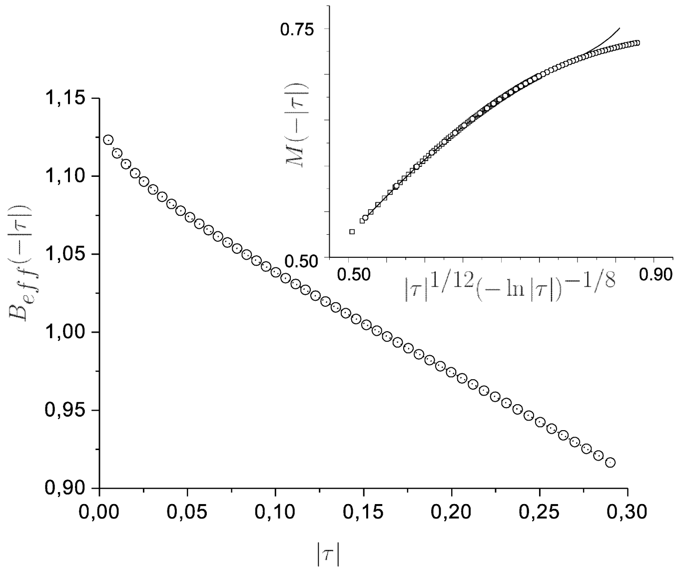

Fig. 2. The effective amplitude of the magnetization M. Insert: The magnetization M as function of $|\tau|^{1/12}(-\ln|\tau|)^{-1/8}$. (Our MC data are represented by open circles, the SE data by boxes and the fit by a solid line.)

$\mathcal{F}(-\ln|\tau|)$. For each line in the tables, several fits have been tried, varying the number of points in the interval $|\tau| \in [0.005, 0.25]$ (total number of points 50) and calculating the χ^2/d.o.f. for each fit. A reasonable balance has to be found between the distance of the points from the critical temperature and their number. It appeared that limiting the fit window to 20 data points, i.e. to the interval $[0.005, 0.1]$, gives the best confidence level. This choice is quite satisfactory, since it corresponds to a close vicinity of the critical point. The criterion that we adopted in order to select a most convincing fit among all possible fits is the stability of the correction-to-scaling amplitudes a and b in Eq. (31) when the temperature window is varied, typically in the range $|\tau| \in [0, 0.06]$ to $|\tau| \in [0, 0.30]$. As long as these numbers have not converged to given values, we cannot pretend that it is meaningful to include such corrections in the analysis. We have to mention that stability of the correction amplitudes is never reached if we stop the correction terms in Eq. (31) at the leading log, or even at the three higher log terms (correction function $\mathcal{E}(-\ln|\tau|)$). Then even the leading amplitude B is questionable. The effective function $\mathcal{F}_{\text{eff}}(-\ln|\tau|)$ is essential to reach convergence of all but the two effective coefficients C_1 and C_2 which still strongly depend on the temperature window.

For a given type of fit defined in the first column, Tables 1 and 2 show the parameters of the fit minimizing χ^2 and the minimization is performed by varying the width and position of the temperature window.

Once our choice is made for C_1 and C_2, the results of the fit for the amplitude B show a remarkable stability. The entry called fit #0 corresponds to a "zeroth-order" fit in which the function $\mathcal{F}(-\ln|\tau|)$ is taken equal to unity. It is presented for comparison, in order to emphasize the improvement occurring in the following lines. Fit #1 keeps all correction coefficients, while the lines which follow are obtained decreasing the number of fit parameters. We favor fits #2 and #3, where the coefficient b (the amplitude of the linear term $|\tau|$) is fixed to zero, since from the first fit (#1) we see that leaving b free leads to a value close to zero and we consider more reliable a fit with fewer parameters. Fit #4 corresponds to another extreme choice including no

Table 1
Various fits of our MC data for the magnetization effective amplitude $M(-|\tau|)|\tau|^{-1/12}(-\ln|\tau|)^{1/8}\mathcal{E}^{1/8}(-\ln|\tau|)$ to the expression (33). The stars in the first column indicate our favorite fits (the reasons for this choice are given in the text).

Fit #	Amplitude	Correction terms			
	B	$\propto \frac{1}{-\ln|\tau|}$	$\propto \frac{\ln(-\ln|\tau|)}{(-\ln|\tau|)^2}$	$\propto |\tau|^{2/3}$	$\propto |\tau|$
MC #0	1.1355(4)	–	–	−0.41(1)	0.41(21)
MC #1	1.1566(5)	−0.740(2)	−0.630(51)	−0.172(4)	−0.018(6)
MC #2*	1.1570(1)	−0.757(1)	−0.522(11)	−0.191(2)	–
MC #3*	1.1559(12)	−0.88(5)	–	−0.21(1)	–
MC #4	1.1593(1)	−0.25(2)	−3.04(5)	–	–

Table 2
Same as Table 1 for the magnetization data obtained by the SE method. A star in the first column indicates our favorite fit with the coefficients C_1 and C_2 (now fixed and shown in bold face in this table and in the forthcoming tables) obtained from the fits of the MC data reported in Table 1.

Fit #	Amplitude	Correction terms			
	B	$\propto \frac{1}{-\ln|\tau|}$	$\propto \frac{\ln(-\ln|\tau|)}{(-\ln|\tau|)^2}$	$\propto |\tau|^{2/3}$	$\propto |\tau|$
SE #0	1.1364(4)	–	–	−0.435(5)	0.097(10)
SE #1	1.1597(1)	−0.637(5)	−1.417(28)	−0.115(2)	0.013(2)
SE #2	1.1589(1)	−0.660(5)	−1.246(25)	−0.126(2)	–
SE #2*	1.1575(1)	**−0.757**	**−0.522**	−0.194(1)	–
SE #3	1.1583(8)	−0.981(34)	–	−0.185(10)	–
SE #3*	1.1575(1)	**−0.88**	–	−0.225(1)	–
SE #4	1.1573(1)	0.164(7)	−4.106(18)	–	–

irrelevant correction at all. It shows that the effective function $\mathcal{F}(-\ln|\tau|)$ is more important than the irrelevant corrections to scaling in order to achieve a stable amplitude B (comparable to the outcomes of fits #1 to #3).

The same procedure is now applied to the SE data. It is a non-conventional approach to fit SE data, which are usually analyzed by approximant methods, but the exercise is tempting. We thus apply exactly the same procedure as in the case of MC data, varying the fitting interval and comparing the values of the χ^2/d.o.f. The best results are collected in Table 2. The agreement between the results quoted in the two tables is amazing. Not only the amplitudes, but also the correction coefficients are very close to each other. In this table (and in the forthcoming tables), we also present the results of this analysis of SE data with C_1 and C_2 *fixed* to their best values extracted in Table 1 from the MC data. They are indicated again with a star (SE #2* and SE #3*) and in order to emphasize the fact that C_1 and C_2 in this case are not free parameters, they are indicated in bold face. A reason for this approach is first to insist on the consistency of the results and second to privilege a fit with less free parameters (and in particular no free log term). For the magnetization amplitude, a compromise between MC and SE data analysis provides our final estimate

$$B = 1.157(1). \qquad (34)$$

As an additional test, we decided to fit also the MC data of Caselle et al. [4], obtained using the Swendsen–Wang cluster algorithm, to our functional expression (33). Notice that the various coefficients reported in Table 3 (not only the critical amplitude, but also the correction terms) are

Table 3
Same as Table 1 but using the MC data of Caselle et al. [4] for the magnetization. The fit marked by a star is performed using the same coefficient C_1 (shown in bold) as in Table 1.

Fit #	Amplitude	Correction terms			
	B	$\propto \frac{1}{-\ln\|\tau\|}$	$\propto \frac{\ln(-\ln\|\tau\|)}{(-\ln\|\tau\|)^2}$	$\propto \|\tau\|^{2/3}$	$\propto \|\tau\|$
CTV #0	1.1386(2)	–	–	−0.518(6)	0.30(2)
CTV #1	1.196 ± 1.499	−7.5 ± 163	19.6 ± 429	−1.09 ± 17.3	1.2 ± 29.2
CTV #2	1.148(6)	0.45(56)	−3.6 ± 1.1	−0.17(4)	–
CTV #3	1.162(9)	−1.13(38)	–	−0.14(12)	–
CTV #3*	1.1561(1)	**−0.88**	–	−0.215(1)	–
CTV #4	1.153(2)	0.73(31)	−5.5 ± 0.77	–	–

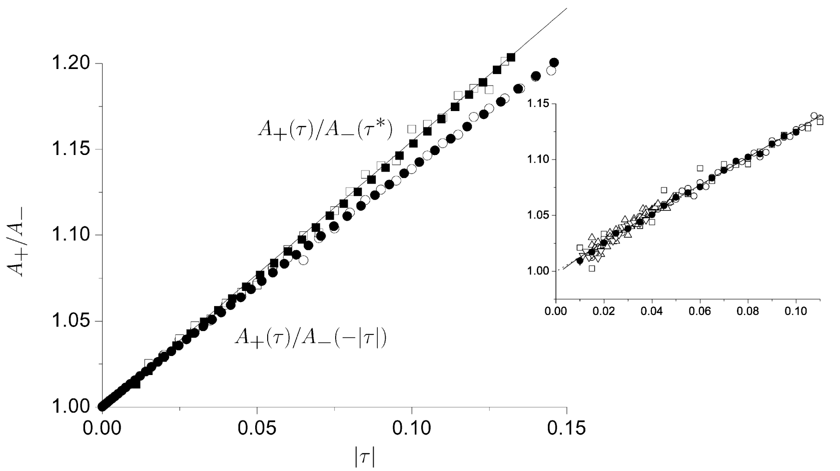

Fig. 3. The specific-heat effective-amplitude ratio computed from the energy ratio $\frac{(E(\beta)-E_0)\tau^{\alpha-1}}{(E_0-E(\beta^*))(\tau^*)^{\alpha-1}}$ as a function of the reduced temperature τ on the dual line. The SE data are represented by boxes, our MC data ($L=100$) by circles. The solid line is given by Eq. (36). The ratio of the effective amplitudes $A_+(\tau)/A_-(-|\tau|)$ is shown for different sizes in the insert (for lattice linear sizes $L=100$ (open circles), $L=200$ (squares), $L=300$ (up triangles), and $L=400$ (down triangles)). The simulations were performed with $N_{\rm th}=10^5$ thermalization steps and $N_{\rm MC}=10^6$ MC steps. The results of a simulation for $L=100$ with $N_{\rm th}=10^6$ and $N_{\rm MC}=10^7$, are represented by closed circles. The SE data are represented by a solid line. The dotted line represents a linear fit of the closed circles.

very close to those reported above in Table 1. In particular this fit gives further support to our choice in favor of fits #2 and #3.

In the following tables, we will refer to the best two fits by the labels #2* and #3* (which means that the coefficients C_1 and/or C_2 are fixed to their values indicated in Table 1) when fitting other quantities. Note that the MC data of Caselle et al. [4] are not fitted with the choice #2*, because they do not extend on a range of temperatures wide enough to apply the corresponding functional expression.

3.3. The specific heat and the energy density

We now turn to the study of the specific-heat amplitudes. Fig. 3 shows the effective-amplitude ratio $A_+(\tau)/A_-(-|\tau|)$ computed at dual and symmetric temperatures following the same prescription as in the case of the 3-state Potts model studied in paper [1]. The same ratio computed from SE data is also shown for comparison. The linear fit of the most accurate MC data (lattice size $L = 100$ computed with 10^7 measurement steps) yields for this ratio the value 0.9999(1), which is remarkably close to the exact value 1 derived from duality.

The ratio

$$\frac{A_+(\tau)}{A_-(\tau^*)} = \frac{(E(\beta) - E_0)\tau^{\alpha-1}}{(E_0 - E(\beta^*))(\tau^*)^{\alpha-1}}, \tag{35}$$

where the constant E_0 is the value of the energy at the transition temperature, $E_0 = E(\beta_c) = -1 - 1/\sqrt{q}$, when expanded close to the transition point leads to

$$\frac{A_+(\tau)}{A_-(\tau^*)} = 1 + \frac{7}{3}\alpha_q\tau + O\big(\tau^{1+\alpha}\big) \tag{36}$$

with $\alpha_q = -E_0\beta_c e^{-\beta_c} = \frac{\ln(1+\sqrt{q})}{\sqrt{q}} \approx 0.5493$. Eq. (36) predicts an asymptotically linear τ-dependence of the effective-amplitude ratio. This linear dependence is observed in Fig. 3 which also confirms that the leading logarithmic corrections in the scaling function $\mathcal{X}_{\mathrm{corr}}(-\ln(|\tau|))$ asymptotically cancel in the ratio $A_+(\tau)/A_-(\tau^*)$. (Of course this is true also for the same quantity computed at symmetric temperatures, since $\tau^* \approx |\tau|$ for small values of τ.) Fig. 3 compares the effective-amplitude ratio obtained from MC simulation and SE data with Eq. (36). The slope of MC data is 1.25, very close to the predicted value 1.28.

Now, we make the natural conjecture (proven in Appendix A in the absence of background corrections) that the cancelation of the leading logarithmic corrections will also occur for the other ratios. For the leading log-correction, $-\ln|\tau|$, and for the next correction in $\ln(-\ln|\tau|)/(-\ln|\tau|)$, this can be shown analytically from the RG as first indicated by Cardy et al. in Ref. [15] and by Salas and Sokal in Ref. [17]. Our statement is stronger since it extends also to the higher order log-terms, such as the next correction in $1/(-\ln|\tau|)$. We believe that Eqs. (A.28) to (A.34) in Appendix A are exact, and since all the log-terms come from Eq. (A.27), they should cancel in the appropriate ratios (i.e. when the same powers of the dilution field appear in the numerator and the denominator. This is always the case when one considers an effective combination tending to a universal ratio as $\tau \to 0$).

According to a RG analysis (see Appendix A), we may write the energy in the critical region as

$$E_\pm\big(\pm|\tau|\big) = E_0 \pm \frac{A_\pm}{\alpha(1-\alpha)\beta_c}\frac{|\tau|^{1/3}}{(-\ln|\tau|)}\frac{1 + a_\pm|\tau|^{2/3}}{\mathcal{E}(-\ln|\tau|)\mathcal{F}(-\ln|\tau|)} + D_{1,\pm}|\tau|. \tag{37}$$

In a fixed range of values of the reduced temperature, the "correction function" $\mathcal{F}(-\ln|\tau|)$ is now fixed and the only remaining freedom is to include background terms (coeff. D) and possibly additive corrections to scaling coming from irrelevant scaling fields (coeff. a). Therefore, once the function $\mathcal{F}(-\ln|\tau|)$ is fixed after our study of the magnetization, a reasonable fit of the energy data needs only three parameters,[8] $A_\pm$, $a_\pm$, and $D_\pm$. The next step is the fit of the mean $\bar{A}(\tau)$ of the effective amplitudes,

$$\begin{aligned}\bar{A}(\tau) &= \frac{1}{2}\alpha(1-\alpha)\beta_c\big(E_+(\tau) - E_-\big(-|\tau|\big)\big) \times \mathcal{G}\big(-\ln|\tau|\big)/|\tau|^{1-\alpha} \\ &= \frac{\beta_c}{9}\big(E_+(\tau) - E_-\big(-|\tau|\big)\big) \times \mathcal{G}\big(-\ln|\tau|\big)/|\tau|^{1/3}.\end{aligned} \tag{38}$$

[8] Like in the case of the magnetization, a fourth parameter in $b_\pm|\tau|$ appears to be unnecessary.

Table 4
Fits of the energy difference (MC data computed at *dual* temperatures) to the expression $\bar{A}(\tau) \simeq$ Ampl. $\times$ (1 + corr. terms) + backgr. terms $\times |\tau|^{-1/3}\mathcal{G}(-\ln|\tau|)$.

Fit #	Amplitude	Correction terms			Background term
	Ampl.	$\propto \frac{1}{-\ln|\tau|}$	$\propto \frac{\ln(-\ln|\tau|)}{(-\ln|\tau|)^2}$	$\propto |\tau|^{2/3}$	$\propto |\tau|$
MC #2*	1.338(3)	**−0.757**	**−0.522**	−4.98(8)	0.920(13)
MC #3*	1.316(10)	**−0.88**	–	−4.88(38)	0.899(62)

We thus fit the MC data to the expression

$$\bar{A}(\tau) = A\big(1 + a|\tau|^{2/3}\big) + D_1|\tau| \times \mathcal{G}\big(-\ln|\tau|\big)/|\tau|^{1/3}. \tag{39}$$

The log corrections, which indeed cancel in the singular part, unfortunately reappear in the background term, albeit suppressed by the power $|\tau|^{2/3}$.

We note that $\bar{A}(\tau)$ is constructed in Eq. (38) using the values of energy density computed at *symmetric* temperatures. The same quantity constructed from the energy densities at *dual* temperatures (with $E_-(\tau^*)$ instead of $E_-(-|\tau|)$ in Eq. (38)) can also be studied and provides better results. In Table 4, we show our results (the best fit is obtained with the choices of C_i's coefficients labeled 2^* in Tables 1 and 2). Again, the agreement between the two fits is quite good, but this time it is more trivial since the same data set is fitted. Taking the average of the parameters from the two fits, we conclude

$$A = 1.327(12), \tag{40}$$

and $a \simeq -4.93(23)$, and $D_1 \simeq 0.910(38)$. Padé approximants of SE data for the specific heat provide $A = 1.35(1)$.

The expansion including corrections to scaling and background terms for the specific heat follows from the expressions of the energy density. There is some disagreement between our amplitude $\frac{A}{\alpha(1-\alpha)\beta_c} \simeq 5.922(40) - 6.021(13)$ and the result reported by Caselle et al. [4], $6A \simeq 7.80(36)$.[9] We have to notice that the amplitudes are very sensitive to the expression used for the fits. Our choice of effective amplitude in Eq. (38) is supported by the quite regular behavior shown in Fig. 4, and also by the natural choice of the fitting expression (39). The comparison between the MC data and the resulting fit is shown in Fig. 5. We agree on this point with Enting and Guttmann [20] who emphasized that their estimates depend *critically* on the form assumed for the logarithmic sub-dominant terms, and on the further assumption that the other sub-dominant terms, including powers of logarithms, powers of logarithms of logarithms, etc., can all be neglected.

3.4. Susceptibilities amplitudes

3.4.1. High temperature susceptibility amplitude

We proceed along the same lines as for the other physical quantities and fit the high-temperature susceptibility to the expression

$$\chi_+(\tau) = \Gamma_+\tau^{-7/6}\mathcal{G}^{3/4}(-\ln\tau)\big(1 + a_+\tau^{2/3} + b_+\tau\big) + D_+. \tag{41}$$

[9] Notice that Caselle et al. use a different definition of the energy.

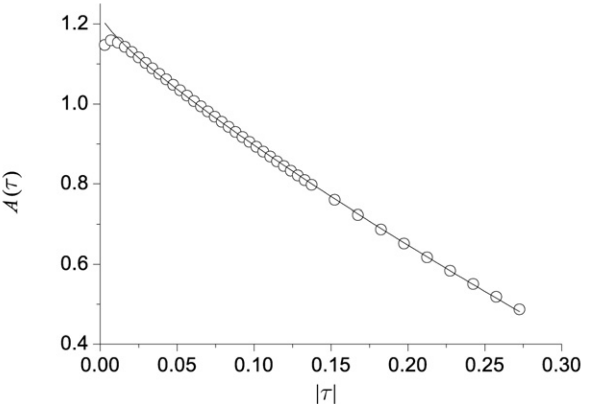

Fig. 4. The effective amplitude $\bar{A}(\tau)$ computed from our MC data using Eq. (38) (open circles) and from the fit to Eq. (39) (solid line).

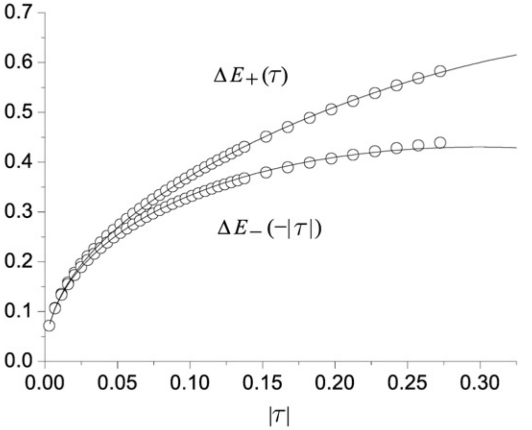

Fig. 5. The energy differences ΔE_+ and ΔE_-, calculated from our MC data for lattice size $L = 100$ (circles) and the fitted expressions (solid lines).

We can easily obtain the amplitude Γ_+ observing that a single constant as a background term D_+ is sufficient for the fit (this will also be the case at low temperature). The effective amplitude

$$\Gamma_{\text{eff}}(\tau) = \chi_+(\tau)\tau^{7/6}\mathcal{G}^{-3/4}(-\ln\tau)$$

is represented in Fig. 6 and Table 5 collects the coefficients determined by the fits. We finally obtain the high-temperature susceptibility amplitude

$$\Gamma_+ = 0.0310(7). \tag{42}$$

The value which follows from differential approximants to SE data, although less accurate, is consistent with it, $\Gamma_+ = 0.033(2)$.

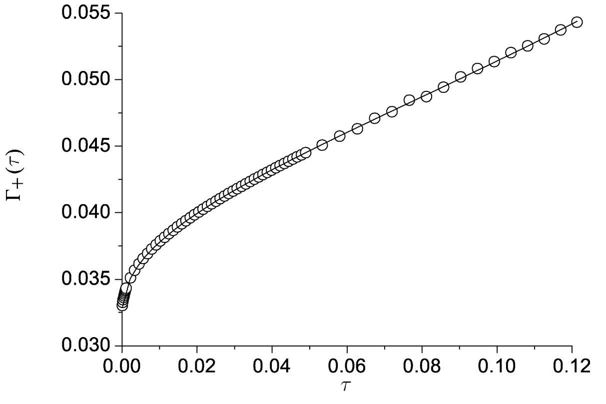

Fig. 6. The effective amplitude of the high-temperature susceptibility $\chi_+(\tau)$. We have shown SE data for $\tau \leqslant 0.05$, our MC data for $\tau > 0.05$ and a fit to Eq. (41) (dotted line).

Table 5
Fits of the high-temperature susceptibility to the expression $\chi_+(\tau) \simeq \text{Ampl.} \times \tau^{-7/6} \times \mathcal{G}^{3/4}(-\ln\tau) \times (1 + \text{corr. terms}) +$ backgr. terms. A star in the first column indicates that the coefficients C_i's are those deduced from the MC fits of Table 1.

Fit #	Amplitude	Correction terms			Backgr.
	Γ_+	$\propto \frac{1}{-\ln\tau}$	$\propto \frac{\ln(-\ln\tau)}{(-\ln\tau)^2}$	$\propto \tau^{2/3}$	$\propto \tau^0$
MC #2*	0.03144(15)	**−0.757**	**−0.522**	0.561(60)	−0.053(17)
MC #3*	0.03178(30)	**−0.88**	–	0.53(23)	0.052(120)
CTV #3*	0.03051(29)	**−0.88**	–	1.48(34)	−0.45(24)
SE #2*	0.03041(1)	**−0.757**	**−0.522**	1.30(1)	−0.362(9)
SE #3*	0.03039(1)	**−0.88**	–	1.67(1)	−0.59(2)

3.4.2. Low temperature susceptibilities amplitudes

The behavior of the longitudinal susceptibility in the low-temperature phase is less easy to analyze [5]. We use the expression

$$\chi_L\big(-|\tau|\big) = \Gamma_L|\tau|^{-7/6}\mathcal{G}\big(-\ln|\tau|\big)^{3/4}\big(1 + a_L|\tau|^{2/3} + b_L|\tau|\big) + D_L \tag{43}$$

and the various coefficients are collected in Table 6. For the transverse susceptibility, the same procedure leads to the amplitudes also listed in Table 6.

One may note that the values of the transverse susceptibility amplitude are more stable than those of the longitudinal amplitude, while the estimates of the corrections to scaling are less scattered in the latter case. Our final estimates are

$$\Gamma_L = 0.00478(24) \tag{44}$$

and

$$\Gamma_T = 0.00074(2). \tag{45}$$

DA analysis of SE data gives approximately $\Gamma_L = 0.005(1)$.

Table 6
Fits of the low-temperature longitudinal susceptibility to the expression $\chi_L(-|\tau|) \simeq \text{Ampl.} \times |\tau|^{-7/6} \times \mathcal{G}^{3/4}(-\ln|\tau|) \times (1 + \text{corr. terms}) + \text{backgr. terms}$ and of the low-temperature transverse susceptibility to the expression $\chi_T(-|\tau|) \simeq \text{Ampl.} \times |\tau|^{-7/6} \times \mathcal{G}^{3/4}(-\ln|\tau|) \times (1 + \text{corr. terms}) + \text{backgr. terms}$. A star in the first column indicates our favorite fit with the coefficients deduced from the MC fits of Table 1.

Fit #	Amplitude	Correction terms			Backgr.
	Γ_L	$\propto \frac{1}{-\ln\tau}$	$\propto \frac{\ln(-\ln\tau)}{(-\ln\tau)^2}$	$\propto \tau^{2/3}$	$\propto \tau^0$
MC #2*	0.00454(2)	**−0.757**	**−0.522**	−2.83(3)	0.050(2)
MC #3*	0.00484(3)	**−0.88**	–	−3.73(14)	0.13(1)
CTV #3*	0.00494(3)	**−0.88**	–	−4.35(15)	0.210(19)
SE #2*	0.00483(1)	**−0.757**	**−0.522**	−3.77(3)	0.116(3)
SE #3*	0.00493(1)	**−0.88**	–	−4.18(5)	0.178(6)
	Γ_T	$\propto \frac{1}{-\ln\tau}$	$\propto \frac{\ln(-\ln\tau)}{(-\ln\tau)^2}$	$\propto \tau^{2/3}$	$\propto \tau^0$
MC #2*	0.00076(1)	**−0.757**	**−0.522**	−0.805(34)	−0.0028(2)
MC #3*	0.00073(1)	**−0.88**	–	−0.25(13)	−0.0050(14)
SE #2*	0.00073(1)	**−0.757**	**−0.522**	−0.577(14)	−0.00373(15)
SE #3*	0.00073(1)	**−0.88**	–	−0.369(15)	−0.00457(16)

3.5. Universal amplitude ratio R_c^-

We use the available MC data for C, M, and χ to estimate the universal amplitude ratio R_C^- in the low-temperature phase. To this purpose, we form the function (compare with Eq. (A.18))

$$R_C^-(-|\tau|) = \alpha\tau^2 \frac{C(-|\tau|)\chi_L(-|\tau|)}{M^2(-|\tau|)} \tag{46}$$

which is an estimator of the universal amplitude ratio in the limit $|\tau| \to 0$. As discussed in Appendix A, we expect that all sets of logarithmic corrections cancel in this ratio. Fig. 7 shows with open symbols the combination from Eq. (46) for two sets of MC data, those of Caselle et al. (CTV) and our simulations. We may fit these data with correction-to-scaling terms starting from $|\tau|^{2/3}$ or, assuming in plain analogy with the energy ratio that such corrections cancel, with terms starting with $|\tau|$. In Table 7 we include these fits for our MC data set varying the temperature window and the number of correction terms.

A similar analysis was also performed for the data from Caselle et al. (not shown here). The results of both analysis are consistent.

More traditionally, we may evaluate the ratio R_C^- using the estimated values of the amplitudes reported in Sections 3.2, 3.3 and 3.4 (see Eq. (14)). The results will be presented later, but anticipating the forthcoming analysis, we can quote as a reliable estimate $R_C^- \simeq 0.0052 \pm 0.0002$ (approximants of SE data lead to 0.0050(2)). One can see from Table 7 that the ratio obtained from the effective function (46) is systematically larger. The difference may be explained by the fact that fitting the effective ratio function (46) without any logarithmic correction, we assume that the background corrections for the longitudinal susceptibility χ_L and for the specific heat C are small in the critical temperature window. While this is indeed the case, these background terms are not negligibly small and their presence leads to systematic deviations of the estimates of R_C^- presented in Table 7. The ratio (46) may be written as $\alpha\tau^2(C_s + C_{\text{bt}})(\chi_s + \chi_{\text{bt}})/M^2$, where C_s and χ_s are the singular parts of the specific heat and of the susceptibility and C_{bt} and χ_{bt} are the corresponding background non-singular terms. Eq. (46) may be rewritten as

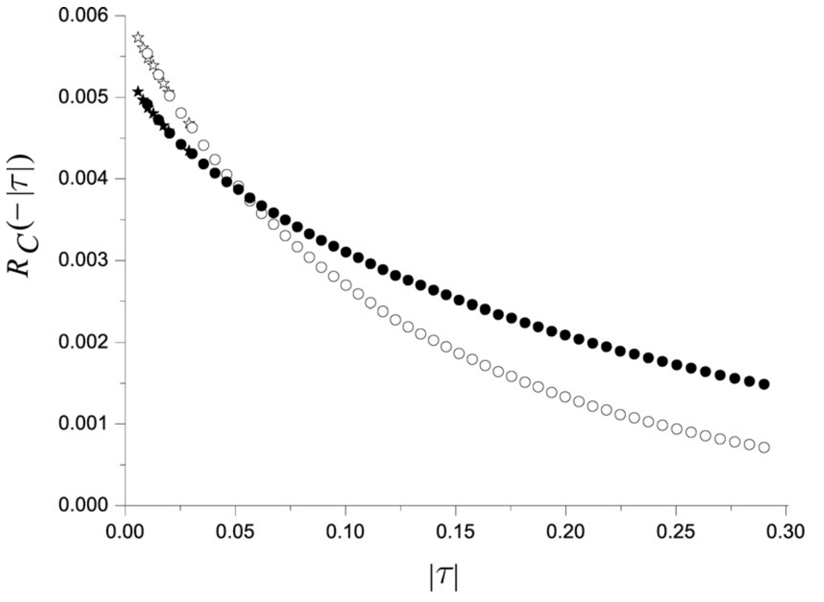

Fig. 7. The functions $R_C^-(-|\tau|)$ (open symbols) and $R_{C*}^-(-\tau)$ (closed symbols) which approaches the universal ratio R_C^- as $\tau \to 0^-$. Our MC data are represented by circles and the CTV data by stars.

Table 7
Estimates of the critical amplitude ratio R_C^- from our MC data using different fits and varying the temperature window.

τ-window	Amplitude	Correction terms			
	R_C^-	$\propto \lvert\tau\rvert^{2/3}$	$\propto \lvert\tau\rvert$	$\propto \lvert\tau\rvert^{4/3}$	$\propto \lvert\tau\rvert^{5/3}$
0.01–0.29	0.00651(3)	−3.04(12)	−1.24(39)	4.18(32)	–
	0.00685(3)	−4.60(3)	3.84(5)	–	–
	0.00619(1)	–	−16.13(11)	29.25(37)	−14.34(31)
	0.00591(2)	–	−11.01(10)	12.13(16)	–
0.01–0.10	0.00628(7)	−1.54(58)	-6.78 ± 2.36	9.41 ± 2.53	–
	0.00654(3)	−3.66(9)	−1.99(18)	–	–
	0.00627(3)	−2.70(2)	–	–	–
	0.00618(3)	–	-15.90 ± 1.26	28.64 ± 5.51	-14.09 ± 6.18
	0.00611(1)	–	−13.05(17)	16.10(35)	–
0.01–0.046	0.00642(6)	−3.09(33)	0.62(80)	–	–
	0.00637(1)	−2.83(2)	–	–	–
	0.00616(4)	–	−14.20(94)	18.99 ± 2.44	–
	0.00588(4)	–	−6.92(18)	–	–

$\alpha\tau^2 C_s\chi_s(1+C_{\rm bt}/C_s)(1+\chi_{\rm bt}/\chi_s)/M^2$. Thus, the background terms $C_{\rm bt}$ and $\chi_{\rm bt}$ contribute when divided by the singular terms (or in other words multiplied by factors $\tau^{2/3}\mathcal{G}$ and $\tau^{7/6}\mathcal{G}^{-3/4}$, respectively). Clearly, in the critical region, the first factor has the dominant contribution. This "large" term may be eliminated completely if we form a quantity equivalent to Eq. (46) from the

Table 8
Estimates of the critical amplitude ratio R^-_{C*} (Expr. (47)) from our MC data using different fits and varying the temperature window.

τ-window	Amplitude	Correction terms			
	R^-_C	$\propto \lvert\tau\rvert^{2/3}$	$\propto \lvert\tau\rvert$	$\propto \lvert\tau\rvert^{4/3}$	$\propto \lvert\tau\rvert^{5/3}$
0.01–0.29	0.00551(9)	−2.53(5)	0.57(15)	1.11(12)	–
	0.00558(3)	−2.97(3)	1.95(2)	–	–
	0.00527(8)	–	−11.44(16)	20.98(51)	−11.25(42)
	0.00508(1)	–	−7.29(9)	7.38(14)	–
0.01–0.10	0.00558(4)	−3.28(36)	3.66 ± 1.45	2.23 ± 1.55	–
	0.00553(1)	−2.77(5)	1.58(9)	–	–
	0.00535(2)	−1.98(2)	–	–	–
	0.00538(2)	–	−16.11(99)	40.39 ± 4.30	31.97 ± 4.81
	0.00525(2)	–	−9.55(24)	11.82(50)	–
0.01–0.046	0.00558(3)	−3.09(20)	2.34(48)	–	–
	0.00543(2)	−2.11(3)	–	–	–
	0.00535(3)	–	−12.40(74)	18.95 ± 1.99	–
	0.00511(4)	–	−5.04(19)	–	–

Table 9
Estimates of the critical amplitude ratio R^-_{C*} from Caselle et al. MC data using different fits and varying the temperature window.

τ-window	Amplitude	Correction terms		
	R^-_C	$\propto \lvert\tau\rvert^{2/3}$	$\propto \lvert\tau\rvert$	$\propto \lvert\tau\rvert^{4/3}$
0.0058–0.029	0.00548(2)	−2.59(17)	1.27(48)	–
	0.00543(1)	−2.14(2)	–	–
	0.00535(1)	–	−13.77(66)	21.79 ± 1.98
	0.00521(2)	–	−5.93(23)	–

energy difference $E_-(|\tau|) - E_0$ instead of the specific heat,

$$R^-_{C^*}\big(-|\tau|\big) = \alpha(\alpha-1)\beta_c\tau\,\frac{(E_-(-|\tau|) - E_0)\chi_L(-|\tau|)}{M^2(-|\tau|)}, \tag{47}$$

which is shown in Fig. 7 with closed symbols. The extrapolation at $\tau \to 0^-$ is obviously different. The results of the fit of MC data to Eq. (47) are given in Table 8. The outcome for the universal combination R^-_C is now fully consistent with the value 0.0052(2) and supports our idea that the specific heat background term spoils the behavior of the estimator (46).

Again, a similar analysis of CTV data (see Table 9) leads to fully consistent results.

4. Discussion

Our final goal is the determination of some universal combinations of amplitudes. This can be done either directly from the values of the amplitudes listed in the various tables of this paper, or also by extrapolating the *effective ratios* to $\tau = 0$. Let us start with an estimate obtained by the second method, and let us concentrate on the most controversial amplitude ratios, those of the

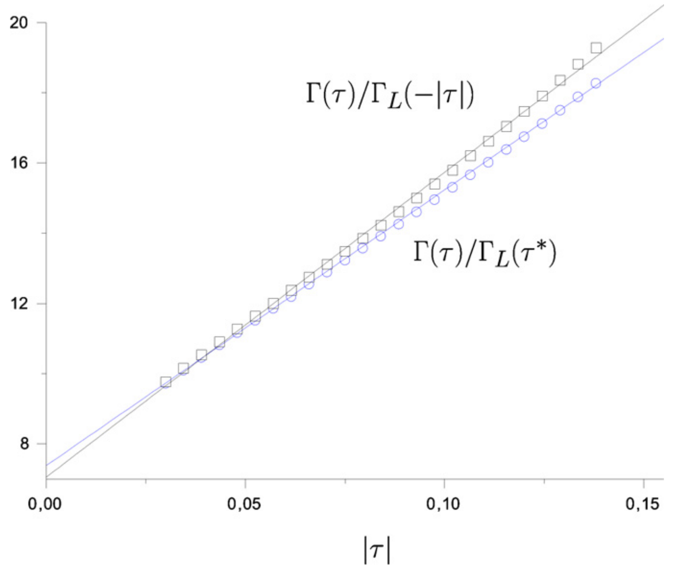

Fig. 8. The ratio of the effective amplitudes $\Gamma_+(\tau)/\Gamma_L(-|\tau|)$ obtained from SE data at symmetric temperatures (boxes) and dual temperatures (circles) together with the corresponding linear fits (solid lines).

susceptibilities. As we have just shown in the section on R_C^-, this method may lead to systematic deviations if the background terms are not handled with care. Later on we shall discuss the ratios of the amplitudes listed in the previous tables.

The ratio Γ_+/Γ_L can be estimated from the ratio of the SE of the susceptibility χ_+ at high-temperature and of the longitudinal susceptibility χ_L in the low-temperature phase. We have again two options to form this ratio, either from quantities computed at temperatures symmetric with respect to the critical temperature $T_c \pm \tau$ or at inverse temperatures β and β^* related by the duality relation (3). Fig. 8 shows both the ratios $\Gamma_+(\tau)/\Gamma_L(-|\tau|)$ and $\Gamma_+(\tau)/\Gamma_L(\tau^*)$, while the straight lines are drawn as a guide for the eye. It would be naive to take the linear fit too seriously, otherwise one should conclude that the background (non-singular) contribution to the ratio is negligible. The value of the universal amplitude ratio Γ_+/Γ_L obtained from the SE data is approximately $\Gamma_+/\Gamma_L \simeq 6.16(1)$ and 6.30(1), when using respectively the fits MC #2* and MC #3*. We have also analyzed the effective-amplitude ratio from MC data obtained by dividing the high-temperature reduced susceptibility by the longitudinal reduced susceptibility computed at temperatures related by the duality relation. Neglecting the constant background terms in the susceptibilities eliminates all logarithms and makes the fit quite simple, leading to a ratio in the range $\Gamma_+/\Gamma_L \simeq 6.30$–6.60. On the other hand, if we keep in the fit the background terms, the logs reappear and we are lead to $\Gamma_+/\Gamma_L \simeq 6.0$–6.1.

Thus we get values which are quite different from the analytical prediction $\Gamma_+/\Gamma_L = 4.013$ of Delfino and Cardy [13], as well as from the value 3.5(4) estimated by Enting and Guttmann from an analysis of the SE data for the susceptibility in both phases, and from the value 3.14(70) estimated by Caselle et al. [4].

Let us now estimate the effective-amplitude ratio $\Gamma_T(-|\tau|)/\Gamma_L(-|\tau|)$. This ratio, shown in Fig. 9, has been computed both by MC simulation, for various lattice sizes, and from SE data. Due to the non-singular correction terms, its behavior is far from being linear in τ as was the ratio $\chi_+(|\tau|)/\chi_L(-|\tau|)$ (compare with Fig. 8). A possible explanation is that there might be

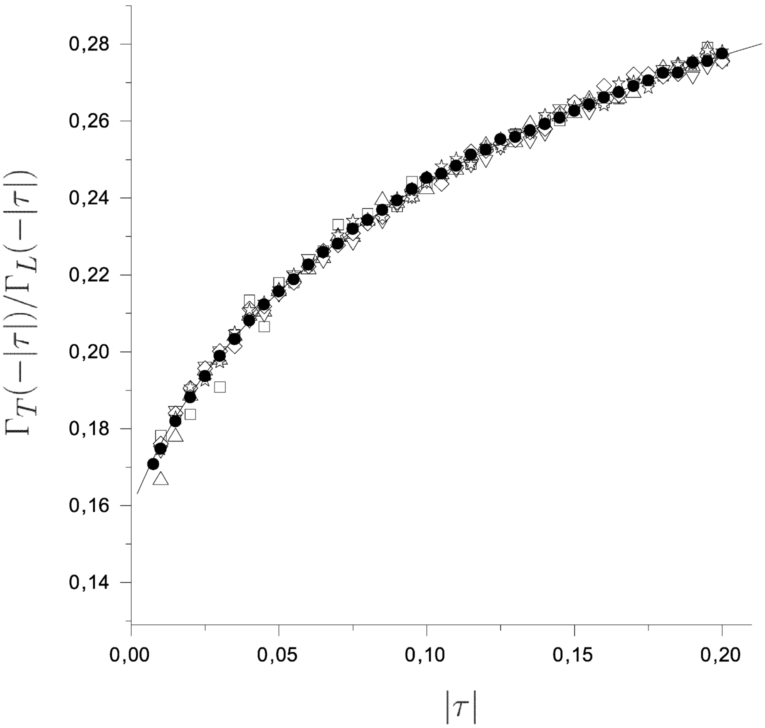

Fig. 9. 4-state Potts model. The ratio of the effective amplitudes $\Gamma_T(-|\tau|)/\Gamma_L(-|\tau|)$ for the 4-state Potts model on square lattices of linear sizes $L = 20$ (boxes), $L = 40$ (up triangles), $L = 60$ (down triangles), $L = 80$ (diamonds), $L = 100$ (stars) computed with $N_{\mathrm{MC}} = 10^5$ MC steps, and $L = 100$ (closed circles) computed with $N_{\mathrm{MC}} = 10^6$. The solid line represents the SE data.

some symmetry in the correction-to-scaling amplitudes occurring in the asymptotic expansion of $\chi_+(|\tau|)$ and $\chi_L(-|\tau|)$, but not of $\chi_T(-|\tau|)$, which introduces here a stronger background term still containing the logs. Following again the same procedure, we arrive at estimates close to 0.146 when neglecting all logarithmic corrections, while we get 0.152–0.153 when allowing for these corrections and from the analysis of SE data. Finally we obtain $\Gamma_T/\Gamma_L = 0.151(3)$ and 0.148(3) from the fits MC #2* and 3*. All these values differ from the analytical prediction $\Gamma_T/\Gamma_L = 0.129$ of Delfino et al. [18] and from the value 0.11(4) of Ref. [20].

Let us now extract what we believe are more reliable estimates for the universal combinations of amplitudes by a direct evaluation of the ratios of the numbers presented in this paper and collected again in Table 10. The universal combinations are presented in Table 11, together with the corresponding results available in the literature. Averaging our different results, we quote the following final estimates:

$$\Gamma_+/\Gamma_L = 6.49 \pm 0.44, \tag{48}$$

$$\Gamma_T/\Gamma_L = 0.154 \pm 0.012, \tag{49}$$

$$R_C^+ = 0.0338 \pm 0.0009, \tag{50}$$

$$R_C^- = 0.0052 \pm 0.0002. \tag{51}$$

These results clearly confirm the above-mentioned limits of effective ratios.

Table 10
Critical amplitudes and correction coefficients for the 4-state Potts model. They are written in the following format Obs.$(\pm|\tau|) \simeq$ Ampl. $\times |\tau|^{◀} \times \mathcal{G}^{★}(-\ln|\tau|) \times (1 +$ corr. terms$) +$ backgr. terms. The results of the MC analysis of Ref. [4] are compiled together with our results obtained by combining the MC and series expansion (SE) data analysis.

Observable	Amplitude	Correction terms, $\times\mathcal{G}^{★}(-\ln|\tau|)$		Background terms		Source
		$\propto |\tau|^{2/3}$	$\propto |\tau|$	$\propto |\tau|^0$	$\propto |\tau|$	
$E_\pm(\tau)$	$1.338(3)/\alpha(1-\alpha)\beta_c$	$-4.98(8)$	α_4	E_0	3.77(6)	this paper MC #2*
	$1.316(9)/\alpha(1-\alpha)\beta_c$	$-4.88(38)$	α_4	E_0	3.68(30)	this paper MC #3*
$\chi_+(\tau)$	$\Gamma_+ = 0.0223(14)$	–	–	0.05(14)	–	[4]
	$\Gamma_+ = 0.031(5)$	–	–	–	–	[20]
	$\Gamma_+ = 0.03144(15)$	0.561(60)	–	$-0.053(17)$	–	this paper MC #2*
	$\Gamma_+ = 0.03178(30)$	0.53(23)	–	0.052(120)	–	this paper MC #3*
	$\Gamma_+ = 0.03041(1)$	1.30(1)	–	$-0.362(9)$	–	this paper SE #2*
	$\Gamma_+ = 0.03039(1)$	1.67(1)	–	$-0.59(2)$	–	this paper SE #3*
$\chi_L(-|\tau|)$	$\Gamma_L = 0.00711(10)$	–	–	0.02(1)	–	[4]
	$\Gamma_L = 0.0088(4)$	–	–	–	–	[20]
	$\Gamma_L = 0.00454(2)$	$-2.83(3)$	–	0.050(2)	–	this paper MC #2*
	$\Gamma_L = 0.00484(3)$	$-3.73(14)$	–	0.13(1)	–	this paper MC #3*
	$\Gamma_L = 0.00483(1)$	$-3.77(3)$	–	0.116(3)	–	this paper SE #2*
	$\Gamma_L = 0.00493(1)$	$-4.18(5)$	–	0.178(6)	–	this paper SE #3*
$\chi_T(\tau)$	$\Gamma_T = 0.0010(3)$	–	–	–	–	[20]
	$\Gamma_T = 0.00076(1)$	$-0.805(34)$	–	$-0.0028(2)$	–	this paper MC #2*
	$\Gamma_T = 0.00073(1)$	$-0.25(13)$	–	$-0.0050(14)$	–	this paper MC #3*
	$\Gamma_T = 0.00073(1)$	$-0.577(14)$	–	$-0.00373(15)$	–	this paper SE #2*
	$\Gamma_T = 0.00073(1)$	$-0.369(15)$	–	$-0.00457(16)$	–	this paper SE #3*
$M(-|\tau|)$	$B = 1.1621(11)$	–	–	0.05(14)	–	[4]
	$B = 1.1570(1)$	$-0.191(2)$	–	–	–	this paper MC #2*
	$B = 1.1559(12)$	$-0.210(10)$	–	–	–	this paper MC #3*
	$B = 1.1575(1)$	$-0.194(1)$	–	–	–	this paper SE #2*
	$B = 1.1575(1)$	$-0.225(1)$	–	–	–	this paper SE #3*

Table 11
Universal combinations of the critical amplitudes in the 4-state Potts model.

A_+/A_-	Γ_+/Γ_L	Γ_T/Γ_L	R_C^+	R_C^-	Source
1.0	4.013	0.129	0.0204	0.00508	[13,18]
–	4.02	0.129	–	–	[19]
–	3.14(70)	–	0.021(5)	0.0068(9)	[4]
–	3.5(4)	0.11(4)	–	–	[20]
1.000(5)	6.93(6)	0.1674(30)	0.03452(25)	0.00499(3)	this paper MC #2*
1.000(13)	6.57(10)	0.1508(26)	0.03439(63)	0.00524(9)	this paper MC #3*
–	6.30(1)	0.1511(24)	0.03336(9)	0.00530(3)	this paper SE #2*
–	6.16(1)	0.1481(23)	0.03279(24)	0.00532(5)	this paper SE #3*

The main outcome of this work are the surprisingly high values of the ratios Γ_+/Γ_L, Γ_T/Γ_L and R_C^+ (and the low value for R_C^-), significantly deviating from the predictions of Delfino and Cardy. We emphasize that our results are also supported by a direct extrapolation of *effective-amplitude ratios* for which most corrections to scaling disappear. We believe that our fitting procedure is reliable, and since the disagreement with the theoretical calculations can hardly be resolved, we suspect that it might be attributed to the approximations made in Ref. [13] in order to predict the susceptibility ratios. Even more puzzling is the fact that Delfino and Cardy argue in favor of a higher robustness of their results for Γ_T/Γ_- than for Γ_+/Γ_-, while the disagreement is indisputable in both cases. Indeed, in the conclusion of their paper, and in a footnote, Delfino et al. [18, p. 533] explain that their results are sensitive to the relative normalization of the order- and disorder-operator form-factors, which could be the origin of some troubles for $q = 3$ and 4 for the ratios Γ_+/Γ_L and R_C only.

As a final argument in favor of our results, we may mention a work of W. Janke and one of us (LNS) on the amplitude ratios in the Baxter–Wu model (expected to belong to the 4-state Potts model universality class), leading to the estimate $\Gamma_+/\Gamma_- \simeq 6.9$ and $R_C^- \approx 0.005$ [30]. This result, obtained from an analysis of MC data shows a similar discrepancy with Delfino and Cardy's result and suggests that further analysis might still be necessary.

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Appendix A. Solution of non-linear RG equations and cancelation of logarithmic corrections in effective-amplitude ratios

For the 4-state Potts model, the non-linear RG equation for the relevant thermal and magnetic fields ϕ and h, with the corresponding RG eigenvalues y_ϕ and y_h, and the marginal dilution field ψ are given by

$$\frac{d\phi}{d\ln b} = (y_\phi + y_{\phi\psi}\psi)\phi, \tag{A.1}$$

$$\frac{dh}{d\ln b} = (y_h + y_{h\psi}\psi)h, \tag{A.2}$$

$$\frac{d\psi}{d\ln b} = g(\psi) \tag{A.3}$$

where b is the length rescaling factor and $l = \ln b$. The function $g(\psi)$ may be Taylor expanded, $g(\psi) = y_{\psi^2}\psi^2(1 + \frac{y_{\psi 3}}{y_{\psi 2}}\psi + \cdots)$. Accounting for marginality of the dilution field, there is no linear term. The first term has been considered by Nauenberg and Scalapino, and later by Cardy, Nauenberg and Scalapino. The second term was introduced by Salas and Sokal. In this appendix, we slightly change the notations of Salas and Sokal, keeping however the notation y_{ij} for all coupling coefficients between the scaling fields i and j. These parameters take the values $y_{\phi\psi} = 3/(4\pi)$, $y_{h\psi} = 1/(16\pi)$, $y_{\psi^2} = 1/\pi$ and $y_{\psi^3} = -1/(2\pi^2)$, while the relevant scaling dimensions are $y_\phi = \nu^{-1} = 3/2$ and $y_h = 15/8$.

The fixed point is at $\phi = h = 0$. Starting from initial conditions ϕ_0, h_0, the relevant fields grow exponentially with l. The field ϕ is analytically related to the temperature, so the temperature behavior follows from the renormalization flow from $\phi_0 \sim |\tau|$ up to some $\phi = O(1)$ outside the critical region. Notice also that the marginal field ψ remains of order $O(\psi_0)$ and ψ_0 is negative, $\psi_0 = O(-1)$. In zero magnetic field, under a change of length scale, the singular part of the free energy density transforms as

$$f(\psi_0, \phi_0) = e^{-Dl} f(\psi, \phi), \tag{A.4}$$

where $D = 2$ is the space dimension. Solving Eq. (A.1) leads to $\ln(\phi/\phi_0) = y_\phi l + y_{\phi\psi} \int \psi\, dl$ where the last integral is obtained from Eq. (A.3) rewritten as $\int_0^l \psi dl = \frac{1}{y_{\psi 2}} \ln(\psi/\psi_0) + \frac{1}{y_{\psi 2}} \ln G(\psi_0, \psi)$. Note that $G(\psi_0, \psi)$ takes the value 1 in Cardy, Nauenberg and Scalapino and the value $\frac{y_{\psi 2} + y_{\psi 3}\psi_0}{y_{\psi 2} + y_{\psi 3}\psi}$ in Salas and Sokal. Since this term appears always in the same combination, we write $z = \psi_0/\psi$, $\bar{z} = \frac{z}{G(\psi_0, \psi)}$ and in the same way we set $x = \phi_0/\phi$. One thus obtains

$$l = -\frac{1}{y_\phi} \ln x + \frac{y_{\phi\psi}}{y_\phi y_{\psi 2}} \ln \bar{z}. \tag{A.5}$$

At the critical temperature $\phi = 0$, the l-dependence on the magnetic field obeys a similar expression and one is led to the equality

$$l = -\nu \ln x + \mu \ln \bar{z} = -\nu_h \ln y + \mu_h \ln \bar{z}, \tag{A.6}$$

where $y = h_0/h$ and for brevity we will denote $\nu = 1/y_\phi = \frac{2}{3}$, $\mu = \frac{y_{\phi\psi}}{y_\phi y_{\psi 2}} = \frac{1}{2}$, $\nu_h = 1/y_h = \frac{8}{15}$ and $\mu_h = \frac{y_{h\psi}}{y_h y_{\psi 2}} = \frac{1}{30}$. We can thus deduce the following behavior for the free energy density in zero magnetic field in terms of the thermal and dilution fields, or at the critical temperature in terms of magnetic and dilution fields

$$f(\phi_0, \psi_0) = x^{D\nu} \bar{z}^{-D\mu} f(\phi, \psi), \tag{A.7}$$
$$f(h_0, \psi_0) = y^{D\nu_h} \bar{z}^{-D\mu_h} f(h, \psi). \tag{A.8}$$

The other thermodynamic properties follow by derivation with respect to the scaling fields, e.g. $E(\phi_0, \psi_0) = \frac{\partial}{\partial \phi_0} f(\psi_0, \phi_0)$, or

$$E(\phi_0, \psi_0) = e^{-Dl} \frac{\partial \phi}{\partial \phi_0} E(\phi, \psi), \tag{A.9}$$

$$C(\phi_0, \psi_0) = e^{-Dl} \left(\frac{\partial \phi}{\partial \phi_0} \right)^2 C(\phi, \psi), \tag{A.10}$$

$$M(\phi_0, \psi_0) = e^{-Dl} \frac{\partial h}{\partial h_0} M(\phi, \psi), \tag{A.11}$$

$$\chi(\phi_0, \psi_0) = e^{-Dl} \left(\frac{\partial h}{\partial h_0} \right)^2 \chi(\phi, \psi). \tag{A.12}$$

The derivatives $\frac{\partial \phi}{\partial \phi_0}$ and $\frac{\partial h}{\partial h_0}$ will thus determine the scaling behavior of all the thermodynamic quantities. The first one is obvious, $\frac{\partial \phi}{\partial \phi_0} = x^{-1}$ and for the second one, $\frac{\partial h}{\partial h_0} = y^{-1}$, we express y in terms of x and z using Eq. (A.6).[10] Altogether, introducing the notations $\lambda = y_h/y_\phi = \frac{5}{4}$ and

[10] It follows that $y = x^{y_h/y_\phi} \bar{z}^{y_{h\psi}/y_{\psi 2} - y_h y_{\phi\psi}/y_\phi y_{\psi 2}}$.

$\kappa = y_h y_{\phi\psi}/y_\phi y_{\psi^2} - y_{h\psi}/y_{\psi^2} = \frac{7}{8}$ one has

$$f(\phi_0,\psi_0) = x^{D\nu}\bar{z}^{-D\mu} f(\phi,\psi), \tag{A.13}$$

$$E(\phi_0,\psi_0) = x^{D\nu-1}\bar{z}^{-D\mu} E(\phi,\psi), \tag{A.14}$$

$$C(\phi_0,\psi_0) = x^{D\nu-2}\bar{z}^{-D\mu} C(\phi,\psi), \tag{A.15}$$

$$M(\phi_0,\psi_0) = x^{D\nu-\lambda}\bar{z}^{-D\mu+\kappa} M(\phi,\psi), \tag{A.16}$$

$$\chi(\phi_0,\psi_0) = x^{D\nu-2\lambda}\bar{z}^{-D\mu+2\kappa} \chi(\phi,\psi). \tag{A.17}$$

What appears extremely useful in these expressions is that when defining appropriate effective ratios,[11] the dependence on the quantity $\bar{z}$ cancels, due to the scaling relations among the critical exponents. This quantity $\bar{z}$ is precisely the only one where the log terms are hidden, and thus we may infer that not only the leading log terms, but all the log terms hidden in the dependence on the marginal dilution field disappear in the conveniently defined effective ratios. For example in an effective ratio like

$$R_C(x) = x^2 \frac{C(x,z)\chi(x,z)}{M^2(x,z)}, \tag{A.18}$$

all corrections to scaling coming from the variable z disappear.

Now we proceed by iterations of $l = -\nu \ln x + \mu \ln \bar{z}$ and $\bar{z} = z\frac{1+(y_{\psi^3}/y_{\psi^2})\psi}{1+(y_{\psi^3}/y_{\psi^2})\psi_0}$. The asymptotic solution of Eq. (A.3) is[12]

$$\frac{\psi}{\psi_0} = \frac{1}{1-\psi_0 y_{\psi^2} l}\left(1 + \frac{y_{\psi^3}}{(y_{\psi^2})^2}\frac{\ln l}{l} + O(1/l)\right). \tag{A.19}$$

We get for the variable z

$$z = \frac{1-\psi_0 y_{\psi^2} l}{1+\frac{y_{\psi^3}}{(y_{\psi^2})^2}\frac{\ln l}{l}} \simeq -\psi_0 y_{\psi^2}\nu\left(-\ln|\tau|\right)\frac{1+\frac{\mu}{\nu}\frac{\ln(-\ln|\tau|)}{-\ln|\tau|} + O(\frac{1}{-\ln|\tau|})}{1+\frac{y_{\psi^3}}{(y_{\psi^2})^2\nu}\frac{\ln(-\ln|\tau|)}{-\ln|\tau|} + O(\frac{1}{-\ln|\tau|})}. \tag{A.20}$$

Similarly, one has the combination

$$\frac{1+(y_{\psi^3}/y_{\psi^2})\psi}{1+(y_{\psi^3}/y_{\psi^2})\psi_0} \simeq \frac{1}{1+(y_{\psi^3}/y_{\psi^2})\psi_0}\left(1 - \frac{y_{\psi^3}}{(y_{\psi^2})^2\nu}\frac{1}{(-\ln|\tau|)} + O\left(\frac{1}{(-\ln|\tau|)^2}\right)\right) \tag{A.21}$$

and eventually one gets for the full correction-to-scaling variable the *heavy* expression

$$\bar{z} = \text{const} \times \left(-\ln|\tau|\right)\frac{1+\frac{\mu}{\nu}\frac{\ln(-\ln|\tau|)}{-\ln|\tau|}}{1+\frac{y_{\psi^3}}{(y_{\psi^2})^2\nu}\frac{\ln(-\ln|\tau|)}{-\ln|\tau|}}$$

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[11] I.e. effective ratios which eventually tend to universal limits when $\tau \to 0$.

[12] When $y_{\psi^3} = 0$ the asymptotic solution of Eq. (A.3) is simply $\frac{\psi_0}{1-\psi_0 y_{\psi^2} l}$. Thus one can try the ansatz $\psi = \frac{\psi_0}{1-\psi_0 y_{\psi^2} l}(1 + X(l))$ with a small correction $X(l)$ to solve asymptotically the full Eq. (A.3). Keeping only terms of order $O(l^{-3})$ at most, we are led to the following expression $X'(l) = -(1/l)X(l) + y_{\psi^3}/((y_{\psi^2})^2 l^2)$ where we use $X(l) = Y(l)/l$ to eventually obtain $Y(l) = (y_{\psi^3}/(y_{\psi^2})^2)\ln l$.

$$\times\left(1-\frac{y_{\psi^3}}{(y_{\psi^2})^2\nu}\frac{1}{(-\ln|\tau|)}\right)\times F\bigl(-\ln|\tau|\bigr)$$

$$=\text{const}\times\bigl(-\ln|\tau|\bigr)\frac{1+\frac{3}{4}\frac{\ln(-\ln|\tau|)}{-\ln|\tau|}}{1-\frac{3}{4}\frac{\ln(-\ln|\tau|)}{-\ln|\tau|}}\times\left(1+\frac{3}{4}\frac{1}{(-\ln|\tau|)}\right)\times\mathcal{F}\bigl(-\ln|\tau|\bigr) \quad \text{(A.22)}$$

where $\mathcal{F}(-\ln|\tau|)$ is a function of the variable $(-\ln|\tau|)$ only where also appears the non-universal constant ψ_0. Using Eq. (A.16), we deduce the behavior of the magnetization for example

$$M\bigl(-|\tau|\bigr)=B|\tau|^{1/12}\bigl(-\ln|\tau|\bigr)^{-1/8}\left[\left(1+\frac{3}{4}\frac{\ln(-\ln|\tau|)}{-\ln|\tau|}\right)\right.$$
$$\left.\times\left(1-\frac{3}{4}\frac{\ln(-\ln|\tau|)}{-\ln|\tau|}\right)^{-1}\left(1+\frac{3}{4}\frac{1}{-\ln|\tau|}\right)\mathcal{F}\bigl(-\ln|\tau|\bigr)\right]^{-1/8}. \quad \text{(A.23)}$$

Since all these log expressions are "lazy functions", it is unsafe to expand such terms, e.g. $(1-\frac{3}{4}\frac{\ln(-\ln|\tau|)}{-\ln|\tau|})^{-1}\simeq 1+\frac{3}{4}\frac{\ln(-\ln|\tau|)}{-\ln|\tau|}$, since the correction term is not small enough in the accessible temperature range $|\tau|\simeq 0.05$–0.10. We can thus only extract an effective function $\mathcal{F}_{\text{eff}}(-\ln|\tau|)$ which mimics the real one $\mathcal{F}(-\ln|\tau|)$ in the convenient temperature range. This is done through a plot of an effective-magnetization amplitude

$$B_{\text{eff}}\bigl(-|\tau|\bigr)=M\bigl(-|\tau|\bigr)|\tau|^{-1/12}\bigl(-\ln|\tau|\bigr)^{1/8}\left[\left(1+\frac{3}{4}\frac{\ln(-\ln|\tau|)}{-\ln|\tau|}\right)\right.$$
$$\left.\times\left(1-\frac{3}{4}\frac{\ln(-\ln|\tau|)}{-\ln|\tau|}\right)^{-1}\left(1+\frac{3}{4}\frac{1}{-\ln|\tau|}\right)\right]^{1/8} \quad \text{(A.24)}$$

which is found to behave as

$$B_{\text{eff}}\bigl(-|\tau|\bigr)=B\left(1-\frac{C_1}{-\ln|\tau|}-\frac{C_2\ln(-\ln|\tau|)}{(-\ln|\tau|)^2}\right)^{1/8} \quad \text{(A.25)}$$

from which one deduces that the function $\mathcal{F}(-\ln|\tau|)$ takes the approximate expression

$$\mathcal{F}\bigl(-\ln|\tau|\bigr)\simeq\left(1+\frac{C_1}{-\ln|\tau|}+\frac{C_2\ln(-\ln|\tau|)}{(-\ln|\tau|)^2}\right)^{-1}. \quad \text{(A.26)}$$

What is remarkable is the stability of the fit to Eq. (A.25). We obtain (see Table 1) $C_1=-0.757$ and $C_2=-0.522$ which yields an amplitude $B=1.1570(1)$. It is also possible to try a simpler choice, fixing $C_1=0$ and approximating the whole series by the C_2-term only. We then find the value $C_2'=-0.88$ and this leads to a very close magnetization-amplitude $B=1.1559(2)$.

For the following, we group all the terms coming from the variable $\bar{z}$ into a single function $\mathcal{G}(-\ln|\tau|)=(-\ln|\tau|)\times\mathcal{E}(-\ln|\tau|)\times\mathcal{F}(-\ln|\tau|)$ where

$$\mathcal{E}\bigl(-\ln|\tau|\bigr)=\left(1+\frac{3}{4}\frac{\ln(-\ln|\tau|)}{-\ln|\tau|}\right)$$
$$\times\left(1-\frac{3}{4}\frac{\ln(-\ln|\tau|)}{-\ln|\tau|}\right)^{-1}\left(1+\frac{3}{4}\frac{1}{-\ln|\tau|}\right) \quad \text{(A.27)}$$

in terms of which the singular parts of the physical quantities take a very compact form,

$$f(\tau)=F_{\pm}|\tau|^{4/3}\mathcal{G}^{-1}\bigl(-\ln|\tau|\bigr), \quad \text{(A.28)}$$

$$M\big(-|\tau|\big) = B|\tau|^{1/12}\mathcal{G}^{-1/8}\big(-\ln|\tau|\big), \tag{A.29}$$

$$\chi_+\big(\pm|\tau|\big) = \Gamma_+|\tau|^{-7/6}\mathcal{G}^{3/4}\big(-\ln|\tau|\big), \tag{A.30}$$

$$\chi_L\big(-|\tau|\big) = \Gamma_L|\tau|^{-7/6}\mathcal{G}^{3/4}\big(-\ln|\tau|\big), \tag{A.31}$$

$$\chi_T\big(-|\tau|\big) = \Gamma_T|\tau|^{-7/6}\mathcal{G}^{3/4}\big(-\ln|\tau|\big), \tag{A.32}$$

$$E_\pm\big(\pm|\tau|\big) = \frac{A_\pm}{\alpha(\alpha-1)}|\tau|^{1/3}\mathcal{G}^{-1}\big(-\ln|\tau|\big), \tag{A.33}$$

$$C_\pm\big(\pm|\tau|\big) = \frac{A_\pm}{\alpha}|\tau|^{-2/3}\mathcal{G}^{-1}\big(-\ln|\tau|\big). \tag{A.34}$$

The function $\mathcal{E}$ is known exactly while the function $\mathcal{F}$ needs to be fitted to the numerical data. In the same range of values of the reduced temperature, the "correction function" $\mathcal{F}(-\ln|\tau|)$ is now *fixed and the only remaining freedom is to include background terms and possibly additive corrections to scaling* coming from irrelevant scaling fields.[13] Among the additive correction terms, we may have those coming from the thermal sector $\Delta_{\phi_n} = -\nu y_{\phi_n}$, where the RG eigenvalues are $y_{\phi_n} = D - \frac{1}{2}n^2$. The first dimension $y_{\phi_1} = y_\phi$ is the temperature RG eigenvalue, the next one, y_{ϕ_2}, vanishes and is responsible for the appearance of the logarithmic corrections, so the first irrelevant correction to scaling in the thermal sector comes from $\Delta_{\phi_3} = -\nu y_{\phi_3} = 5/3$. One can also imagine a coupling of the magnetic sector to irrelevant scaling fields. The magnetic scaling dimensions x_{σ_n} lead to RG eigenvalues $y_{h_n} = D - x_{\sigma_n}$. The first dimension $y_{h_1} = y_h$ is the magnetic field RG eigenvalue. The second one is still relevant, $y_{h_2} = 7/8$, and it could lead, if admissible by symmetry, to corrections generically governed by the *difference* of relevant eigenvalues $(y_{h_1} - y_{h_2})/y_\phi = 2/3$. The next contribution comes from $y_{h_3} = -9/8$ and leads to a Wegner correction-to-scaling exponent [29] $\Delta_{h_3} = -\nu y_{h_3} = 3/4$. Eventually, spatial

[13] To introduce corrections to scaling, let us consider the case of an irrelevant scaling field, let say g, coupled to the temperature field through

$$\frac{d\phi}{dl} = y_\phi\phi + y_{\phi\psi}\phi\psi + y_{\phi g}\phi g \quad \text{and} \quad \frac{dg}{dl} = y_g g$$

($\Delta > 0$ above plays the rôle of $-y_g/y_\phi$, and is thus linked to the corresponding negative RG eigenvalue y_g). Solving for g gives $g = g_0 e^{y_g l}$ (the irrelevant scaling field decays exponentially when one approaches the fixed point). Solving for ψ gives $\psi = \frac{\psi_0}{1-\psi_0 y_{\psi^2} l}$, and for ϕ,

$$l = \frac{1}{y_\phi}\ln(\phi/\phi_0) - \frac{y_{\phi\psi}}{y_\phi y_{\psi^2}}\ln(\psi/\psi_0) + \frac{y_{\phi g}}{y_\phi y_g} g_0\big(e^{y_g l} - 1\big).$$

Iteration now leads to

$$l = -\frac{1}{y_\phi}\ln|\tau| + \frac{y_{\phi\psi}}{y_\phi y_{\psi^2}}\ln\big(-\ln|\tau|\big) + \frac{y_{\phi\psi}}{y_\phi y_{\psi^2}}\ln\frac{|\psi_0|y_{\psi^2}}{y_\phi} + \frac{y_{\phi g} g_0}{y_\phi |y_g|}\big(1 - |\tau|^{|y_g|/y_\phi}\big)$$

and thus a free energy density including the additive correction term

$$f \simeq e^{-Dl} = \text{const} \times |\tau|^{D/y_\phi}\big(-\ln|\tau|\big)^{-Dy_{\phi\psi}/y_\phi y_{\psi^2}}\left(1 + \frac{Dy_{\phi g} g_0}{y_\phi |y_g|}|\tau|^{|y_g|/y_\phi}\right).$$

In our case, the $\ln|\tau|$ terms are due to the first scaling field (marginal) through the complicated variable $\bar{z}$ and other correction terms could be added, e.g.

$$f(\tau) = F_\pm|\tau|^{4/3}\big(-\ln|\tau|\big)^{-1}\mathcal{E}^{-1}\big(-\ln|\tau|\big)\mathcal{F}^{-1}\big(-\ln|\tau|\big)\big(1 + D|\tau|^{\frac{2}{3}|y_g|}\big).$$

inhomogeneities of primary fields (higher order derivatives) bring the extra possibility of integer correction exponents $y_n = -n$ in the conformal tower of the identity. The first one of these irrelevant terms corresponds to a Wegner exponent $\Delta_1 = -\nu(-1) = 2/3$ and it is always present. We may thus possibly include the following corrections: $|\tau|^{2/3}$, $|\tau|^{3/4}$, $|\tau|^{4/3}$, $|\tau|^{5/3}, \ldots$, the first and third ones being always present, while the other corrections depend on the symmetry properties of the observables.

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