

Logarithmic Corrections and Finite-Size Scaling in the Two-Dimensional 4-State Potts Model

Jesús Salas¹ and Alan D. Sokal¹

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We analyze the scaling and finite-size-scaling behavior of the two-dimensional 4-state Potts model. We find new multiplicative logarithmic corrections for the susceptibility, in addition to the already known ones for the specific heat. We also find additive logarithmic corrections to scaling, some of which are universal. We have checked the theoretical predictions at criticality and off criticality by means of high-precision Monte Carlo data.

KEY WORDS: Scaling; finite-size scaling; critical phenomena; renormalization group; logarithmic corrections; corrections to scaling; Potts model; Ashkin-Teller model; Swendsen-Wang algorithm; cluster algorithm; Monte Carlo.

1. INTRODUCTION

The two-dimensional (2D) q -state ferromagnetic Potts model is one of the most intensively studied systems in statistical mechanics. Although this model is very simple to formulate, it has a rich phase diagram. Baxter⁽¹⁾ showed that for $q \leq 4$ this model undergoes a second-order phase transition at the self-dual point, while for $q > 4$ the transition is of first order.

The borderline case $q = 4$ is the most difficult: here the transition is second-order, but the leading power-law scaling behavior is modified by multiplicative logarithms, as was first observed by Nauenberg and Scalapino⁽²⁾ and Cardy, Nauenberg and Scalapino.⁽³⁾² These authors

¹ Department of Physics, New York University, New York, New York 10003; e-mail: salas@mafalda.physics.nyu.edu, sokal@nyu.edu. Current address for J. Salas: Departamento de Física Teórica, Facultad de Ciencias, Universidad de Zaragoza, Zaragoza 50009, Spain; e-mail: jesus@jupiter.unizar.es.

² In addition to these analytical works, the possible existence of multiplicative logarithmic corrections was proposed almost contemporaneously by Rebbi and Swendsen⁽⁴⁾ on the basis of numerical Monte Carlo renormalization group data.

studied an extended Potts model (the dilute Potts model⁽⁵⁾) in which, in addition to the usual q spin states, vacancies are allowed. The density of the vacancies is governed by a fugacity (“dilution field”). For each $q < 4$, one finds the following phase diagram for low vacancy fugacity, there is an ordinary critical point belonging to the universality class of the pure Potts model; for high vacancy fugacity, there is a first-order transition at which the energy, the magnetization and the vacancy density are all discontinuous; these two transition curves meet at a tricritical point. In the renormalization-group (RG) framework, there is for each $q < 4$ an ordinary critical fixed point, a tricritical fixed point, and a discontinuity fixed point (governing the first-order transition). At $q = 4$, the critical and tricritical fixed points merge, and the dilution field becomes marginal: this is the cause of the multiplicative logarithmic corrections. For $q > 4$, only the discontinuity fixed point survives.

The quantitative analysis of Cardy *et al.*^(2, 3) is based on studying the RG flow for the q -state dilute Potts model, as a function of the continuous parameter q , in a neighborhood of $q = 4$. First, by using a nonlinear transformation to appropriate scaling fields, they obtain the RG equations in Poincaré normal form through second order in the scaling fields and first order in $\epsilon \equiv q - 4$. Next they fix the free parameters in this normal form by matching the RG predictions to leading order in ϵ with the exactly known results for the critical exponents when $q < 4$ ^(6, 8) and for the latent heat when $q > 4$.⁽¹⁾³ Finally, by integrating the RG equations at $q = 4$ with suitable boundary conditions, they obtain predictions for the leading-order critical behavior of: a) the specific heat, the correlation length, and the magnetization as functions of the thermal field at zero ordering field; b) the critical magnetization as a function of the ordering field; and c) the critical two-point correlator as a function of the distance between the two points. In all these cases, the power-law dependence expected generically for a second-order phase transition is modified by multiplicative logarithmic corrections.

In this paper we show that by extending the analysis of Cardy *et al.* through third order in the fields, we can obtain not only the leading critical behavior but also the *universal* leading corrections to scaling: these are additive terms of the generic form $\log \log / \log$, with universal amplitudes that we can compute exactly. In addition, there are nonuniversal subleading correction-to-scaling terms of order $1/\log$. A similar behavior arises in

³ At that time that refs. 2 and 3 were written, the exact formulae for the critical exponents were only conjectured. They have now been confirmed by both Coulomb-gas and conformal-field-theory methods: see Appendix A.1 for a brief review.

other models with marginally irrelevant operators, such as the four-dimensional φ^4 (or Ising) model,^(9, 10) the three-dimensional tricritical φ^6 (or spin-1 Ising) model,⁽¹¹⁾ and the three-dimensional ferromagnet with strong dipolar interactions.^(12, 13)

A second goal of this paper is to extend the renormalization-group analysis of Cardy *et al.* to obtain the finite-size-scaling (FSS) behavior, as well as the leading corrections to finite-size scaling, for the 4-state Potts model in a periodic $L \times L$ box. Finite-size scaling⁽¹⁴⁻¹⁶⁾ plays an important role in the analysis of Monte Carlo simulations, which of course deal with finite systems and must thus be extrapolated to the infinite-volume limit. This extrapolation⁽¹⁷⁻¹⁹⁾ is a very delicate procedure, and the corrections to finite-size scaling induce systematic errors in the extrapolation.

For $q < 4$ the FSS behavior of the Potts model is well understood. The critical singularities are rounded-off: at finite volume, the specific heat (resp. the susceptibility) has a peak of height $\sim L^{\alpha/\nu}$ (resp. $L^{\gamma/\nu}$), and this peak is shifted from the critical point by an amount of order $L^{-1/\nu}$. The corrections to this leading behavior are suppressed by a factor $L^{-\omega}$, where ω is a correction-to-scaling exponent.

For $q > 4$ the FSS behavior is that appropriate to a first-order phase transition: the height of the peak in the specific heat scales as $\sim L^d$, and the shift as $\sim L^{-d}$, where d is the dimensionality of the lattice. The corrections are of order L^0 and L^{-2d} , respectively. This behavior has been proven rigorously for $q \gg 1$ by Borgs, Kotecký and Miracle-Solé,⁽²⁰⁻²²⁾ and has been confirmed numerically by Billoire *et al.*⁽²³⁾ for $q = 20$.

For $q = 4$ the FSS behavior is more complicated, but it can be obtained by a relatively trivial extension of the infinite-volume RG analysis. Not surprisingly, we find multiplicative logarithmic corrections to the leading power-law behavior (some of which have been found previously⁽²⁴⁾); in addition, we find additive corrections of orders $\log \log L / \log L$ and $1 / \log L$. In all cases we try to distinguish which corrections are universal and which are nonuniversal.

We remark that the FSS behavior of the eigenvalues of the transfer matrix in an $L \times \infty$ strip is also known:^(25, 26) there are additive logarithmic corrections to scaling due to the marginal dilution field.

The third goal of this paper is to test the predicted finite-size-scaling behavior for the 4-state Potts model by means of a high-precision Monte Carlo simulation using a Swendsen–Wang-type algorithm. We find that our Monte Carlo data are consistent with theory if we include *both* the predicted multiplicative logarithms *and* the additive logarithmic corrections. However, it would have been impossible to *deduce* the theory from these data, which are also consistent with other functional forms. In particular, we are unable to observe numerically in an unequivocal way the

correct powers on the multiplicative logarithms or the correct universal amplitudes on the additive $\log \log L / \log L$ corrections: these features are obscured by the presence of the nonuniversal $1 / \log L$ corrections.

The plan of this paper is as follows: In Section 2 we carry out the RG analysis for the 4-state Potts model in infinite volume, with emphasis on the multiplicative logarithms and on the universal additive logarithmic corrections. In Section 3 we extend this analysis to determine the finite-size-scaling behavior and the leading corrections to it. In Section 4 we describe our Monte Carlo simulations. In Section 5 we compare our numerical data, both on and off criticality, to the RG predictions. In Section 6 we report briefly our data on the dynamic critical behavior of our Swendsen–Wang-type algorithm. In the Appendix we show how the Cardy *et al.* RG analysis for $q \approx 4$ can be extended to cubic order in the fields, yielding the universal third-order term in the RG flow for the dilution field.

2. SCALING EQUATIONS IN INFINITE VOLUME

2.1. Renormalization-Group Flow

It is well known^(2, 3, 24) that the scaling behavior of the two-dimensional 4-state Potts model has logarithmic corrections. This is due to the presence in this model of a marginal operator, which is absent in any other two-dimensional Potts model.

Cardy, Nauenberg and Scalapino^(2, 3) described the renormalization-group flow for the q -state dilute Potts model by using three scaling fields: a thermal field ϕ , an ordering field h , and a dilution field ψ .⁴ The pure Potts model corresponds to a large negative value of the dilution field. Near criticality, the thermal field is proportional to the temperature deviation from criticality ($\phi \sim J_c - J$). The fields ϕ and h are relevant, and the field ψ is marginal when $q = 4$. The critical point is found at $\phi = h = 0$. In the larger space (q, ϕ, h, ψ) , the point $q = 4, \phi = h = \psi = 0$ is a multicritical point, at which a curve of critical points [$q < 4, \phi = h = 0, \psi \sim -(4 - q)^{1/2}$] meets a curve of tricritical points [$q < 4, \phi = h = 0, \psi \sim +(4 - q)^{1/2}$].

Cardy *et al.* found that the renormalization-group equations for $q = 4$ under an infinitesimal change of scale dl , keeping terms through second order in the fields, are

⁴Of course, in addition to these three fields there will be an infinite number of irrelevant scaling fields. But these will produce corrections to scaling that are suppressed by powers of the length scale, hence are negligible compared to the logarithmic corrections arising from the marginal operator ψ .

$$\frac{d\psi(l)}{dl} = a\psi(l)^2 \quad (2.1a)$$

$$\frac{d\phi(l)}{dl} = [y_T + b\psi(l)] \phi(l) \quad (2.1b)$$

$$\frac{dh(l)}{dl} = [y_H + c\psi(l)] h(l) \quad (2.1c)$$

where

$$y_T = \frac{3}{2}, y_H = \frac{15}{8}, a = \frac{1}{\pi}, b = \frac{3}{4\pi}, c = \frac{1}{16\pi} \quad (2.2)$$

The solution of these equations is:

$$\psi(l) = \frac{\psi(0)}{1 - a\psi(0)l} \quad (2.3a)$$

$$\phi(l) = \frac{\phi(0) e^{3l/2}}{(1 - a\psi(0)l)^{3/4}} \quad (2.3b)$$

$$h(l) = \frac{h(0) e^{15l/8}}{(1 - a\psi(0)l)^{1/16}} \quad (2.3c)$$

where l is the logarithm of the length-rescaling factor. From (2.3b, c) it is clear that the thermal and ordering fields are relevant (i.e., they grow exponentially as $l \rightarrow \infty$). The dilution field ψ is marginally irrelevant when $\psi(0) < 0$, in the sense that $\psi(l) \rightarrow 0$ as $l \rightarrow \infty$ but at a subexponential rate. This induces multiplicative logarithmic corrections (i.e., powers of l) in ϕ and h ; only when $\psi(0) = 0$ do we have a pure power-law (i.e., exponential-of- l) behavior for the two relevant fields. This latter behavior occurs in the Baxter-Wu model,⁽²⁷⁾ which is believed to be in the same universality class as the 4-state Potts model but does not exhibit any multiplicative logarithmic correction. We shall henceforth assume without comment that $\psi(0) < 0$.

The equations (2.1) are the Poincaré normal form of the RG flow at $q = 4$, taking into account terms through second order in the fields.⁽³⁾ The analysis of these equations yields the correct leading terms (power and multiplicative logarithm) for all the critical observables (correlation length, specific heat, etc.). However, we should include more terms in order to be

able to analyze the corrections to scaling to these quantities. Equation (2.1a) should be replaced by

$$\frac{d\psi(l)}{dl} \equiv F(\psi(l)) = a\psi(l)^2 + a'\psi(l)^3 + \dots \quad (2.4)$$

where a' is some constant, and the dots \dots stand for higher powers of $\psi(l)$. Note that the ratio a'/a^2 is universal, in the sense that it cannot be altered by any smooth change of variable; the coefficients of order ψ^4 and higher, by contrast, can be set to any desired values (e.g. zero) by a smooth change of variable $\psi \rightarrow \psi + \alpha_2\psi^2 + \alpha_3\psi^3 + \dots$. The solution of (2.4) has the following asymptotic behavior for large l :

$$\psi(l) = -\frac{1}{al} \left[1 + \frac{a' \log l}{a^2} + O\left(\frac{1}{l}\right) \right] \quad (2.5)$$

Note that the $\log l/l$ correction term here is *universal*: it does not depend on $\psi(0)$ or on the parametrization of ψ . By contrast, the $1/l$ corrections are nonuniversal, as their value depends explicitly on $\psi(0)$. The terms of order ψ^4 and higher in (2.4), even if present, affect only the $1/l$ corrections.

The effect of the term $a'\psi(l)^3$ in (2.4) on the solutions of (2.1b, c) can be computed easily. Let us define the function $f_{A,B}(l; \psi(0))$ to be the ratio $\theta(l)/\theta(0)$ when solving the generic equation

$$\frac{d\theta}{dl} = [A + Ba\psi(l)] \theta(l) \quad (2.6)$$

where $\psi(l)$ is the *exact* solution of (2.4) with the specified initial value $\psi(0)$. Namely, the function $f_{A,B}$ is given by the integral

$$f_{A,B}(l; \psi(0)) = \exp \left(\int_0^l [A + Ba\psi(l')] dl' \right) \quad (2.7a)$$

$$= \exp \left(\int_{\psi(0)}^{\psi(l)} [A + Ba\psi'] \frac{d\psi'}{F(\psi')} \right) \quad (2.7b)$$

The asymptotic behavior of $f_{A,B}$ for large l is

$$f_{A,B}(l; \psi(0)) = e^{Al} (-a\psi(0)l)^{-B} \left[1 + \frac{a' \log l}{a^2} + O\left(\frac{1}{l}\right) \right]^B \quad (2.8)$$

Thus, the solutions (2.3b, c) are replaced by

$$\begin{aligned}\phi(l) &= \phi(0) f_{3/2, 3/4}(l; \psi(0)) \\ &= \frac{\phi(0) e^{3l/2}}{(-a\psi(0)l)^{3/4}} \left[1 + \frac{a' \log l}{a^2 l} + O\left(\frac{1}{l}\right) \right]^{3/4}\end{aligned}\quad (2.9a)$$

$$\begin{aligned}h(l) &= h(0) f_{15/8, 1/16}(l; \psi(0)) \\ &= \frac{h(0) e^{15l/8}}{(-a\psi(0)l)^{1/16}} \left[1 + \frac{a' \log l}{a^2 l} + O\left(\frac{1}{l}\right) \right]^{1/16}\end{aligned}\quad (2.9b)$$

One must also include higher powers of $\psi(l)$ inside the square brackets in (2.1b, c), but these terms cause only subleading corrections, multiplying (2.9) by factors $1 + O(1/l)$.

The value of a' can be obtained by studying the RG flow in a neighborhood of the multicritical point $q = q_c = 4$, and matching the exponents with the exactly known value⁽²⁸⁾ of the next-to-leading thermal exponent as a function of q . The details of this computation are given in Appendix A; the result is

$$a' = -\frac{1}{2\pi^2}\quad (2.10)$$

2.2. Correlation Length

In infinite volume one can define various different correlation lengths: the most important of these are the exponential correlation length (=inverse mass gap)

$$\xi_{\infty}^{(\text{exp})} \equiv \lim_{|x| \rightarrow \infty} \frac{-|x|}{\log G(x)}\quad (2.11)$$

(where x is taken to infinity along a coordinate axis) and the second-moment correlation length

$$\xi_{\infty}^{(2)} \equiv \left(\frac{1}{2d} \frac{\sum_{\nu} |x|^2 G(x)}{\sum_{\nu} G(x)} \right)^{1/2}\quad (2.12)$$

where $G(x)$ is the two-point correlation function and d is the spatial dimension. (We have appended a subscript ∞ to emphasize that these quantities are defined in infinite volume, in order to distinguish them from the finite-volume quantities to be introduced in the next section.) Both of these

correlation lengths, as well as other similar ones, are expected to scale in the same way near the critical point (but with different prefactors).

Let, therefore, ξ_∞ be any one of these correlation lengths. It behaves under a change of scale l as

$$\xi_\infty(\phi(0), h(0), \psi(0)) = e^l \xi_\infty(\phi(l), h(l), \psi(l)) \quad (2.13)$$

[Henceforth we shall drop the arguments 0 on the initial values of the fields, and simply write $\phi \equiv \phi(0)$, $h \equiv h(0)$, $\psi \equiv \psi(0)$.] Substituting the solutions (2.9), we get the scaling form

$$\xi_\infty(\phi, h, \psi) = e^l \xi_\infty(\phi f_{3/2, 3/4}(l; \psi), h f_{15/8, 1/16}(l; \psi), \psi(l)) \quad (2.14)$$

where $\psi(l)$ is given by (2.5).

Let us now define $l^* \equiv l^*(\phi, \psi)$ as the solution of the equation

$$\phi f_{3/2, 3/4}(l^*; \psi) = \begin{cases} +1 & \text{if } \phi > 0 \\ -1 & \text{if } \phi < 0 \end{cases} \quad (2.15)$$

(This solution is unique when $|\phi|$ is sufficiently small.) The exact form of l^* as a function of ϕ and ψ cannot be obtained in closed form. However, we can get the following asymptotic expansion for small ϕ (and fixed $\psi < 0$):

$$\begin{aligned} l^*(\phi, \psi) = & -\frac{2}{3} \log |\phi| + \frac{1}{2} \log(-\log |\phi|) + \frac{1}{2} \log\left(\frac{-2a\psi}{3}\right) \\ & + \left(\frac{3}{8} - \frac{3a'}{4a^2}\right) \frac{\log(-\log |\phi|)}{-\log |\phi|} + O\left(\frac{1}{\log |\phi|}\right) \end{aligned} \quad (2.16)$$

Note that the first, second and fourth terms in (2.16) are universal, while the third term and the $O(1/\log |\phi|)$ correction are nonuniversal (they depend on ψ). It follows from (2.16) that for any exponents A, B we can write

$$F_{A, B}(\phi; \psi) \equiv f_{A, B}(l^*(\phi, \psi); \psi) \quad (2.17a)$$

$$\begin{aligned} & = |\phi|^{-2A/3} (-\log |\phi|)^{(A/2 - B)} \left(\frac{-2a\psi}{3}\right)^{(A/2 - B)} \\ & \times \left[1 - \left(\frac{3}{4} + \frac{3a'}{2a^2}\right) \left(\frac{A}{2} - B\right) \frac{\log(-\log |\phi|)}{-\log |\phi|} \right. \\ & \left. + O\left(\frac{1}{\log |\phi|}\right) \right] \end{aligned} \quad (2.17b)$$

Note that the leading power and log are universal, as is the additive correction proportional to $\log(-\log|\phi|)/\log|\phi|$; the constant factor and the $1/\log|\phi|$ additive correction are nonuniversal.

Let us now insert $l=l^*(\phi, \psi)$ into (2.14): using (2.16)/(2.17), and restricting for simplicity to zero field ($h=0$), the result is

$$\xi_{\infty}(\phi, 0, \psi) = F_{1,0}(\phi; \psi) \xi_{\infty} \left(\pm 1, 0, \frac{3}{2a \log |\phi|} + \dots \right) \quad (2.18a)$$

$$= |\phi|^{-2/3} \left(\frac{2a\psi}{3} \log |\phi| \right)^{1/2} \left[1 + \left(\frac{3}{8} - \frac{3a'}{4a^2} \right) \frac{\log(-\log|\phi|)}{-\log|\phi|} + O\left(\frac{1}{\log|\phi|}\right) \right] \xi_{\infty} \left(\pm 1, 0, \frac{3}{2a \log |\phi|} + \dots \right) \quad (2.18b)$$

$$\approx C_{\pm} |\phi|^{-2/3} (-\log|\phi|)^{1/2} \left[1 + \left(\frac{3}{8} - \frac{3a'}{4a^2} \right) \frac{\log(-\log|\phi|)}{-\log|\phi|} + O\left(\frac{1}{\log|\phi|}\right) \right] \quad (2.18c)$$

where

$$C_{\pm} \equiv \left(\frac{-2a\psi}{3} \right)^{1/2} \xi_{\infty}(\pm 1, 0, 0) \quad (2.19)$$

is a nonuniversal amplitude; here the + (resp. -) sign corresponds to the high-temperature (resp. low-temperature) side of criticality. In the passage from (2.18b) to (2.18c) we have assumed that $\xi_{\infty}(\pm 1, 0, 0) \neq 0$ and that $\xi_{\infty}(\pm 1, 0, \psi)$ is a *smooth* function of ψ near $\psi=0$: together these assumptions imply that $\xi_{\infty}(\pm 1, 0, 3/(2a \log|\phi|) + \dots) = \text{const} + O(1/\log|\phi|)$. Physically, this amounts to assuming that ψ is a *non-dangerous* irrelevant variable.⁽²⁹⁻³¹⁾ We shall henceforth make this assumption without further comment. The leading power and multiplicative logarithm in (2.18c) were first obtained in ref. 3; the universal $\log(-\log|\phi|)/\log|\phi|$ additive correction is new.

If we invert (2.18c) we get

$$\phi \approx \pm C'_{\pm} \xi_{\infty}^{-3/2} (\log \xi_{\infty})^{3/4} \left[1 - \frac{3a'}{4a^2} \frac{\log \log \xi_{\infty}}{\log \xi_{\infty}} + O\left(\frac{1}{\log \xi_{\infty}}\right) \right] \quad (2.20)$$

where

$$C'_{\pm} \equiv (-a\psi)^{3/4} \xi_{\infty}(\pm 1, 0, 0)^{3/2} \quad (2.21)$$

is a nonuniversal amplitude. Again, the correction of order $\log \log \xi_\infty / \log \xi_\infty$ is universal, while the correction of order $1/\log \xi_\infty$ is nonuniversal.

To study the critical isotherm (with $h > 0$) we first define the scale $l^{**} \equiv l^{**}(h, \psi)$ to be the solution of the equation

$$hf_{15/8, 1/16}(l^{**}; \psi) = 1 \quad (2.22)$$

This solution is given asymptotically for small h by

$$\begin{aligned} l^{**}(h, \psi) = & -\frac{8}{15} \log h + \frac{1}{30} \log(-\log h) + \frac{1}{30} \log\left(\frac{-2a\psi}{15}\right) \\ & + \left(\frac{1}{480} - \frac{a'}{16a^2}\right) \frac{\log(-\log h)}{-\log h} + O\left(\frac{1}{\log h}\right) \end{aligned} \quad (2.23)$$

We can also define a function analogous to $F_{A, B}$:

$$G_{A, B}(h; \psi) \equiv f_{A, B}(l^{**}(h, \psi); \psi) \quad (2.24a)$$

$$\begin{aligned} & = h^{-8A/15} (-\log h)^{A/30 - B} \left(\frac{-8a\psi}{15}\right)^{A/30 - B} \\ & \times \left[1 + \left(\frac{1}{16} - \frac{15a'}{8a^2}\right) \left(\frac{A}{30} - B\right) \frac{\log(-\log h)}{-\log h} + O\left(\frac{1}{\log h}\right) \right] \end{aligned} \quad (2.24b)$$

If we now choose $l = l^{**}(h, \psi)$ in (2.14), we get on the critical isotherm ($\phi = 0$)

$$\xi_\infty(0, h, \psi) = G_{1, 0}(h; \psi) \xi_\infty\left(0, 1, \frac{15}{8a} \frac{1}{\log h} + \dots\right) \quad (2.25a)$$

$$\sim h^{-8/15} (-\log h)^{1/30} \left[1 + \left(\frac{1}{480} - \frac{a'}{16a^2}\right) \frac{\log(-\log h)}{-\log h} + O\left(\frac{1}{\log h}\right) \right] \quad (2.25b)$$

2.3. The Free Energy and Its Derivatives

The singular piece of the free energy per unit volume behaves under a change of scale l as

$$f_{\text{sing}}(\phi(0), h(0), \psi(0)) = e^{-2l} f_{\text{sing}}(\phi(l), h(l), \psi(l)) \quad (2.26)$$

If we plug the solution (2.9) of the renormalization-group equations (2.1) into (2.26), we get

$$f_{\text{sing}}(\phi, h, \psi) = e^{-2l} f_{\text{sing}}(\phi f_{3/2, 3/4}(l; \psi), h f_{15/8, 1/16}(l; \psi), \psi(l)) \quad (2.27)$$

where $\psi(l)$ is given by (2.5).

Let us now choose the scale $l = l^*(\phi, \psi)$ as in (2.15); using (2.16)/(2.17), we get

$$f_{\text{sing}}(\phi, h, \psi) = F_{-2, 0}(\phi; \psi) f_{\text{sing}}\left(\pm 1, h F_{15/8, 1/16}(\phi; \psi), \frac{3}{2a \log |\phi|} + \dots\right) \quad (2.28)$$

where the + (resp. -) sign corresponds to the high-temperature (resp. low-temperature) side of criticality. At zero field ($h = 0$) this expression can be written as

$$f_{\text{sing}}(\phi, 0, \psi) \approx D_{\pm} |\phi|^{4/3} (-\log |\phi|)^{-1} \times \left[1 - \left(\frac{3}{4} - \frac{3a'}{2a^2} \right) \frac{\log(-\log |\phi|)}{-\log |\phi|} + O\left(\frac{1}{\log |\phi|}\right) \right] \quad (2.29)$$

where

$$D_{\pm} \equiv \left(\frac{-2a\psi}{3} \right)^{-1} f_{\text{sing}}(\pm 1, 0, 0) \quad (2.30)$$

is a nonuniversal amplitude. The leading power and multiplicative logarithm in (2.29) were first obtained in ref. 2; the universal $\log(-\log |\phi|)/\log |\phi|$ additive correction is new.

If we differentiate (2.28) twice with respect to ϕ , we get the specific heat. At zero field ($h = 0$) we get

$$C_H(\phi, 0, \psi) \sim |\phi|^{-2/3} (-\log |\phi|)^{-1} \times \left[1 - \left(\frac{3}{4} - \frac{3a'}{2a^2} \right) \frac{\log(-\log |\phi|)}{-\log |\phi|} + O\left(\frac{1}{\log |\phi|}\right) \right] \quad (2.31)$$

The leading behavior of the specific heat was previously obtained in ref. 2.

If we differentiate (2.28) once with respect to the ordering field h , we get the magnetization. The result at zero ordering field ($h \downarrow 0$) in the low-temperature regime ($\phi < 0$) is

$$M(\phi, 0, \psi) \sim F_{-2,0}(\phi; \psi) F_{15/8, 1/16}(\phi; \psi) = F_{-1/8, 1/16}(\phi; \psi) \quad (2.32a)$$

$$\begin{aligned} &\sim (-\phi)^{1/12} (-\log(-\phi))^{-1/8} \\ &\times \left[1 - \left(\frac{3}{32} - \frac{3a'}{16a^2} \right) \frac{\log(-\log(-\phi))}{-\log(-\phi)} + O\left(\frac{1}{\log|\phi|}\right) \right] \end{aligned} \quad (2.32b)$$

If we differentiate (2.28) twice with respect to the ordering field h , we get the susceptibility. The result at $h=0$ is

$$\chi(\phi, 0, \psi) \sim F_{-2,0}(\phi; \psi) F_{15/8, 1/16}(\phi; \psi)^2 = F_{7/4, 1/8}(\phi; \psi) \quad (2.33a)$$

$$\begin{aligned} &\sim |\phi|^{-7/6} (-\log|\phi|)^{3/4} \\ &\times \left[1 - \left(\frac{9}{16} - \frac{9a'}{8a^2} \right) \frac{\log(-\log|\phi|)}{-\log|\phi|} + O\left(\frac{1}{\log|\phi|}\right) \right] \end{aligned} \quad (2.33b)$$

The leading power and multiplicative logarithms in (2.32b) were first obtained in ref. 3. The result (2.33b) did not appear in ref. 3, but it can of course be obtained directly from their approach. The universal $\log(-\log|\phi|)/\log|\phi|$ additive corrections are all new.

Finally, we can write the asymptotic behavior of the specific heat, the magnetization, and the susceptibility as functions of ξ_∞ . Using (2.20) we get

$$C_H \sim \frac{\xi_\infty}{(\log \xi_\infty)^{3/2}} \left[1 + \frac{3a'}{2a^2} \frac{\log \log \xi_\infty}{\log \xi_\infty} + O\left(\frac{1}{\log \xi_\infty}\right) \right] \quad (2.34a)$$

$$M \sim \frac{\xi_\infty^{-1/8}}{(\log \xi_\infty)^{1/16}} \left[1 + \frac{a'}{16a^2} \frac{\log \log \xi_\infty}{\log \xi_\infty} + O\left(\frac{1}{\log \xi_\infty}\right) \right] \quad (2.34b)$$

$$\chi \sim \frac{\xi_\infty^{7/4}}{(\log \xi_\infty)^{1/8}} \left[1 + \frac{a'}{8a^2} \frac{\log \log \xi_\infty}{\log \xi_\infty} + O\left(\frac{1}{\log \xi_\infty}\right) \right] \quad (2.34c)$$

Note that the (universal) corrections of order $\log \log \xi_\infty / \log \xi_\infty$ are proportional to the ratio a'/a^2 and to the exponent of the multiplicative logarithm, since the other terms of the same order cancel out.

Finally, we observe that the following two relations hold:

$$C_H \xi_\infty^2 \sim \phi^{-2} \left[1 + O\left(\frac{1}{\log|\phi|}\right) \right] \quad (2.35a)$$

$$M^2 \xi_\infty^2 \sim \chi \left[1 + O\left(\frac{1}{\log|\phi|}\right) \right] \quad (2.35b)$$

Note that in these relations there are *neither* multiplicative logarithmic corrections *nor* additive $\log(-\log|\phi|)/\log|\phi|$ corrections. It follows that the hyperscaling laws

$$dv = 2 - \alpha \quad (2.36a)$$

$$dv = \gamma + 2\beta \quad (2.36b)$$

are satisfied without logarithmic corrections.

The magnetization on the critical isotherm ($\phi = 0, h > 0$) can be calculated by first choosing the scale $l = l^{**}(h, \psi)$ as in (2.22). Plugging (2.23)–(2.24) into (2.27) we get

$$f_{\text{sing}}(0, h, \psi) = G_{-2,0}(h; \psi) f_{\text{sing}}\left(0, 1, \frac{15}{8a \log h} + \dots\right) \quad (2.37a)$$

$$\begin{aligned} &\sim h^{16/15} (-\log h)^{-1/15} \\ &\times \left[1 - \left(\frac{1}{240} - \frac{a'}{8a^2} \right) \frac{\log(-\log h)}{-\log h} + O\left(\frac{1}{\log h}\right) \right] \end{aligned} \quad (2.37b)$$

By differentiating this equation with respect to h we get the critical magnetization:

$$M(0, h, \psi) \sim h^{1/15} (-\log h)^{-1/15} \left[1 - \left(\frac{1}{240} - \frac{a'}{8a^2} \right) \frac{\log(-\log h)}{-\log h} + O\left(\frac{1}{\log h}\right) \right] \quad (2.38)$$

The leading power and multiplicative logarithm in this result were first obtained also in ref. 3. The universal $\log(-\log h)/\log h$ correction is new.

2.4. Two-Point Correlators

The authors of ref. 3 also included the following behavior for the two-point correlation function at criticality:

$$G(x; 0, 0, \psi) \sim \frac{1}{|x|^{1/4} (\log |x|)^{1/8}} \quad \text{as } |x| \rightarrow \infty \quad (2.39)$$

If we assume a natural scaling law of the form

$$G(x; \phi, 0, \psi) \approx \frac{1}{|x|^{1/4} (\log |x|)^{1/8}} F_G\left(\frac{|x|}{\xi_\infty(\phi, 0, \psi)}\right) \quad (2.40)$$

where F_G is some scaling function, then we can deduce equation (2.34c) through the integral

$$\chi = \int d^2x G(x) \quad (2.41)$$

Moreover, we can deduce the relation (2.34b) by taking $|x| \sim \xi_\infty$ and using the hyperscaling relation

$$G(|x| \sim \xi_\infty) \sim \lim_{|x| \rightarrow \infty} G(x) \equiv M^2 \quad (2.42)$$

3. FINITE-SIZE SCALING

In this section we analyze the finite-size-scaling behavior of the two-dimensional 4-state Potts model on an $L \times L$ lattice with periodic boundary conditions.

3.1. Renormalization-Group Flow in Finite Volume

To obtain the finite-size scaling of this model we only have to adjoin a new “scaling field” L^{-1} , where L is the linear size of the system. The fixed-point value of this field obviously is $L^{-1} = 0$, corresponding to the infinite-volume limit. The behavior of this scaling field under a change of scale is trivial: to (2.1a–c) we need to adjoin the flow

$$\frac{dL^{-1}(l)}{dl} = L^{-1}(l) \quad (3.1)$$

3.2. Correlation Length

Not all of the correlation lengths employed in infinite volume have sensible analogues in a fully finite lattice: for example, the exponential correlation length (2.11) makes sense only if the lattice is infinite in at least one direction. However, the second-moment correlation length (2.12) does have a sensible extension to finite volume; this extension is, however, not unique. One reasonable definition for a periodic lattice of linear size L is

$$\xi^{(2)} \equiv \frac{(\chi/F - 1)^{1/2}}{2 \sin(\pi/L)} \quad (3.2)$$

where χ is the susceptibility (i.e., the Fourier-transformed two-point correlation function at zero momentum) and F is the corresponding quantity at the smallest nonzero momentum ($2\pi/L, 0$):

$$\chi \equiv \sum_x G(x; L) \quad (3.3)$$

$$F \equiv \sum_x e^{2i\pi x_1/L} G(x; L) \quad (3.4)$$

where $G(x; L)$ is, of course, the two-point correlation function on the finite lattice. Another definition could be

$$\xi' \equiv \left(\frac{1}{2} \frac{\sum_x (L^2/\pi^2) \sin^2(\pi x_1/L) G(x; L)}{\sum_x G(x; L)} \right)^{1/2} = \frac{L}{2\pi} \left(1 - \frac{F}{\chi} \right)^{1/2} \quad (3.5)$$

Hereafter, ξ will denote any reasonable finite-volume correlation length.

The generalization of (2.13)/(2.14) is

$$\xi(\phi, h, \psi, L^{-1}) = e^{l\xi}(\phi(l), h(l), \psi(l), L^{-1}(l)) \quad (3.6a)$$

$$= e^{l\xi} \left(\phi_{f_{3/2, 3/4}}(l; \psi), h_{f_{15/8, 1/16}}(l; \psi), \psi(l), \frac{e^l}{L} \right) \quad (3.6b)$$

where $\psi(l)$ is given by (2.5). Let us now choose the scale

$$l = \log L \quad (3.7)$$

so that (3.6) becomes

$$\xi(\phi, h, \psi, L^{-1}) = L\xi(\phi_{f_{3/2, 3/4}}(\log L; \psi), h_{f_{15/8, 1/16}}(\log L; \psi), \psi(\log L), 1) \quad (3.8)$$

One quantity of interest is the L -dependence of the correlation length at criticality ($\phi = h = 0$). From (3.8) and (2.5) it is trivial to see that

$$\xi(0, 0, \psi, L^{-1}) = L\xi(0, 0, \psi(\log L), 1) \quad (3.9a)$$

$$= L \left[x^* + \frac{A}{\log L} + B \frac{\log \log L}{(\log L)^2} + O\left(\frac{1}{(\log L)^2}\right) \right] \quad (3.9b)$$

where

$$x^* \equiv \xi(0, 0, 0, 1) \quad (3.10a)$$

$$A \equiv -\frac{1}{a} \frac{\partial \xi}{\partial z}(0, 0, z, 1) \Big|_{z=0} \quad (3.10b)$$

$$B \equiv \frac{a'}{a^2} A \quad (3.10c)$$

are all universal; the corrections of order $1/(\log L)^2$ are nonuniversal.

We can also obtain a finite-size-scaling law off criticality. For simplicity let us restrict attention to $h=0$. From (3.8) we know that at zero field

$$\frac{\xi(\phi, 0, \psi, L^{-1})}{L} = \xi \left(\phi f_{3/2, 3/4}(\log L; \psi), 0, -\frac{1}{a \log L} + \dots, 1 \right) \quad (3.11)$$

And from (2.8) we know that

$$\phi f_{3/2, 3/4}(\log L; \psi) = \phi L^{3/2} (-a\psi \log L)^{-3/4} \left[1 + \frac{a'}{a^2} \frac{\log \log L}{\log L} + O\left(\frac{1}{\log L}\right) \right] \quad (3.12)$$

where the $O(1/\log L)$ correction term is nonuniversal. Therefore, we obtain the FSS law

$$\frac{\xi(\phi, 0, \psi, L^{-1})}{L} = \bar{F}_\xi(\phi L^{3/2} (\psi \log L)^{-3/4}) + O\left(\frac{\log \log L}{\log L}\right) \quad (3.13)$$

where the function \bar{F}_ξ is universal modulo a nonuniversal rescaling of its argument.

The disadvantage of this approach is that the corrections to FSS are of order $\log \log L / \log L$. A better way to write the FSS law is to consider the relation between the finite-volume and infinite-volume correlation lengths at the same ϕ, h, ψ . Again restricting for simplicity to $h=0$, let us insert in (3.11) the expression (2.20) for ϕ as a function of $\xi_\infty \equiv \xi_\infty(\phi, 0, \psi)$. The first argument on the right-hand side of (3.11) can be written (for $L, \xi_\infty \gg 1$) as

$$\begin{aligned} & \phi f_{3/2, 3/4}(\log L; \psi) \\ &= \pm E_\pm \left(\frac{\xi_\infty}{L} \right)^{-3/2} \left(\frac{\log \xi_\infty}{\log L} \right)^{3/4} \\ & \quad \times \left[1 + \frac{3a'}{4a^2} \left(\frac{\log \log L}{\log L} - \frac{\log \log \xi_\infty}{\log \xi_\infty} \right) + \frac{A'}{\log L} + \frac{B'}{\log \xi_\infty} + \dots \right] \end{aligned} \quad (3.14)$$

where $E_{\pm} \equiv \xi_{\infty}(\pm 1, 0, 0)^{3/2}$ is a universal amplitude, the coefficients A' and B' are nonuniversal (they depend on ψ), and the dots denote corrections of order $\log \log L/(\log L)^2$ and $\log \log \xi_{\infty}/(\log \xi_{\infty})^2$. If we denote by $\eta \equiv \eta(\psi)$ the coefficient of the nonuniversal $1/l$ correction in the formula (2.8) for $f_{A, B}$, then the values of A' and B' are given by

$$A' = \frac{3}{4} \eta(\psi) \tag{3.15a}$$

$$B' = -\frac{3}{4} \eta(\psi) - \frac{3}{4} \log \xi_{\infty}(\pm 1, 0, 0) - \frac{1}{a} \frac{\partial}{\partial x} \log \xi_{\infty}(\pm 1, 0, x) \Big|_{x=0} \tag{3.15b}$$

If we now consider the finite-size-scaling limit $\phi \rightarrow 0$, ψ fixed, $L \rightarrow \infty$ with ξ_{∞}/L fixed, we get

$$\phi f_{3/2, 3/4}(\log L; \psi) = \pm E_{\pm} \left(\frac{\xi_{\infty}}{L} \right)^{-3/2} \left[1 + \frac{A' + B' + 3/4 \log(\xi_{\infty}/L)}{\log L} + \dots \right] \tag{3.16}$$

Miraculously, the combination $A' + B'$ appearing here does *not* depend on ψ . Therefore, inserting this into (3.11), we obtain

$$\frac{\xi(\phi, 0, \psi, L^{-1})}{L} = F_{\xi} \left(\frac{\xi_{\infty}(\phi, 0, \psi)}{L} \right) + \hat{F}_{\xi} \left(\frac{\xi_{\infty}(\phi, 0, \psi)}{L} \right) \frac{1}{\log L} + \dots \tag{3.17}$$

where the functions F_{ξ} and \hat{F}_{ξ} are *universal* (they do not contain any piece depending on ψ). It is quite remarkable that not only the leading finite-size-scaling function, but also the leading correction to it, is universal (in amplitude as well as in shape). This is a special feature of the logarithmic corrections to scaling induced by a marginally irrelevant operator, and is not observed in the more common context of power-law corrections to scaling induced by irrelevant operators.

The equation (3.17) can be formally inverted, yielding

$$\frac{\xi_{\infty}(\phi, 0, \psi)}{L} = G_{\xi} \left(\frac{\xi(\phi, 0, \psi, L^{-1})}{L} \right) + \hat{G}_{\xi} \left(\frac{\xi(\phi, 0, \psi, L^{-1})}{L} \right) \frac{1}{\log L} + \dots \tag{3.18}$$

Again both functions G_{ξ} and \hat{G}_{ξ} are *universal*.

3.3. The Free Energy and Its Derivatives

The finite-volume generalization of (2.27) is

$$f_{\text{sing}}(\phi, h, \psi, L^{-1}) = e^{-2l} f_{\text{sing}} \left(\phi f_{3/2, 3/4}(l; \psi), h f_{15/8, 1/16}(l; \psi), \psi(l), \frac{e^l}{L} \right) \quad (3.19)$$

where $\psi(l)$ is given by (2.5). As in (3.7) we choose $l = \log L$, and get

$$\begin{aligned} f_{\text{sing}}(\phi, h, \psi, L^{-1}) \\ = L^{-2} f_{\text{sing}} \left(\phi f_{3/2, 3/4}(\log L; \psi), h f_{15/8, 1/16}(\log L; \psi), -\frac{1}{a \log L} + \dots, 1 \right) \end{aligned} \quad (3.20)$$

The finite-size behavior near criticality of the specific heat, magnetization, and susceptibility can be obtained by performing the appropriate derivatives with respect to ϕ or h . For simplicity let us restrict attention to zero field, where we get⁵

$$\begin{aligned} C_H(\phi, 0, \psi, L^{-1}) = \frac{L}{(-a\psi \log L)^{3/2}} \left[1 + \frac{3a' \log \log L}{2a^2 \log L} + \frac{k_{C_H}}{\log L} + \dots \right] \\ \times \left. \frac{\partial^2 f_{\text{sing}}}{\partial x^2} \left(x, 0, -\frac{1}{a \log L} + \dots, 1 \right) \right|_{x = \phi f_{3/2, 3/4}(\log L; \psi)} \end{aligned} \quad (3.21)$$

⁵ We refrain from writing also

$$\begin{aligned} M(\phi, 0, \psi, L^{-1}) = \frac{L^{-1/8}}{(-a\psi \log L)^{1/16}} \left[1 + \frac{a' \log \log L}{16a^2 \log L} + \frac{k_M}{\log L} + \dots \right] \\ \times \left. \frac{\partial f_{\text{sing}}}{\partial y} \left(\phi f_{3/2, 3/4}(\log L; \psi), y, -\frac{1}{a \log L} + \dots, 1 \right) \right|_{y=0} \end{aligned}$$

because the finite-volume magnetization of course *vanishes* at $h=0$, for all ϕ (by virtue of the Potts symmetry). This scaling is indeed valid, but the prefactor $(\partial f_{\text{sing}}/\partial h)(\phi, h, \psi, 1)$ *vanishes* at $h=0$.

The scaling $L^{-1/8}(\log L)^{-1/16}$ at criticality applies not to the usual magnetization $M \equiv L^{-2} \langle \mathcal{M} \rangle$, but rather to the “absolute magnetization” $\tilde{M} \equiv L^{-2} \langle |\mathcal{M}| \rangle$. These two quantities are essentially identical in the low-temperature phase ($h \downarrow 0$ at fixed $\phi < 0$), but are very different in the critical regime. Unfortunately, much of the literature (especially numerical work) has sloughed over the distinction between M and \tilde{M} .

$$\chi(\phi, 0, \psi, L^{-1}) = \frac{L^{7/4}}{(-a\psi \log L)^{1/8}} \left[1 + \frac{a'}{8a^2} \frac{\log \log L}{\log L} + \frac{k'_\chi}{\log L} + \dots \right] \times \frac{\partial^2 f_{\text{sing}}}{\partial y^2} \left(\phi f_{3/2, 3/4}(\log L; \psi), y, -\frac{1}{a \log L} + \dots, 1 \right) \Big|_{y=0} \tag{3.22}$$

For future convenience, we have denoted by k_c the coefficient of the nonuniversal $1/\log L$ correction term within the square brackets, which arises from the nonuniversal $1/l$ term in (2.8). In addition to the two correction terms within the square brackets, we have (through order $1/\log L$) three other corrections arising from the factors involving f_{sing} : a *universal* $1/\log L$ term arising from the derivative of the relevant scaling function with respect to ψ at $\psi = 0$; and a *universal* $\log \log L/\log L$ term plus a *nonuniversal* $1/\log L$ term, both arising from the fact that the first argument of f_{sing} is not exactly proportional to $\phi L^{3/2}(\log L)^{-3/4}$, but is rather given by (3.12). The simplest case is *at* criticality ($\phi = 0$): then the second and third terms vanish, and the first one gets amalgamated with the nonuniversal terms $k_c/\log L$. We thus get

$$C_H(0, 0, \psi, L^{-1}) \sim \frac{L}{(\log L)^{3/2}} \left[1 + \frac{3a'}{2a^2} \frac{\log \log L}{\log L} + \frac{k'_{c_H}}{\log L} + \dots \right] \tag{3.23}$$

$$\chi(0, 0, \psi, L^{-1}) \sim \frac{L^{7/4}}{(\log L)^{1/8}} \left[1 + \frac{a'}{8a^2} \frac{\log \log L}{\log L} + \frac{k'_\chi}{\log L} + \dots \right] \tag{3.24}$$

where k'_{c_H} and k'_χ are nonuniversal.

In conclusion, all the observables which are computed through derivatives of the free energy have at criticality a multiplicative logarithmic piece, proportional to some power of $\log L$. They also have additive corrections of order $\log \log L/\log L$, the coefficient of which is $-a'/a^2$ times the exponent of the multiplicative logarithm. These corrections arise together from the fact that with each derivative we gain a factor $f_{A, B}(\log L; \psi)$. On the other hand, the $1/\log L$ corrections in (3.23)/(3.24) are nonuniversal because the corresponding terms in $f_{A, B}(\log L; \psi)$ are nonuniversal. Both the multiplicative logarithm and the additive $\log \log L/\log L$ term are absent in the correlation length (3.9). The leading power and multiplicative logarithm in (3.23) were obtained previously in ref. 24. It is noteworthy to remark that in some of the literature it was (wrongly!) assumed that the leading term for the susceptibility had no such logarithmic corrections. ⁽³²⁻³⁴⁾

Off criticality, we get FSS laws

$$C_H(\phi, 0, \psi, L^{-1}) \sim \frac{L}{(\log L)^{3/2}} \left[\bar{F}_{C_H}(\phi L^{3/2}(\psi \log L)^{-3/4}) + O\left(\frac{\log \log L}{\log L}\right) \right] \quad (3.25)$$

$$\chi(\phi, 0, \psi, L^{-1}) \sim \frac{L^{7/4}}{(\log L)^{1/8}} \left[\bar{F}_\chi(\phi L^{3/2}(\psi \log L)^{-3/4}) + O\left(\frac{\log \log L}{\log L}\right) \right] \quad (3.26)$$

The disadvantage of (3.25)/(3.26) is that the corrections to FSS are of order $\log \log L / \log L$. A better way to write the FSS last is to use ξ_∞ / L as the argument of the scaling function. Using the relation (3.16), we get

$$\begin{aligned} C_H(\phi, 0, \psi, L^{-1}) &\sim \frac{L}{(\log L)^{3/2}} \left[1 + \frac{3a'}{2a^2} \frac{\log \log L}{\log L} + \frac{k_{C_H}}{\log L} + \dots \right] \\ &\times \left[F_{C_H}\left(\frac{\xi_\infty(\phi, 0, \psi)}{L}\right) + \hat{F}_{C_H}\left(\frac{\xi_\infty(\phi, 0, \psi)}{L}\right) \frac{1}{\log L} + \dots \right] \end{aligned} \quad (3.27)$$

$$\begin{aligned} \chi(\phi, 0, \psi, L^{-1}) &\sim \frac{L^{7/4}}{(\log L)^{1/8}} \left[1 + \frac{a'}{8a^2} \frac{\log \log L}{\log L} + \frac{k_\chi}{\log L} + \dots \right] \\ &\times \left[F_\chi\left(\frac{\xi_\infty(\phi, 0, \psi)}{L}\right) + \hat{F}_\chi\left(\frac{\xi_\infty(\phi, 0, \psi)}{L}\right) \frac{1}{\log L} + \dots \right] \end{aligned} \quad (3.28)$$

where the scaling functions F_c and \hat{F}_c are *universal* and can be expressed in terms of derivatives of f_{sing} . Thus, the nonuniversal terms $k_c / \log L$ appear only in the prefactor in square brackets. There is of course, also a nonuniversal prefactor multiplying everything.

Finally, we can re-express ξ_∞ / L as a function of $\xi(\phi, L) / L \equiv \xi(\phi, 0, \psi, L^{-1}) / L$, using (3.18), and get

$$\begin{aligned} C_H(\phi, 0, \psi, L^{-1}) &\sim \frac{L}{(\log L)^{3/2}} \left[1 + \frac{3a'}{2a^2} \frac{\log \log L}{\log L} + \frac{k_{C_H}}{\log L} + \dots \right] \\ &\times \left[G_{C_H}\left(\frac{\xi(\phi, L)}{L}\right) + \hat{G}_{C_H}\left(\frac{\xi(\phi, L)}{L}\right) \frac{1}{\log L} + \dots \right] \end{aligned} \quad (3.29)$$

$$\chi(\phi, 0, \psi, L^{-1}) \sim \frac{L^{7/4}}{(\log L)^{1/8}} \left[1 + \frac{a'}{8a^2} \frac{\log \log L}{\log L} + \frac{k_x}{\log L} + \dots \right] \\ \times \left[G_x \left(\frac{\xi(\phi, L)}{L} \right) + \hat{G}_x \left(\frac{\xi(\phi, L)}{L} \right) \frac{1}{\log L} + \dots \right] \quad (3.30)$$

The scaling functions G_c and \hat{G}_c are universal.

If we study the ratio $C_H(\phi, 0, \psi, L^{-1})/C_H(0, 0, \psi, L^{-1})$, we can see easily from (3.29) that the prefactor in square brackets cancels out, and we have

$$\frac{C_H(\phi, 0, \psi, L^{-1})}{C_H(0, 0, \psi, L^{-1})} \approx G_{C_H} \left(\frac{\xi(\phi, L)}{L} \right) + \hat{G}_{C_H}^{(1)} \left(\frac{\xi(\phi, L)}{L} \right) \frac{1}{\log L} + \dots \quad (3.31)$$

where both scaling functions are *universal*. Therefore, both the universal $\log \log L/\log L$ corrections and the nonuniversal $1/\log L$ corrections to the specific heat $C_H(\phi, 0, \psi, L^{-1})$ come from its value *at* criticality. Similar reasoning applies to the susceptibility.

4. DESCRIPTION OF THE SIMULATIONS

4.1. The Monte Carlo Algorithm

The Monte Carlo (MC) algorithm we used in our simulations was actually an algorithm^(33, 34) to simulate the Ashkin-Teller (AT) model.^(35, 36) This model is a generalization of the Ising model to a four-state model, and it includes as a particular case the 4-state Potts model. The general AT model assigns to each lattice site x two Ising spins $\sigma_x = \pm 1$ and $\tau_x = \pm 1$, and they interact through the Hamiltonian

$$H_{AT} = -J \sum_{\langle xy \rangle} \sigma_x \sigma_y - J' \sum_{\langle xy \rangle} \tau_x \tau_y - K \sum_{\langle xy \rangle} \sigma_x \tau_x \sigma_y \tau_y \quad (4.1)$$

where the sums run over nearest-neighbor pairs $\langle xy \rangle$. The line $J = J' = K$ is the 4-state Potts model with $\beta = 4J$:

$$H_{\text{Potts}} = -J \sum_{\langle xy \rangle} (\sigma_x \sigma_y + \tau_x \tau_y + \sigma_x \tau_x \sigma_y \tau_y) \\ = -4J \sum_{\langle xy \rangle} \delta_{\sigma_x, \sigma_y} \delta_{\tau_x, \tau_y} + \text{const} \quad (4.2)$$

The critical point of the square-lattice 4-state Potts model lies at $J = J' = K = \frac{1}{4} \log 3$. The plane $K = 0$ of the general AT model corresponds

to two non-interacting Ising models with nearest-neighbor constants J and J' , respectively.

Wiseman and Domany⁽³²⁾ proposed an algorithm of Swendsen–Wang (SW) type for the general AT model. This algorithm (called the “direct algorithm” in refs. 33 and 34) reduces to the standard SW algorithm⁽³⁷⁾ at the Ising and 4-state Potts subspaces. In refs. 33 and 34 we proposed an embedding variant of their algorithm; it reduces to the standard SW algorithm at the Ising plane, but not at the 4-state Potts line. However, we gave numerical evidence that the two algorithms lie in the same dynamic universality class. In particular, we found that at criticality

$$\frac{\tau_{\text{int}, \mathcal{E}}^{\text{direct}}}{\tau_{\text{int}, \mathcal{E}}^{\text{embedd}}} = 1.516 \pm 0.035 \quad (4.3)$$

where $\tau_{\text{int}, \mathcal{E}}$ denotes the integrated autocorrelation time of the energy (this is roughly the slowest mode in SW-type dynamics). However, because the embedding algorithm requires 1.9 times as much CPU time per iteration as the direct algorithm (since in the AT formulation there are twice as many spin variables as in the Potts formulation), our algorithm is about 25% less efficient than the standard SW algorithm.

Let us review briefly our embedding algorithm (more details can be found in ref. 34). First, consider the Boltzmann weight of a given bond $\langle xy \rangle$, conditional on the $\{\tau\}$ configuration (i.e., the τ spins are kept fixed): it is

$$W_{\text{bond}}(\sigma_x, \sigma_y; \tau_x, \tau_y) = e^{-2J(1 + \tau_x \tau_y)} + [1 - e^{-2J(1 + \tau_x \tau_y)}] \delta_{\sigma_x, \sigma_y} \quad (4.4)$$

We can simulate this system of σ spins using a standard SW algorithm. The effective nearest-neighbor coupling

$$J_{xy}^{\text{eff}} = J(1 + \tau_x \tau_y) \quad (4.5)$$

is no longer translation-invariant, but this does not matter. The key point is that the effective coupling is always *ferromagnetic*. An exactly analogous argument applies to the $\{\tau\}$ spins when the $\{\sigma\}$ spins are held fixed.

The embedding algorithm for the 4-state Potts model has therefore two parts:

Step 1: Update of $\{\sigma\}$ Spins. Given the $\{\tau\}$ configuration (which we hold fixed), we perform a standard SW iteration on the σ spins. The probability p_{xy} arising in the SW algorithm takes the value $p_{xy} = 1 - \exp[-2J(1 + \tau_x \tau_y)]$.

Step 2: Update of $\{\tau\}$ Spins. Given the $\{\sigma\}$ configuration (which we hold fixed), we perform a standard SW iteration on the τ spins. The probability p_{xy} arising in the SW algorithm takes the value $p_{xy} = 1 - \exp[-2J(1 + \sigma_x \sigma_y)]$.

One iteration of the embedding algorithm consists, by definition, of a single application of Step 1 followed by a single application of Step 2.

4.2. Observables to Be Measured

Let us begin by defining some basic observables. The observables of interest involving only the σ spins are

$$\mathcal{M}_\sigma \equiv \sum_x \sigma_x \quad (4.6)$$

$$\mathcal{E}_\sigma \equiv \sum_{\langle xy \rangle} \sigma_x \sigma_y \quad (4.7)$$

$$\mathcal{F}_\sigma \equiv \frac{1}{2} \left[\left| \sum_x \sigma_x e^{2i\pi x_1/L} \right|^2 + \left| \sum_x \sigma_x e^{2i\pi x_2/L} \right|^2 \right] \quad (4.8)$$

where L is the linear size of the system (we always use periodic boundary conditions) and (x_1, x_2) are the Cartesian coordinates of the point x . The observable \mathcal{F}_σ can be also seen as the square of the Fourier transform of σ at the smallest allowed non-zero momenta [i.e., $(\pm 2\pi/L, 0)$ and $(0, \pm 2\pi/L)$ for the square lattice]; it is normalized to be comparable to its zero-momentum analogue \mathcal{M}_σ^2 . We define analogous observables for the τ spins and for the composite operator $\sigma\tau$.

At the 4-state Potts line we have a symmetry under permutations of $(\sigma, \tau, \sigma\tau)$. Thus, the natural choice of observables are those invariant under this symmetry. We have measured the following observables:

$$\mathcal{M}^2 \equiv \frac{1}{3} (\mathcal{M}_\sigma^2 + \mathcal{M}_\tau^2 + \mathcal{M}_{\sigma\tau}^2) \quad (4.9)$$

$$\mathcal{E} \equiv \frac{1}{3} (\mathcal{E}_\sigma + \mathcal{E}_\tau + \mathcal{E}_{\sigma\tau}) \quad (4.10)$$

$$\mathcal{F} \equiv \frac{1}{3} (\mathcal{F}_\sigma + \mathcal{F}_\tau + \mathcal{F}_{\sigma\tau}) \quad (4.11)$$

These observables coincide with the usual ones for the 4-state Potts model up to some multiplicative constants. We then define the magnetic susceptibility

$$\chi = \frac{1}{V} \langle \mathcal{M}^2 \rangle \quad (4.12)$$

the two-point correlation at the smallest nonzero momentum

$$F = \frac{1}{V} \langle \mathcal{F} \rangle \quad (4.13)$$

the second-moment correlation length

$$\xi^{(2)} = \frac{(\chi/F - 1)^{1/2}}{2 \sin \pi/L} \quad (4.14)$$

the energy density (per bond)

$$E = \frac{1}{2V} \langle \mathcal{E} \rangle \quad (4.15)$$

and the specific heat

$$C_H = \frac{1}{2V} (\langle \mathcal{E}^2 \rangle - \langle \mathcal{E} \rangle^2) \quad (4.16)$$

In all these formulae, $V = L^2$ is the number of lattice sites and $2V$ is the number of bonds (we have a square lattice with periodic boundary conditions).

Finally, let us define the quantities associated with the Monte Carlo dynamics. Given an observable \mathcal{O} , we define the corresponding unnormalized autocorrelation function as

$$C_{\mathcal{O}\mathcal{O}}(t) = \langle \mathcal{O}_s \mathcal{O}_{s+t} \rangle - \langle \mathcal{O} \rangle^2 \quad (4.17)$$

where all the expectation values $\langle \cdot \rangle$ are taken in equilibrium, and t is the "time" in units of MC steps. The associated normalized autocorrelation function is

$$\rho_{\mathcal{O}\mathcal{O}} = \frac{C_{\mathcal{O}\mathcal{O}}(t)}{C_{\mathcal{O}\mathcal{O}}(0)} \quad (4.18)$$

The integrated autocorrelation time for the observable \mathcal{O} is defined as

$$\tau_{\text{int}, \mathcal{O}} = \frac{1}{2} \sum_{t=-\infty}^{\infty} \rho_{\mathcal{O}\mathcal{O}}(t) \quad (4.19)$$

The integrated autocorrelation time controls the statistical error in MC estimates of the mean $\langle \mathcal{O} \rangle$. Given a time series of measurements $\{\mathcal{O}_1, \mathcal{O}_2, \dots, \mathcal{O}_n\}$ (in equilibrium), the sample mean

$$\bar{\mathcal{O}} \equiv \frac{1}{n} \sum_{i=1}^n \mathcal{O}_i \quad (4.20)$$

constitutes an unbiased estimator of $\langle \mathcal{O} \rangle$, and its variance (when $n \gg \tau_{\text{int}, \mathcal{O}}$) is

$$\text{var}(\bar{\mathcal{O}}) = \frac{1}{n} 2\tau_{\text{int}, \mathcal{O}} C_{\mathcal{O}\mathcal{O}}(0) \quad (4.21)$$

Thus, the variance of $\bar{\mathcal{O}}$ is $2\tau_{\text{int}, \mathcal{O}}$ larger than it would be if the measurements were uncorrelated. We can numerically obtain reliable estimates of both $\tau_{\text{int}, \mathcal{O}}$ and its error bar (from the autocorrelation function) by using a self-consistent truncation procedure (see Appendix C of ref. 38). We have used a window of width $6\tau_{\text{int}, \mathcal{O}}$, which is sufficient whenever the autocorrelation function decays roughly exponentially. This almost-exponential decay has been confirmed numerically in ref. 34.

To compute the specific-heat error-bar we used the following procedure: first we computed the mean energy $\langle \mathcal{E} \rangle$, and then considered the observable $\mathcal{O} \equiv (\mathcal{E} - \langle \mathcal{E} \rangle)^2$ using the general procedure described in this section.

4.3. Summary of the Simulations

We have simulated the 4-state Potts model on an $L \times L$ square lattice with periodic boundary conditions, using the “embedding” algorithm described in Section 4.1. We performed the simulation at 194 pairs (J, L) . The values of the coupling constant J range from 0.261 to the critical point $J_c = \frac{1}{4} \log 3 \approx 0.274653$. The lattice sizes L range from 16 to 1024 at the critical point, and from 32 to 512 off criticality. In all cases we have started our simulations with a random configuration, and we have discarded the first 10^5 iterations to allow the system to reach equilibrium. This discard interval is more than sufficient: in the worst case ($L = 1024$ at J_c) it is roughly equal to $190\tau_{\text{int}, \mathcal{E}}$ (or $160\tau_{\text{exp}, \mathcal{E}}$ ⁽³⁴⁾) and in all other cases it is at least $300\tau_{\text{int}, \mathcal{E}}$.

The length of the runs ranges from 9×10^5 to 10^7 iterations. For $L = 512$ this run length corresponds to 10^4 times $\tau_{\text{int}, \mathcal{E}}$; for $L = 256$ it is at least $2 \times 10^4\tau_{\text{int}, \mathcal{E}}$; for $L = 128$, at least $3 \times 10^4\tau_{\text{int}, \mathcal{E}}$; and for $L = 64$, at least

Table 1. Monte Carlo Data for the 4-State Potts Model at Criticality^a

L	MCS	χ	C_H	$\zeta^{(2)}$	$\tau_{\text{int}, \sigma}$
16	0.9	141.41 ± 0.29	2.513 ± 0.013	15.758 ± 0.056	12.86 ± 0.24
32	1.9	474.23 ± 0.94	4.170 ± 0.020	31.681 ± 0.100	23.13 ± 0.40
64	9.9	1587.70 ± 1.90	6.971 ± 0.020	63.704 ± 0.115	41.58 ± 0.42
128	6.9	5321.74 ± 10.55	11.730 ± 0.055	128.153 ± 0.368	77.13 ± 1.26
256	4.4	17764.70 ± 60.96	19.936 ± 0.158	256.291 ± 1.243	143.00 ± 3.99
512	2.9	59876.54 ± 334.67	33.969 ± 0.467	519.102 ± 4.078	252.83 ± 11.57
1024	0.8	196872.43 ± 3137.60	60.135 ± 2.091	1020.767 ± 21.680	534.44 ± 67.68

^aFor each lattice size L we show the number of measurements (MCS) in units of 10^5 , the susceptibility χ , the specific heat C_H , the second-moment correlation length $\zeta^{(2)}$, and the integrated autocorrelation time for the energy $\tau_{\text{int}, \sigma}$. The quoted error bars correspond to one standard deviation (i.e., confidence level $\sim 68\%$).

$4 \times 10^4 \tau_{\text{int}, \sigma}$. These run lengths are more than sufficient to get a fairly good determination of the dynamic quantities, and to get high-precision data for the static quantities. Unfortunately, for $L = 1024$ we were able to achieve only $1500 \tau_{\text{int}, \sigma}$, as the autocorrelation time is quite large.⁽³⁴⁾

The data at the critical point were employed already in our previous work^(33, 34) to extract the dynamic critical behavior of our SW-type algorithm. Here we have improved the statistics at $L = 64, 128, 256$; the revised data at criticality are displayed in Table 1. The whole set of data, including the 187 runs off criticality, can be obtained from the authors.

The CPU time required by our program is approximately $10L^2 \mu\text{s}$ /iteration on an IBM RS-6000/370. The total CPU time used in this project was approximately 8.5 years on this machine. The simulations were mainly run on the CAPC cluster at New York University, the IBM SP2 cluster at the Cornell Theory Center, and the DEC Alpha cluster at the Pittsburgh Supercomputing Center.

5. NUMERICAL RESULTS

5.1. Finite-Size Scaling at Criticality

In this subsection we are going to test the FSS predictions (3.9)/(3.23)/(3.24) for the 4-state Potts model *at criticality*. In refs. 33 and 34 we presented some preliminary results. However, we have now made significant extensions of these runs, in some cases doubling the statistics. More importantly, we now have a better *theoretical* knowledge of the FSS behavior of this model, which includes both multiplicative and additive logarithmic corrections.

For each quantity ϑ , we shall carry out fits to several different Ansätze using the standard weighted least-squares method. As a precaution against corrections to scaling, we impose a lower cutoff $L \geq L_{\min}$ on the data points admitted in the fit, and we study systematically the effects of varying L_{\min} on both the estimated parameters and the χ^2 . In general, our preferred fit corresponds to the smallest L_{\min} for which the goodness of fit is reasonable (e.g., the confidence level⁶ is ≥ 10 –20 %) and for which subsequent increases in L_{\min} do not cause the χ^2 to drop vastly more than one unit per degree of freedom.

5.1.1. Second-Moment Correlation Length. The quantity $\xi^{(2)}/L$ is expected to approach a constant x^* as $L \rightarrow \infty$, with additive $O(1/\log L)$ corrections (3.9). The constant x^* can be in principle computed via conformal field theory, but to our knowledge this calculation has not yet been done.

A fit of this ratio to a constant is reasonably good only for $L_{\min} = 128$:

$$\frac{\xi^{(2)}}{L} = x^* = 1.0022 \pm 0.0023 \quad (5.1)$$

with $\chi^2 = 2.38$ (3 DF, level = 50 %). However, if we take into account the $1/\log L$ corrections we get a good fit already for $L_{\min} = 16$:

$$\frac{\xi^{(2)}}{L} = (1.0221 \pm 0.0061) - \frac{0.1077 \pm 0.0239}{\log L} \quad (5.2)$$

with $\chi^2 = 2.32$ (5 DF, level = 80 %). On the other hand, an equally good fit can be obtained using a power-law correction $L^{-\Delta}$ with $0 < \Delta \lesssim 0.5$; this is to be expected, as a logarithm can be well mimicked by a small power. We can conclude conservatively that

$$x^* = 1.02 \pm 0.03 \quad (5.3)$$

5.1.2. Susceptibility. The expected behavior of the critical susceptibility at finite L is given by (3.24). Thus, in addition to the standard $L^{\gamma/\nu}$ term with $\gamma/\nu = 7/4$, we have a multiplicative logarithmic correction $(\log L)^{-1/8}$, and also additive logarithmic corrections of orders $\log \log L/\log L$ and $1/\log L$. All these features make the accurate numerical estimation of the exponent γ/ν quite difficult.

⁶“Confidence level” is the probability that χ^2 would exceed the observed value, assuming that the underlying statistical model is correct. An unusually low confidence level (e.g., less than 5%) thus suggests that the underlying statistical model is *incorrect*—the most likely cause of which would be corrections to scaling.

If we fit the susceptibility to the naive power law AL^p , we get a reasonably good fit for $L_{\min} = 16$:

$$\frac{\chi}{\nu} = 1.744 \pm 0.001 \quad (5.4)$$

with $\chi^2 = 2.21$ (5 DF, level = 82%). The difference from the exact result 1.75 is not large, but it is six standard deviations and thus strongly statistically significant. The fact that the estimate (5.4) estimate is *smaller* than the exact value is consistent with the existence of a multiplicative logarithmic correction raised to a *negative* power. However, without the theoretical knowledge of a multiplicative logarithmic correction, we could equally well conclude that this small discrepancy is due to additive corrections to scaling.⁽³⁴⁾

If we try to fit the quantity $\chi/L^{7/4}$ to an arbitrary power of $\log L$ [i.e., $\chi/L^{7/4} = A(\log L)^p$] we obtain a reasonable fit already for $L_{\min} = 16$:

$$p = -0.0236 \pm 0.0040 \quad (5.5)$$

with $\chi^2 = 3.64$ (5 DF, level = 60%). This result differs drastically from the theoretical prediction $p = -1/8 = -0.125$. Alternatively, we can try to fit $\chi/L^{7/4}$ to a power-law $AL^{\nu/p}$; the result for $L_{\min} = 128$ is

$$\frac{\chi}{\nu} = 1.765 \pm 0.003 \quad (5.6)$$

with $\chi^2 = 1.83$ (2 DF, level = 40%). Once again this differs by five standard deviations from the exact value 1.75.

Looking at the FSS prediction (3.24), it is plausible to think that the reason why (5.5)/(5.6) differ so radically from the leading-order theoretical prediction $L^{7/4}(\log L)^{-1/8}$ are the large corrections to scaling. To test this idea, we have fitted $\chi/[L^{7/4}(\log L)^{-1/8}]$ to $A + B \log \log L / \log L$. The fit is reasonable for $L_{\min} = 64$:

$$\frac{\chi}{L^{7/4}(\log L)^{-1/8}} = (1.673 \pm 0.033) - (1.056 \pm 0.098) \frac{\log \log L}{\log L} \quad (5.7)$$

with $\chi^2 = 2.76$ (3 DF, level = 43%). However, the ratio $B/A \approx -0.63$ is quite different from the expected value $a'/(8a^2) = -1/16 = -0.0625$.

Furthermore, if we try fitting $\chi/[L^{7/4}(\log L)^{-1/8}]$ to $A + B/\log L$, we obtain an equally good (even slightly better) fit: with the same $L_{\min} = 64$, we get

$$\frac{\chi}{L^{7/4}(\log L)^{-1/8}} = (1.454 \pm 0.013) - \frac{0.600 \pm 0.055}{\log L} \quad (5.8)$$

with $\chi^2 = 1.94$ (3 DF, level = 59%). Clearly, at these modest values of L , it is virtually impossible to disentangle numerically the $\log \log L / \log L$ and $1 / \log L$ contributions, both of which are predicted theoretically to be present. Indeed, the small value ($-1/16$) of the universal $\log \log L / \log L$ coefficient makes it undetectable in the presence of the much larger (~ -0.4) nonuniversal $1 / \log L$ coefficient. To distinguish these two contributions, we would need to reach at least $\log \log L \approx 5$, i.e. $L \approx 10^{64}$! Note, finally, the large discrepancy between the estimates (5.7) and (5.8) of the leading amplitude A : it is virtually impossible to estimate the correct limiting value in the presence of such strong corrections.

5.1.3. Specific Heat. The FSS behavior of the specific heat at criticality is given by (3.23); it is of the same $L^p(\log L)^{-q}$ form as the susceptibility, but with a much larger logarithmic exponent q . This makes it extremely difficult to estimate accurately the leading exponent $\alpha/\nu = 1$, as was found already in ref. 34.

A naive power-law fit to $AL^{\alpha/\nu}$ gives a reasonably good result for $L_{\min} = 128$:

$$\frac{\alpha}{\nu} = 0.770 \pm 0.008 \quad (5.9)$$

with $\chi^2 = 1.15$ (2 DF, level = 57%). This estimate is far below the exact value; this deviation is roughly consistent with the predicted multiplicative logarithmic correction in both sign and magnitude: a behavior $(\log L)^{-3/2}$ can be well mimicked over the interval $128 \leq L \leq 1024$ by a power $L^{-0.23}$.

We can try to estimate the power of the logarithmic term by fitting C_H/L to $A \log^p L$. The result is good for $L_{\min} = 128$:

$$p = -1.258 \pm 0.044 \quad (5.10)$$

with $\chi^2 = 0.66$ (2 DF, level = 72%). We obtain a much better result than for the susceptibility, but (5.10) is still six standard deviations away from the predicted value -1.5 . We can also try to compute α/ν by fitting $C_H \log^{3/2} L$ to the power-law $AL^{\alpha/\nu}$. The result for $L_{\min} = 128$ is

$$\frac{\alpha}{\nu} = 1.044 \pm 0.008 \quad (5.11)$$

with $\chi^2 = 0.97$ (2 DF, level = 62%). This is still five standard deviations away from the exact value $\alpha/\nu = 1$.

Finally, we have fitted the function $C_H/[L(\log L)^{-3/2}]$ to the Ansatz $A + B \log \log L/\log L$. The fit is good for $L_{\min} = 128$:

$$\frac{C_H}{L(\log L)^{-3/2}} = (1.607 \pm 0.113) - (1.926 \pm 0.354) \frac{\log \log L}{\log L} \quad (5.12)$$

with $\chi^2 = 0.72$ (2 DF, level = 70%). Again the ratio $B/A \approx -1.2$ is rather different from the expected universal value $3a'/(2a^2) = -3/4 = -0.75$ from (3.23).

If, instead, we try to fit $C_H/[L(\log L)^{-3/2}]$ to the Ansatz $A + B/\log L$, the fit is reasonable already for $L_{\min} = 64$:

$$\frac{C_H}{L(\log L)^{-3/2}} = (1.291 \pm 0.022) - \frac{1.526 \pm 0.096}{\log L} \quad (5.13)$$

with $\chi^2 = 1.22$ (3 DF, level = 75%). Again, we are unable to disentangle the two types of corrections.

5.1.4. The Combination $\chi/C_H^{1/12}$. From (3.23)/(3.24) we see that the combination $\chi/C_H^{1/12}$ does not show any multiplicative logarithmic correction, nor any additive correction of order $\log \log L/\log L$. Rather,

$$\frac{\chi}{C_H^{1/12}}(0, 0, \psi, L^{-1}) \sim L^{5/3} \left[1 + O\left(\frac{1}{\log L}\right) \right] \quad (5.14)$$

It is therefore of some interest to see whether the fits for this particular combination are at all “cleaner” than those for χ and C_H separately. To compute the error bars on $\chi/C_H^{1/12}$, we took into account the cross-correlations between the specific heat and the susceptibility. We can thus trust χ^2 value in these the fits.

To test the prediction (5.14), we first tried a power-law Ansatz AL^p . The fit is already good for $L_{\min} = 16$:

$$p = 1.682 \pm 0.001 \quad (5.15)$$

with $\chi^2 = 3.60$ (5 DF, level = 61%). This exponent is 15 standard deviations away from the expected value $5/3 = 1.666667$. This discrepancy might be due to a rather strong correction to scaling.

If we assume that the corrections to scaling are of order $1/\log L$, the fit is reasonable for $L_{\min} = 64$:

$$\frac{\chi C_H^{-1/12}}{L^{5/3}} = (1.422 \pm 0.013) - \frac{0.429 \pm 0.057}{\log L} \quad (5.16)$$

with $\chi^2 = 2.23$ (3 DF, level = 53%). However, a correction of order $\log \log L / \log L$ gives an even better fit: already with $L_{\min} = 32$ we have

$$\frac{\chi C_H^{-1/12}}{L^{5/3}} = (1.588 \pm 0.026) - (0.785 \pm 0.078) \frac{\log \log L}{\log L} \quad (5.17)$$

with $\chi^2 = 2.37$ (4 DF, level = 67%). Again, we find it impossible to distinguish clearly between these two corrections to scaling, even when we know on theoretical grounds that only $1/\log L$ corrections are present.

5.2. Finite-Size Scaling off Criticality

In this section we are going to test the FSS predictions for the 4-state Potts model off criticality. In particular, from (3.11) we see that

$$\frac{\xi(\phi, 0, \psi, L^{-1})}{L} = \xi(\phi f_{3/2, 3/4}(\log L; \psi), 0, 0, 1) + O\left(\frac{1}{\log L}\right) \quad (5.18)$$

The first argument on the right-hand side is equal (for large L) to

$$\phi f_{3/2, 3/4}(\log L; \psi) = \frac{\phi L^{3/2}}{(-a\psi \log L)^{3/4}} \left[1 + \frac{a' \log \log L}{a^2 \log L} + O\left(\frac{1}{\log L}\right) \right] \quad (5.19)$$

This means that if we plot $\xi^{(2)}/L$ as a function of $\phi L^{3/2} \log^{-3/4} L$, the points will collapse onto a single curve. Of course, the expected deviations of order $\log \log L / \log L$ may make this collapse less than perfect.⁷

Analogously, from (3.21)–(3.22) we obtain similar predictions for the specific heat and the susceptibility:

$$\frac{C_H(\phi, 0, \psi, L^{-1})}{L(\log L)^{-3/2}} = \tilde{F}_{C_H} \left(\frac{\phi L^{3/2}}{(\log L)^{3/4}}, 0, 0, 1 \right) + O\left(\frac{\log \log L}{\log L}\right) \quad (5.20)$$

$$\frac{\chi(\phi, 0, \psi, L^{-1})}{L^{7/4}(\log L)^{-1/8}} = \tilde{F}_\chi \left(\frac{\phi L^{3/2}}{(\log L)^{3/4}}, 0, 0, 1 \right) + O\left(\frac{\log \log L}{\log L}\right) \quad (5.21)$$

where \tilde{F}_{C_H} and \tilde{F}_χ are certain derivatives of the free energy f_{sing} . Again, plotting the l.h.s. of (5.20) or (5.21) versus $\phi L^{3/2}(\log L)^{-3/4}$ will collapse the corresponding data onto a single curve, modulo corrections $O(\log \log L / \log L)$.

⁷ One could also plot $\xi^{(2)}/L$ as a function of $\phi L^{3/2}(\log L)^{-3/4} [1 + (a'/a^2) \log \log L / \log L]$, and get only $1/\log L$ corrections. However, we have seen in the preceding subsection that it is very hard to disentangle these two effects at criticality. Thus, we expect no gain in introducing explicitly the $\log \log L / \log L$ correction.

The effect of the marginal scaling field ψ on the FSS equations is thus threefold: 1) The specific heat and the susceptibility have a multiplicative logarithmic correction. 2) The scaled-temperature variable appearing on the r.h.s. of the FSS equations is not merely $L^{1/\nu}(J - J_c)$, but has a multiplicative logarithmic correction $(\log L)^{-3/4}$ [the same for all observables]. 3) The corrections to finite-size scaling are not $O(L^{-\omega})$, but rather $O(\log \log L / \log L)$, which makes the numerical analysis much harder.

The naive approach to off-criticality FSS—neglecting all multiplicative logarithms—would be to plot $\xi^{(2)}/L$, C_H/L , and $\chi/L^{7/4}$ versus $L^{3/2}(J - J_c)$. These plots are displayed in Fig. 1. The results are quite poor: there is no

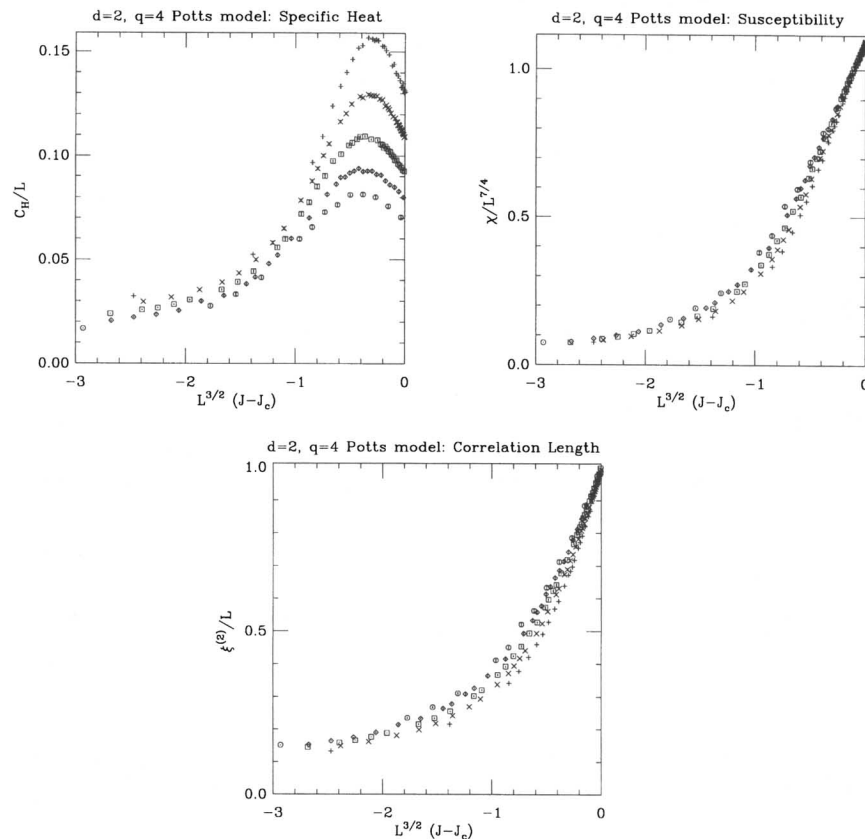


Fig. 1. Naive finite-size scaling plots, neglecting all multiplicative logarithms, for the specific heat C_H , the susceptibility χ , and the second-moment correlation length $\xi^{(2)}$. Note that the abscissa $L^{3/2}(J - J_c)$, where $J_c = \frac{1}{4} \log 3 = 0.274653\dots$, also lacks the predicted multiplicative logarithms. Symbols denote the different lattice sizes: $L = 32$ (+), $L = 64$ (\times), $L = 128$ (\square), $L = 256$ (\diamond), and $L = 512$ (\circ).

data-collapse for the specific heat; and for the susceptibility and the correlation length the data collapse only close to J_c .

A slightly less naive approach is to incorporate the predicted multiplicative logarithms for the specific heat and the susceptibility, while still ignoring the multiplicative logarithmic corrections to the abscissa $L^{3/2}(J - J_c)$. But if we do this, we get even worse plots (see Fig. 2), with the exception of the specific heat near J_c (where the rescaling of the abscissa makes no difference anyway, and the multiplicative logarithm in C_H helps a lot). The slight deterioration in the susceptibility plot near J_c is a reflection of our inability (5.5) to verify the correct power of $\log L$.

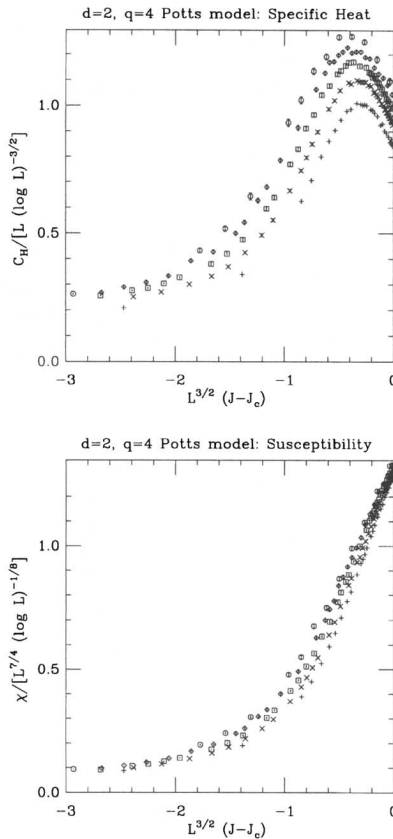


Fig. 2. Finite-size scaling plots that include the predicted multiplicative logarithms $C_H \sim L(\log L)^{-3/2}$ and $\chi \sim L^{7/4}(\log L)^{-1/8}$ but do not include any multiplicative logarithms in the abscissa $L^{3/2}(J - J_c)$. Symbols denote the different lattice sizes: $L = 32$ (+), $L = 64$ (x), $L = 128$ (□), $L = 256$ (◇), and $L = 512$ (○). Note that the fits are worse than in Fig. 1.

However, when we try to verify the correct FSS equations (5.18)–(5.21), the result is very different (see Fig. 3). The data for the specific heat exhibit a good collapse away from J_c . Close to the critical point we see large deviations, presumably due to the $\log \log L/\log L$ and $1/\log L$ corrections. For the susceptibility, we get a good (though not perfect) data-collapse along the entire curve; the data-collapse is even better for the correlation length. We conclude that the data are in reasonable agreement with the predicted multiplicative logarithms, if we make allowance for the additive logarithmic corrections to scaling.

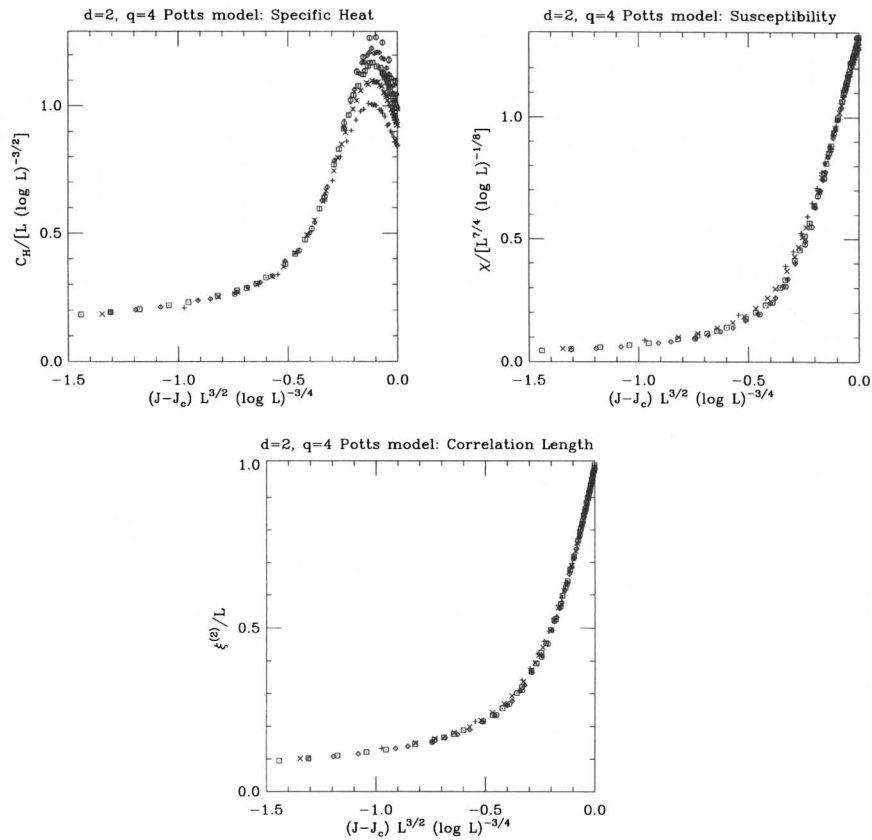


Fig. 3. Finite-size scaling plots for the specific heat C_H , the susceptibility χ , and the second-moment correlation length $\xi^{(2)}$ that take into account *all* predicted multiplicative logarithms. Note that the correct abscissa variable is $(J - J_c) L^{3/2} (\log L)^{-3/4}$. Symbols denote the different lattice sizes: $L = 32$ (+), $L = 64$ (\times), $L = 128$ (\square), $L = 256$ (\diamond), and $L = 512$ (\circ).

Remark. In most situations, FSS plots of this type are difficult to obtain because of the uncertainties in the determination of J_c : a small error on J_c ruins the data-collapse. Fortunately, in our case we *do* know the exact value of J_c . This fact allows us to test the FSS predictions very accurately.

Another way to present FSS data is to avoid using the “bare” variable $J - J_c$, and to use instead the physical observable $\xi^{(2)}(L)/L$. From (3.29)–(3.30) we conclude that plotting $C_H/[L(\log L)^{-3/2}]$ or $\chi/[L^{7/4}(\log L)^{-1/8}]$ versus $\xi^{(2)}/L$ will provide a single curve for each observable, modulo corrections of order $\log \log L/\log L$. In Fig. 4 we display the FSS plots of

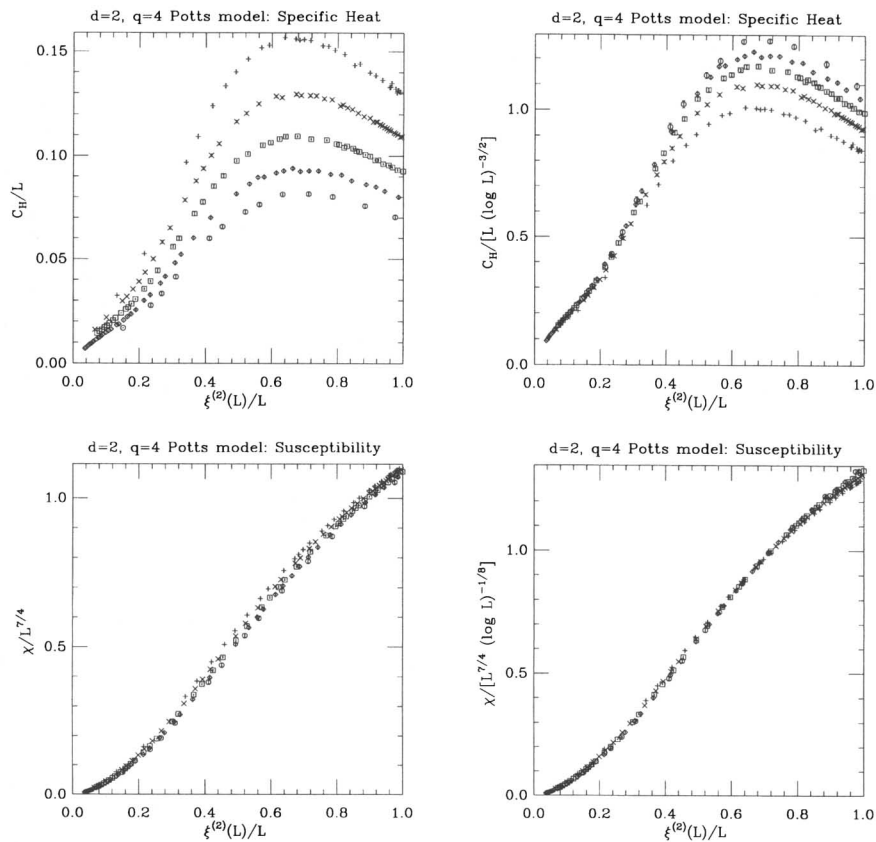


Fig. 4. Finite-size scaling plots for the specific heat C_H and the susceptibility χ as functions of $\xi^{(2)}(L)/L$. For each observable, the plot in the left column includes only the leading power law, while the plot in the right column takes into account the predicted multiplicative logarithmic correction. The improvement is clear. Symbols denote the different lattice sizes: $L = 32$ (+), $L = 64$ (\times), $L = 128$ (\square), $L = 256$ (\diamond), and $L = 512$ (\circ).

these two observables, when we neglect the multiplicative logarithmic corrections (left column) and with the full leading terms (right column). Including the multiplicative logarithmic corrections makes a big improvement, especially for the specific heat. Again we see large corrections to scaling near the critical point (namely, at $\xi^{(2)}/L \approx x^* \approx 1.02$), in agreement with the behavior found in Section 5.1.

The main drawback of this type of plot is that data with small $\xi^{(2)}/L$ are artificially compressed. One way to overcome this difficulty is to replace L by $\xi^{(2)}$ in the y -axis. That is, we can plot $C_H/[\xi^{(2)}(\log \xi^{(2)})^{-3/2}]$ and $\chi/[\xi^{(2)7/4}(\log \xi^{(2)})^{-1/8}]$ versus $\xi^{(2)}/L$ (see Fig. 5). We emphasize that these

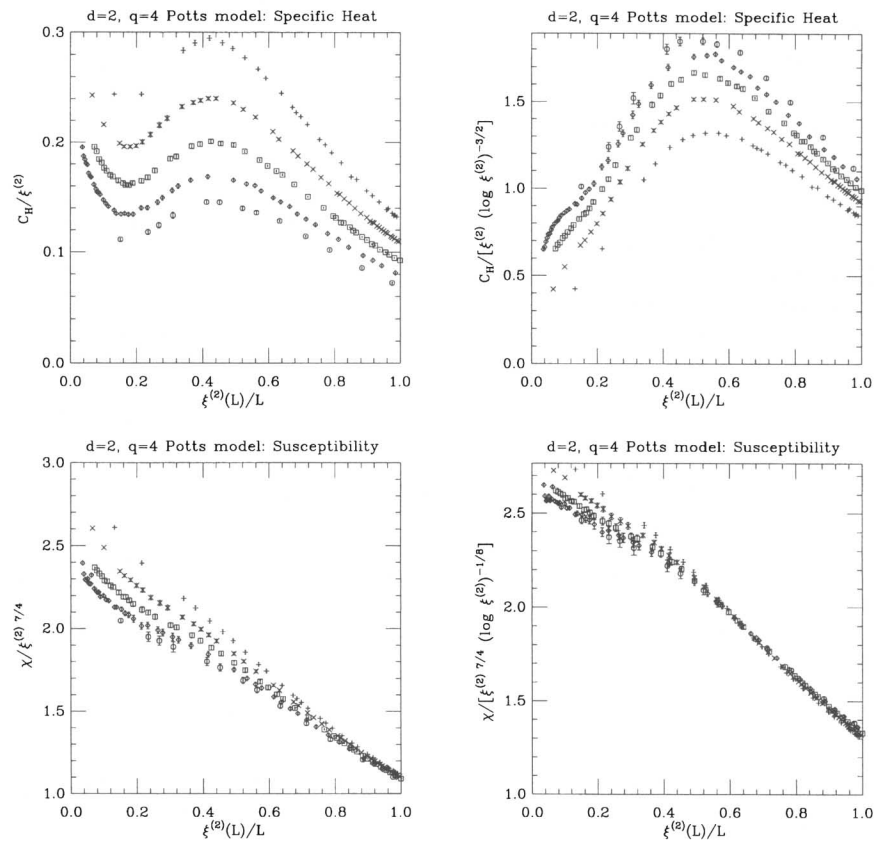


Fig. 5. Finite-size scaling plots for the specific heat C_H and the susceptibility χ as functions of $\xi^{(2)}(L)/L$. These are the same plots as in Fig. 4, with the lattice size L replaced by the second-moment correlation length $\xi^{(2)}(L)$ on the y -axis. Symbols denote the different lattice sizes: $L = 32$ (+), $L = 64$ (x), $L = 128$ (□), $L = 256$ (◇), and $L = 512$ (○).

plots are identical to those in Fig. 4, except that the scale of the y -axis is changed in a way depending on $x \equiv \xi^{(2)}/L$. We see that the data-collapse at small $\xi^{(2)}/L$ is not in fact as good as it had appeared in Fig. 4: in reality, it is mediocre for the susceptibility and quite poor for the specific heat. Nevertheless, there is a clear improvement in both cases when we include the predicted multiplicative logarithmic correction.

5.3. Extrapolation Techniques

We have also considered how well the extrapolation scheme introduced in ref. 19 works in the presence of logarithmic corrections. This method makes use of the following FSS equation for an arbitrary long-distance observable \mathcal{O} :

$$\frac{\mathcal{O}(J, 2L)}{\mathcal{O}(J, L)} = F_c \left(\frac{\xi(J, L)}{L} \right) + O(\xi^{-\omega}, L^{-\omega}) \quad (5.22)$$

where F_c is an unknown scaling function and ω is a correction-to-scaling exponent. (Here we have chosen a size-scaling factor $s = 2$; a similar equation holds, of course, for any s .)

Let us first check the analogous equations for our case. To simplify the notation, we will write only two arguments for the observables: $\mathcal{O}(J, L) \equiv \mathcal{O}(\phi, h = 0, \psi, L^{-1})$. From (3.17) we conclude that

$$\frac{\xi(J, 2L)}{\xi(J, L)} = \tilde{A}_\xi \left(\frac{\xi_\infty(J)}{L} \right) + \tilde{B}_\xi \left(\frac{\xi_\infty(J)}{L} \right) \frac{1}{\log L} + \dots \quad (5.23)$$

where \tilde{A}_ξ and \tilde{B}_ξ are universal (albeit unknown) scaling functions. Using the relation (3.18) we arrive at

$$\frac{\xi(J, 2L)}{\xi(J, L)} = A_\xi \left(\frac{\xi(J, L)}{L} \right) + B_\xi \left(\frac{\xi(J, L)}{L} \right) \frac{1}{\log L} + \dots \quad (5.24)$$

where A_ξ and B_ξ are again universal. Thus, we get the same equation as (5.22), but the corrections to scaling are much larger ($\sim 1/\log L$).

The same type of equation can be derived for the specific heat and the susceptibility, using (3.29)–(3.30): although there are corrections of order $\log \log L/\log L$, these cancel out in forming the ratio between lattice sizes L and $2L$. Notice that the nonuniversal $k_c/\log L$ contribution also cancels

out in the ratio $\mathcal{O}(J, 2L)/\mathcal{O}(J, L)$. This means that the leading correction to scaling is universal. That is, we have

$$\frac{\mathcal{O}(J, 2L)}{\mathcal{O}(J, L)} = A_c \left(\frac{\xi(J, L)}{L} \right) + B_c \left(\frac{\xi(J, L)}{L} \right) \frac{1}{\log L} + \dots \quad (5.25)$$

where both scaling functions A_c and B_c are *universal*.

The $1/\log L$ corrections in (5.25) make a numerical determination of the finite-size-scaling functions A_c very difficult. Unfortunately, these functions are the basic objects needed to extrapolate from finite L to the infinite-volume limit.⁽¹⁹⁾ Thus, a naive application of the method of ref. 19

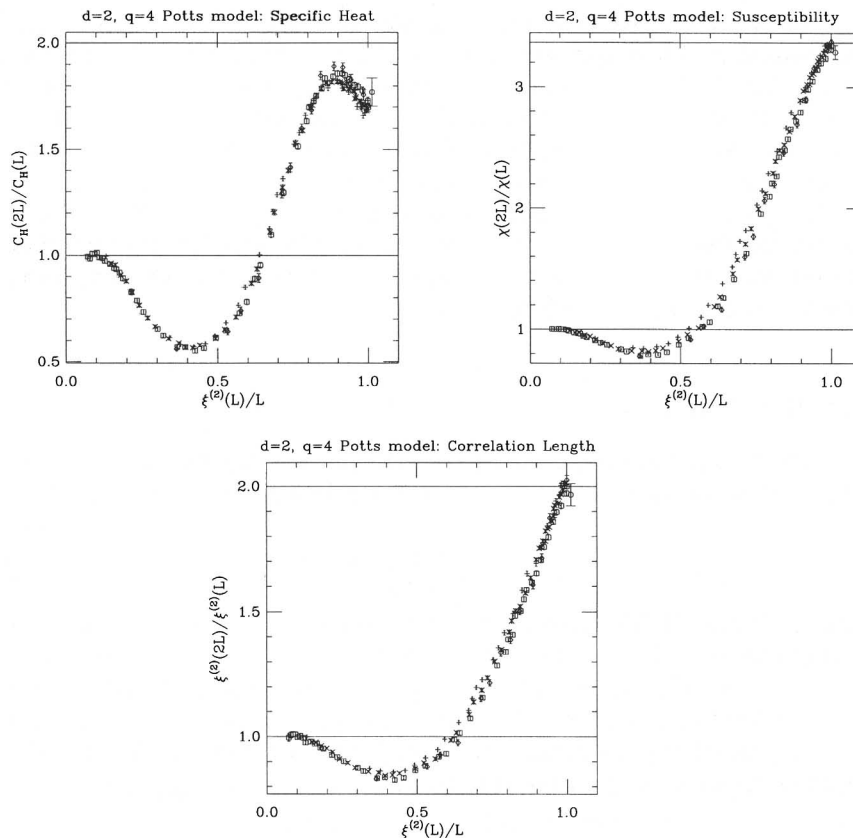


Fig. 6. “ $L/2L$ ” finite-size scaling plots, of the kind employed in ref. 19, for the specific heat C_H , the susceptibility χ and the second-moment correlation length $\xi^{(2)}$. For each observable \mathcal{O} , we plot the quantity $\mathcal{O}(2L)/\mathcal{O}(L)$ versus $\xi^{(2)}/L$. Symbols denote the different lattice sizes: $L = 32$ (+), $L = 64$ (x), $L = 128$ (□), $L = 256$ (◇), and $L = 512$ (○).

is not expected to work well. Figure 6 shows the plots of $\mathcal{O}(J, 2L)/\mathcal{O}(J, L)$ versus $\xi^{(2)}/L$ for the specific heat, the susceptibility and the second-moment correlation length. The data collapse is notably inferior to that observed in most other models.⁽¹⁹⁾ Note also that the specific-heat curve is *very far* from its correct value $2^{\alpha/\nu} = 2$ at the critical point $\xi^{(2)}/L = x^* \approx 1.02$; rather, it takes the value $2^{(\alpha/\nu)_{\text{eff}}} = 2^{\approx 0.770} \approx 1.71$. This is another indication of the very strong corrections to scaling.

6. DYNAMIC CRITICAL BEHAVIOR OF THE SWENDSEN–WANG-TYPE ALGORITHM

In this section we shall analyze briefly the dynamic critical behavior of our Swendsen–Wang-type algorithm for the two-dimensional 4-state Potts model. Recall that we have used the “embedding” variant of the SW-type algorithm for the Ashkin–Teller model.^(33, 34) This algorithm does *not* coincide with the standard Swendsen–Wang⁽³⁷⁾ algorithm for the 4-state Potts model, but it is expected heuristically (and confirmed numerically⁽³⁴⁾ at criticality) to lie in the same dynamic universality class. We therefore expect the dynamic critical exponents to be identical for the two algorithms; and we also expect the dynamic finite-size-scaling functions to be identical modulo a multiplicative factor.

6.1. Dynamic Finite-size Scaling at Criticality

We first fit the integrated autocorrelation time for the energy, $\tau_{\text{int}, \mathcal{E}}$, to a pure power law $\tau_{\text{int}, \mathcal{E}} = AL^{z_{\text{int}, \mathcal{E}}}$. We obtain a good fit for $L_{\text{min}} = 32$:

$$z_{\text{int}, \mathcal{E}} = 0.876 \pm 0.011 \quad (6.1)$$

with $\chi^2 = 2.54$ (4 DF, level = 64%). However, this *cannot* be the true asymptotic behavior, because the Li–Sokal bound^(34, 39) guarantees that $\tau_{\text{int}, \mathcal{E}} \geq \text{const} \times C_H$, and we know from (3.23) that the specific heat diverges at criticality like $L(\log L)^{-3/2}$.⁸ Rather, this *apparent* exponent $z_{\text{int}, \mathcal{E}} < 1$ is probably an effect of multiplicative logarithmic corrections (with a negative exponent), just as it is for the specific heat.

⁸ The Li–Sokal bound has been proven for the original Swendsen–Wang algorithm⁽³⁹⁾ and more generally for the *direct* form of the Ashkin–Teller SW algorithm.⁽³⁴⁾ But the embedding form of the AT algorithm is believed (and observed numerically⁽³⁴⁾) to be in the same dynamic universality class as the direct algorithm. So the bound should apply for it as well.

In refs. 34 and 40 we showed that there are only two likely behaviors for the autocorrelation time of the Swendsen–Wang algorithm for the 2D Potts models:

$$\tau_{\text{int}, \mathcal{E}} = \begin{cases} AL^p & \text{with } p \text{ small} \\ A + B \log L & \end{cases} \quad (6.2)$$

With the available statistics it is very hard to distinguish between these two scenarios. If we fit the quantity $\tau_{\text{int}, \mathcal{E}}/[L(\log L)^{-3/2}]$ to a pure power law AL^p , we obtain a reasonable fit for $L_{\min} = 128$:

$$p = 0.153 \pm 0.028 \quad (6.3)$$

with $\chi^2 = 1.30$ (2 DF, level = 52%). On the other hand, if we fit the same quantity to the logarithmic Ansatz $A + B \log L$, the fit is very good already for $L_{\min} = 16$:

$$\frac{\tau_{\text{int}, \mathcal{E}}}{L(\log L)^{-3/2}} = (0.197 \pm 0.173) + (1.278 \pm 0.044) \log L \quad (6.4)$$

with $\chi^2 = 1.53$ (5 DF, level = 77%). Thus, our MC data supports slightly better the logarithmic scenario compared to the power-law scenario.

One can also study directly the ratio $\tau_{\text{int}, \mathcal{E}}/C_H$, and fit the results to the Ansätze (6.2). Unfortunately, we do not know the correct error bar on this ratio, as we do not know the covariance between the estimator of the specific heat and the estimator of $\tau_{\text{int}, \mathcal{E}}$. Instead, we shall use the *upper bound* on the error bar provided by the triangle inequality. Our error bars are thus overestimated—by how much we do not know—and, consequently, the χ^2 values of the fits are expected to be artificially small. We can, however, compare the *relative* χ^2 values for the two Ansätze. (See ref. 34 for a complete discussion concerning these points.) If we try to fit $\tau_{\text{int}, \mathcal{E}}/C_H$ to a pure power law AL^p , we get a good result for $L_{\min} = 16$:

$$p = 0.119 \pm 0.011 \quad (6.5)$$

with $\chi^2 = 1.06$ (5 DF, level = 96%). With the logarithmic Ansatz $A + B \log L$, the fit is less good: for the same L_{\min} we obtain $\chi^2 = 1.99$ (5 DF, level = 85%). Thus, for $L_{\min} = 16$ the power-law fit gives a χ^2 a factor of two better than the logarithmic fit. However, for $L_{\min} = 32$, the two fits give more nearly equal values of χ^2 : 0.98 and 1.27, respectively.

6.2. Dynamic Finite-Size Scaling off Criticality

The FSS behavior of the dynamic observables off criticality is expected to be similar to that discussed previously for the static observables. That is,

we expect multiplicative logarithmic corrections, as well as additive logarithmic corrections to scaling. In this section we have considered the two scenarios discussed in the previous subsection, with the aim of distinguishing between them.

First, we have made the FSS plots analogous to those of Figs. 1 and 2. That is, we have plotted the leading behavior— $\tau_{\text{int},\sigma}/L^{z_{\text{int},\sigma}}$ or $\tau_{\text{int},\sigma}/[L(\log L)^{-3/2}(1+6.501\log L)]$ —versus $L^{3/2}(J-J_c)$ (left column in Fig. 7). In both cases, we obtain terrible fits. However, the situation improves dramatically when we consider the correct abscissa $L^{3/2}(\log L)^{-3/4}(J-J_c)$

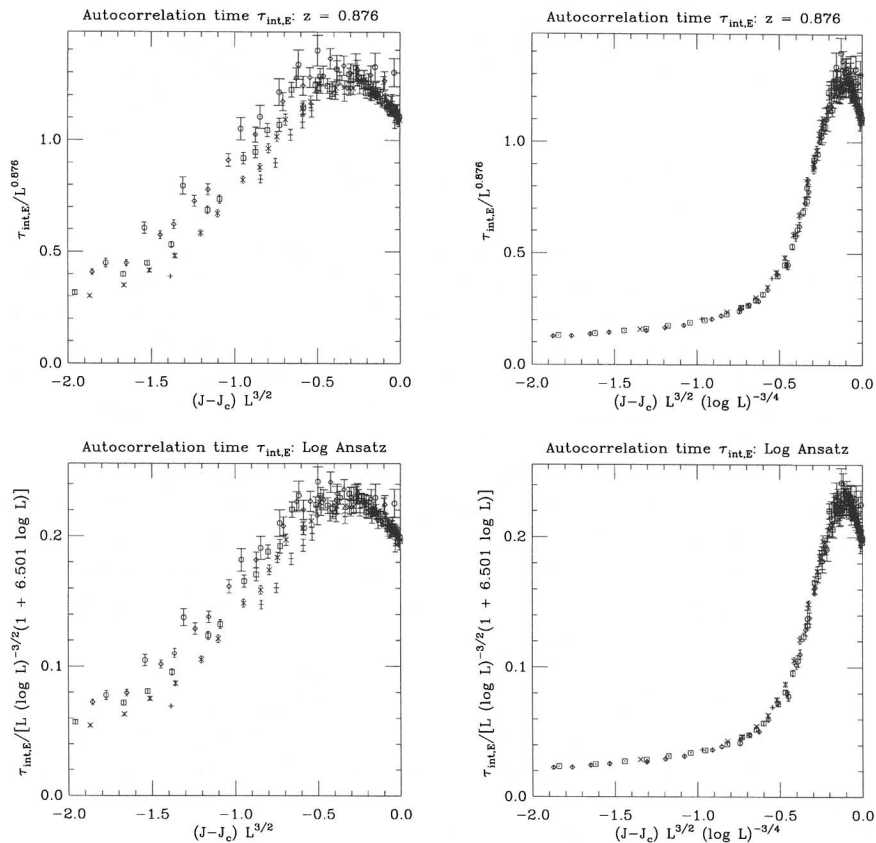


Fig. 7. Finite-size scaling plots for the integrated autocorrelation time $\tau_{\text{int},\sigma}$ as a function of $L^{3/2}(J-J_c)$ (left column) and $(J-J_c)L^{3/2}(\log L)^{-3/4}$ (right column). We show the two most likely scenarios: $\tau_{\text{int},\sigma} \sim L^{z_{\text{int},\sigma}}$ with $z_{\text{int},\sigma} = 0.876 \pm 0.011$ (upper row), and $\tau_{\text{int},\sigma} \sim L(\log L)^{-3/2}(1+6.501\log L)$ (lower row). Symbols denote the different lattice sizes: $L = 32$ (+), $L = 64$ (x), $L = 128$ (□), $L = 256$ (◇), and $L = 512$ (○).

(right column in Fig. 7). Unfortunately, from these plots corresponding to the two most likely scenarios, it is impossible to tell which one is more likely.

Alternatively, we can plot the same quantities as functions of the physical observable $\xi^{(2)}(L)/L$ (left column in Fig. 8). Again, the plots are very similar, and there is no objective reason to prefer one over the other. The corrections to scaling for small $\xi^{(2)}/L$ appear to be quite small; they grow slightly in size as we approach larger values of $\xi^{(2)}/L$. To check that this behavior is not an artifact of the compression of the vertical axis at

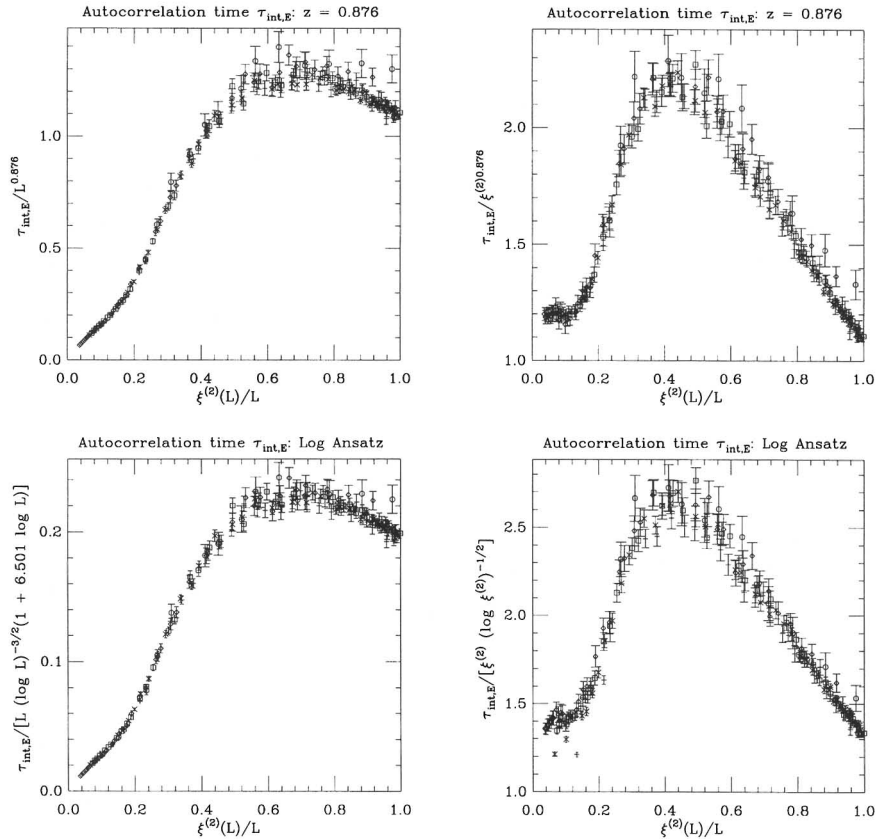


Fig. 8. Finite-size scaling plots for the integrated autocorrelation time $\tau_{\text{int},\sigma}$ as a function of the physical observable $\xi^{(2)}(L)/L$. The upper row shows the Ansatz $\tau_{\text{int},\sigma} \sim L^{z_{\text{int},\sigma}}$ with $z_{\text{int},\sigma} = 0.876 \pm 0.011$, while the lower row shows the scenario $\tau_{\text{int},\sigma} \sim L(\log L)^{-3/2} (1 + 6.501 \log L)$. In the left column we show the usual FSS plots; in the right column we have substituted the variable L in the y -axis denominator by $\xi^{(2)}$ in order to amplify the region with smaller $\xi^{(2)}/L$. Symbols denote the different lattice sizes: $L = 32$ (+), $L = 64$ (\times), $L = 128$ (\square), $L = 256$ (\diamond), and $L = 512$ (\circ).

small $\xi^{(2)}/L$, we have tried replacing L by $\xi^{(2)}$ in the y -axis denominators (right column in Fig. 8). We emphasize that these plots are identical to those in the left column, except that the scale of the y -axis is changed in a way depending on $x \equiv \xi^{(2)}/L$. Contrary to what we observed for the static observables, the corrections to scaling for small $\xi^{(2)}/L$ are not so large compared to the error bars, except for a few points at very small $\xi^{(2)}$ in the logarithmic Ansatz (where the neglect of the additive constant A in $A + B \log \xi^{(2)}$ obviously plays a role). Note, finally, that the scaling function tends to a nonzero constant when $\xi^{(2)}/L \rightarrow 0$, as expected on general theoretical grounds.

APPENDIX A. CALCULATION OF THE COEFFICIENT a'

In this appendix we derive the value (2.10) of the cubic coefficient a' in the RG flow for the 4-state Potts model. The method is identical to that of Cardy *et al.*,⁽³⁾ carried to one higher order: namely, we study the renormalization-group flow for the q -state dilute Potts model in a neighborhood of the multicritical point $q = 4$, $\phi = h = \psi = 0$; we then match this flow with the exactly known⁽²⁸⁾ values of the critical exponents as a function of q , expanded now through *second* order in $(4 - q)^{1/2}$.

A.1. Exactly Known Values of Critical Exponents

The leading thermal exponent $y_{T,1}$, the next-to-leading thermal exponent $y_{T,2}$, the leading magnetic exponent $y_{H,1}$ and the next-to-leading magnetic exponent $y_{H,2}$ of the q -state dilute Potts model are known exactly, both for the ordinary critical point (arising in the pure Potts model) and for the tricritical point (arising in the dilute model). Their values are:

$$y_{T,1} = \frac{3 + 3x}{2 + x} \quad (\text{A.1})$$

$$y_{T,2} = \frac{4x}{2 + x} \quad (\text{A.2})$$

$$y_{H,1} = \frac{15 + 8x + x^2}{4(2 + x)} \quad (\text{A.3})$$

$$y_{H,2} = \frac{7 + 8x + x^2}{4(2 + x)} \quad (\text{A.4})$$

where

$$x = \frac{2}{\pi} \arccos\left(\frac{\sqrt{q}}{2}\right) \quad (\text{A.5})$$

with $-1 \leq x \leq 0$ corresponding to the ordinary critical points and $0 \leq x \leq 1$ corresponding to the tricritical points. The value of $y_{T,1}$ for the ordinary critical point was conjectured by den Nijs;⁽⁶⁾ this conjecture was extended to the tricritical branch of the dilute Potts model by Nienhuis *et al.*⁽⁵⁾ It has now been derived by Coulomb-gas methods^(41,42) for both the critical⁽²⁴⁾ and tricritical⁽²⁸⁾ branches. The expression (A.2) for the next-to-leading thermal exponent was first conjectured by Burkhardt,⁽⁴³⁾ it was derived using Coulomb-gas methods by Nienhuis.⁽²⁸⁾ Finally, the expressions (A.3)/(A.4) for the leading and next-to-leading magnetic exponents were first conjectured by Nienhuis *et al.*⁽⁷⁾ and Pearson,⁽⁸⁾ their validity was established by den Nijs⁽⁴⁴⁾ using the Coulomb-gas approach. In the Coulomb-gas formulation, all these formulae are naturally parametrized in terms of the variable $t = 1/(2+x)$, which is proportional to the temperature of the associated Gaussian model; the thermal (resp. magnetic) exponents are linear (resp. quadratic) polynomials in t .

These exponents can also be understood in terms of conformal field theory.^(45,47) Let us consider a conformal field theory (CFT) with central charge $c < 1$, which we parametrize as

$$c = 1 - \frac{6}{m(m+1)} \quad (\text{A.6})$$

with $0 < m < \infty$ (not necessarily integer). Then the conformal weight of a primary field $\phi_{r,s}$ (r, s integer) is given by the Kac formula⁹

$$\Delta_{r,s} = \frac{[(m+1)r - ms]^2 - 1}{4m(m+1)} \quad (\text{A.7})$$

The corresponding critical exponent is $y_{r,s} = 2 - 2\Delta_{r,s}$. If m is a rational (resp. irrational) number, then the corresponding CFT has a finite (resp. infinite) operator algebra. If m is an integer ≥ 2 , then the corresponding QFT is *unitary*, at least as long as we restrict attention to the fields $\phi_{r,s}$ satisfying $1 \leq s \leq r \leq m-1$.

⁹ We follow the notation of refs. 46 and 47. In ref. 48 the indices r and s are interchanged with respect to this notation.

The *critical* q -state Potts model can be represented^(48, 49) by a CFT with central charge

$$c = 1 - \frac{3x^2}{2+x} \quad (\text{A.8})$$

where the parameter x is given by (A.5) with $-1 \leq x \leq 0$.¹⁰ From (A.6)/(A.8) we see that

$$x = -2/(m+1) \quad (\text{A.9})$$

and the Kac formula (A.7) reduces to

$$A_{r,s} = \frac{[2(r-s) + sx]^2 - x^2}{8(2+x)} \quad (\text{A.10})$$

The unitary theories $m = 2, 3, 4, 5, \dots$ correspond to $q = 1, 2, 4 \cos^2(\pi/5), 3, \dots$

The energy operator ε is identified with $\phi_{2,1}$. This means that $y_{T,1} = 2 - 2A_{2,1}$, and we obtain the result (A.1). From the conformal algebra $\varepsilon\varepsilon \sim \phi_{2,1}\phi_{2,1} \sim I + \phi_{3,1}$, and we identify the operator $\phi_{3,1}$ as the one giving the next-to-leading thermal corrections. This implies that $y_{T,2} = 2 - 2A_{3,1}$, and we get (A.2). Finally, the spin operator s is identified with $\phi_{(m+1)/2, (m+1)/2}$ (or alternatively $\phi_{(m+1)/2-1, (m+1)/2}$). Therefore, $y_{H,1} = 2 - 2A_{(m+1)/2, (m+1)/2} = 2 - 2A_{(m+1)/2, (m+1)/2-1}$, and this yields (A.3). The second magnetic exponent $y_{H,2}$ can be derived from the conformal weight of the operator $\phi_{(m+1)/2+1, (m+1)/2}$ (or alternatively $\phi_{(m+1)/2-2, (m+1)/2}$). More generally, we can obtain the full spectrum of thermal exponents

$$y_{T,n} = 2 - 2A_{n+1,1} = \frac{(4-n^2) + (n+2)x}{2+x} \quad (\text{A.11})$$

and magnetic exponents

$$\begin{aligned} y_{H,n} &= 2 - 2A_{(m+1)/2+n-1, (m+1)/2} = 2 - 2A_{(m+1)/2-n, (m+1)/2} \\ &= \frac{[16 - (2n-1)^2] + 8x + x^2}{4(2+x)} \end{aligned} \quad (\text{A.12})$$

However, this identification of the magnetic operators makes sense only when m is an odd integer $1, 3, 5, 7, \dots$, corresponding to $q = 0, 2, 3, 2 + \sqrt{2}, \dots$

¹⁰ Our parameter x is equal to minus the parameter y appearing in refs. 46 and 48.

The *tricritical* Potts model can be obtained by the analytic continuation of the preceding formulae to $0 \leq x \leq 1$.⁽⁴⁶⁾ The nonformal charge continues to be given by (A.8), but we must now identify

$$x = 2/m \quad (\text{A.13})$$

The Kac formula for the tricritical models is thus given by

$$A_{r,s} = \frac{[2(r-s) + rx]^2 - x^2}{8(2+x)} \quad (\text{A.14})$$

The energy operator is now identified with the operator $\phi_{1,2}$, which reproduces (A.1). More generally, the thermal exponents are given by the operators $\phi_{1,1+n}$, while the magnetic exponents come from the operators $\phi_{m/2, (m/2)+n}$ (or equivalently from $\phi_{m/2, (m/2)+1-n}$). Notice that the magnetic operators make sense only when m is an *even* integer 2, 4, 6, 8, ..., corresponding to the *same* series $q = 0, 2, 3, 2 + \sqrt{2}, \dots$ as in the critical case.

A.2. Renormalization-Group Flow for the q -State Dilute Potts Model

Following Cardy *et al.* [ref. 3, Section II], we study the RG flow for the q -state dilute Potts model in a neighborhood of the multicritical point $\epsilon \equiv q - 4 = 0$, $\phi = h = \psi = 0$. Cardy *et al.* showed that the RG equations can be brought by a series of smooth changes of variable into the form

$$\frac{d\psi}{dl} = a(\psi^2 + \epsilon) + O(f^3, \epsilon f, \epsilon^2) \quad (\text{A.15a})$$

$$\frac{d\phi}{dl} = (y_T + b\psi)\phi + O(f^3, \epsilon f, \epsilon^2) \quad (\text{A.15b})$$

$$\frac{dh}{dl} = (y_H + c\psi)h + O(f^3, \epsilon f, \epsilon^2) \quad (\text{A.15c})$$

where a, b, c, y_T, y_H are universal parameters. Here f stands collectively for the fields ψ, ϕ and h ; and we consider ϵ to be of order ψ^2 because that is its magnitude at the fixed points $\psi_{\pm}^2 = -\epsilon + O((-\epsilon)^{3/2})$.

By a similar argument one can treat the terms of cubic order in the fields; as before, the ψ equation decouples from the others, and becomes

$$\frac{d\psi}{dl} = a(\psi^2 + \epsilon) + a'\psi^3 + a''\epsilon\psi + O(\psi^4, \epsilon\psi^2, \epsilon^2) \quad (\text{A.16})$$

For $\epsilon < 0$ there are fixed points at

$$\psi_{\pm} = \pm (-\epsilon)^{1/2} + \frac{a'' - a'}{2a} (-\epsilon) + O((-\epsilon)^{3/2}) \quad (\text{A.17})$$

with eigenvalues

$$y_{\pm} = \pm 2a(-\epsilon)^{1/2} + 2a'(-\epsilon) + O((-\epsilon)^{3/2}) \quad (\text{A.18})$$

Here the $+$ sign corresponds to the tricritical point, with a *relevant* second thermal exponent $y_+ > 0$ controlling the tricritical-to-critical crossover; and the $-$ sign corresponds to the ordinary critical point, with an *irrelevant* second thermal exponent $y_- < 0$ controlling the leading corrections to scaling. Matching (A.18) to the known second thermal exponent (A.2)/(A.5), we find

$$a = \frac{1}{\pi} \quad (\text{A.19})$$

$$a' = -\frac{1}{2\pi^2} \quad (\text{A.20})$$

This reasoning gives an independent (and consistent!) derivation of the quadratic coefficient a , which was derived previously by Nauenberg and Scalapino^(2,3) by matching (A.15a, b) to Baxter's⁽¹⁾ exact result for the latent heat in the pure Potts model for $q > 4$; and it gives the promised derivation of a' .

Remark. This reasoning does not fix the value of a'' . Indeed, by a smooth change of variable $\psi = \psi' + \alpha_2 \psi'^2$, the coefficient a'' can be set to *any* desired value: for example, $a'' = 0$ or $a'' = a'$. The latter choice has the property of placing the fixed points at $\psi_{\pm} = \pm (-\epsilon)^{1/2}$ with *no* correction $O(-\epsilon)$. This approach can also be extended to higher order: e.g. starting from the fourth-order equation

$$\begin{aligned} \frac{d\psi}{dl} = & a(\psi^2 + \epsilon) + a'\psi^3 + a''\epsilon\psi \\ & + a^{(3)}\psi^4 + a^{(4)}\epsilon\psi^2 + a^{(5)}\epsilon^2 + O(\psi^5, \epsilon\psi^3, \epsilon^2\psi, \epsilon^3) \end{aligned} \quad (\text{A.21})$$

we can make a smooth change of variable $\psi = (1 + \alpha_{11}\epsilon)\psi' + \alpha_2\psi'^2 + \alpha_3\psi'^3$ and fix *three* of the four coefficients a'' , $a^{(3)}$, $a^{(4)}$, $a^{(5)}$ to any desired values.

For example, if we choose to fix $a'' = a'$, $a^{(3)} = a^{(4)}$, $a^{(5)} = 0$ we then have the normal form

$$\frac{d\psi}{dl} = (\psi^2 + \epsilon) \tilde{F}(\psi) + O(\psi^5, \epsilon\psi^3, \epsilon^2\psi, \epsilon^3) \quad (\text{A.22})$$

with \tilde{F} independent of ϵ . Alternatively, we can choose $a'' = a'$, $a^{(3)} = 0$, $a^{(4)} = a^{(5)}$ to yield the normal form

$$\frac{d\psi}{dl} = (\psi^2 + \epsilon)[A_0(\epsilon) + A_1(\epsilon)\psi] + O(\psi^5, \epsilon\psi^3, \epsilon^2\psi, \epsilon^3) \quad (\text{A.23})$$

with A_0, A_1 independent of ψ . It would be interesting to know whether either (or both) of these normal forms can be established to all orders in ψ and ϵ . If so, the functions $\tilde{F}(\psi)$, $A_0(\epsilon)$ and $A_1(\epsilon)$ would then be *completely determined* from the known exponent (A.2)/(A.5).

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