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Finite-size scaling above the upper critical dimension revisited: the case of the five-dimensional Ising model

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Abstract. Monte-Carlo results for the moments $\langle M^k \rangle$ of the magnetization distribution of the nearest-neighbor Ising ferromagnet in a L^d geometry, where L $(4 \leq L \leq 22)$ is the linear dimension of a hypercubic lattice with periodic boundary conditions in $d = 5$ dimensions, are analyzed in the critical region and compared to a recent theory of Chen and Dohm (CD) [X.S. Chen and V. Dohm, Int. J. Mod. Phys. C **9**, 1007 (1998)]. We show that this finite-size scaling theory (formulated in terms of two scaling variables) can account for the longstanding discrepancies between Monte-Carlo results and the so-called "lowest-mode" theory, which uses a single scaling variable $tL^{d/2}$ where $t = T/T_c - 1$ is the temperature distance from the critical temperature, only to a very limited extent. While the CD theory gives a somewhat improved description of corrections to the "lowest-mode" results (to which the CD theory can easily be reduced in the limit $t \to 0$, $L \to \infty$, $tL^{d/2}$ fixed) for the fourth-order cumulant, discrepancies are found for the susceptibility $(L^d \langle M^2 \rangle)$. Reasons for these problems are briefly discussed.

PACS. 05.70.Jk Critical point phenomena – 64.60.-i General studies of phase transitions – 75.40.Mg Numerical simulation studies

1 Introduction

Since about 15 years the five-dimensional Ising model is used as a "laboratory" [1–8] to test theoretical concepts about critical phenomena, in particular the concept of finite-size scaling [9–32], which has become an extremely valuable and indispensable tool for the study of phase transitions in condensed matter [22,33,34] and gauge theories of elementary particle physics [35,36]. In this context, the $d = 5$ Ising model is of particular interest, since it exceeds the upper critical dimension, $d^* = 4$, and hence the Landau mean-field exponents exactly describe the critical behavior [37,38]. Also correction-to-scaling exponents [39] are known precisely [38] and fluctuations around the leading mean-field description can be dealt with by simple perturbation theory; a renormalization-group treatment of fluctuation effects is not required here [37,38]. While for $d > d^*$ the hyperscaling relation $d\nu = \gamma + 2\beta$ (ν, γ, β being the standard critical exponents for correlation length ξ, susceptibility χ and order parameter M, respectively) does not hold and hence finite-size scaling in its standard version ("the linear dimension L scales with ξ" [9–12,16,20,23]) does not hold either [12–14], a simple extension was proposed [1,2,17,18] which can be phrased as [2] "the linear dimension L scales asymptotically with a thermodynamic length $\ell_T = (M_b^2/\chi_b)^{-1/d} \propto t^{-2/d}$". Moreover it was suggested that ratios of moments of the order parameter distribution, such as $Q \equiv \langle M^2 \rangle^2 / \langle M^4 \rangle$ or $\langle |M| \rangle^2 / \langle M^2 \rangle$ can easily be calculated from the so-called lowest-mode approximation [17], which was believed to be exact for the limit $L \to \infty$, $t \to 0$, L/ℓ_T fixed and should yield, apart from scale factors, universal finite-size scaling functions of L/ℓ_T.

In view of these rather definite predictions [17], apparent discrepancies between the theoretical results and the Monte-Carlo simulations [1–3] have been disturbing and it has been a matter of debate [4–8,27,29–31] whether the discrepancies reflect corrections to finite-size scaling. In reference [8] it was shown that the Monte-Carlo data for Q are indeed compatible with the predictions of Brézin and Zinn-Justin [17] if one takes into account two, theoretically predicted, corrections to scaling. However, this still left the very slow convergence of Q as a function of L toward its predicted asymptotic value as a remarkable feature (in Ref. [3] the data for Q for the considered range of system sizes appeared to have a common intersection point unequal to this value). More importantly, the correctness of the treatment in reference [17] has recently been doubted [31] (see below). This controversy is cumbersome because the fact that it is apparently very difficult to disentangle the leading and subleading terms in finite-size scaling analyses even in a case where all involved critical exponents are known precisely naturally leads to

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some doubt on analyses where one wants to extract unknown critical exponents from finite-size scaling [22,23,26,34]. In addition, the problem also is of interest in the context of physical systems that are nearly described by Landau theory, such as systems with a long but finite range of interaction [25,28], polymer mixtures near their critical point of unmixing [40], etc.

New light has been shed on this state of affairs by Chen and Dohm (CD) [29–31], who presented detailed arguments that for $d > d^*$ the standard treatment of the ϕ^4 field theory in continuous space [17,18,38] yields a misleading description of finite-size behavior, different from the finite-size behavior of a ϕ^4 model on a lattice, which one believes to be equivalent to an Ising model [37,38]. Chen and Dohm emphasized that therefore the justification given for the lowest-mode theory is invalid, and stated that the moment ratios mentioned above "do not have the universal properties predicted previously and that recent analyses of Monte-Carlo results for the five-dimensional Ising model are not conclusive" [31].

In view of this criticism, a reanalysis of the available Monte-Carlo results (including also some recent unpublished results [41] used in [42]) is clearly warranted. Such an analysis, where we compare the Monte-Carlo data in detail with the result of the CD theory (which treats order parameter fluctuations perturbatively to one-loop order for the Ising case [31]) is given here. For the sake of a coherent presentation, we summarize the pertinent theoretical results in Section 2, while Section 3 gives a detailed comparison of the results for Q and for the susceptibility $\chi = L^d\langle M^2\rangle$ with the CD theory. Section 4 summarizes our conclusions.

2 Theoretical background

The singular part of the free-energy density f_L of a system with linear size L in an external field h is written as (see, *e.g.*, Ref. [14])

$$f_L = L^{-d} f\left(tL^{y_\mathrm{t}}, hL^{y_\mathrm{h}}, uL^{y_\mathrm{i}}\right), \quad L\to\infty, \tag{1}$$

where $t = T/T_\mathrm{c} - 1$ and u is an irrelevant variable, in the renormalization-group sense (exponents $y_\mathrm{t} > 0$, $y_\mathrm{h} > 0$, $y_\mathrm{i} < 0$). Now for $d > d^* = 4$ we have $y_\mathrm{t} = 2$, $y_\mathrm{h} = (d+2)/2$ and $y_\mathrm{i} = 4-d$, but u is a "dangerous irrelevant variable" (see, *e.g.*, Refs. [43,44]), which means that the scaling function $f(x_1, x_2, x_3)$ is singular in the limit $x_3 \to 0$ and cannot simply be replaced by $f(x_1, x_2, 0)$. In terms of the bulk correlation length $\xi_\mathrm{b} = \xi_0 t^{-\nu}$ (above T_c in zero field), the first argument of equation (1) can be interpreted as $(L/\xi_\mathrm{b})^2$. Taking suitable derivatives of equation (1) with respect to the field we can thus write for the order parameter, the susceptibility and the ratio Q (in zero field)

$$\langle|M|\rangle = L^{-(d-2)/2} P_M\left\{t(L/\xi_0)^2, (L/\ell_0)^{4-d}\right\}, \tag{2}$$

$$\chi = \left(\frac{\partial^2 f_L}{\partial h^2}\right) = L^d\langle M^2\rangle = L^2 P_\chi\left\{t(L/\xi_0)^2, (L/\ell_0)^{4-d}\right\} \tag{3}$$

and

$$Q = \frac{\langle M^2\rangle^2}{\langle M^4\rangle} = P_Q\left\{t(L/\xi_0)^2, (L/\ell_0)^{4-d}\right\}, \tag{4}$$

where P_M, P_χ and P_Q are the (universal [22]) finite-size scaling functions of the quantities $\langle|M|\rangle$, χ and Q. The correlation-length amplitude ξ_0 of the bulk correlation length now appears as a scale factor for the variable x_1 and for the variable x_3 we have introduced the correlation-length amplitude ℓ_0 of the bulk correlation length at T_c in a small field [31] as a scale factor. In this way, the arguments of the scaling functions P_M, P_χ and P_Q are dimensionless, as they should be. Note that $u \propto \ell_0^{d-4}$.

For large L the variable $x_3 \propto (L/\ell_0)^{4-d}$ clearly becomes very small, and hence it is an obvious question to ask how all these functions f_L, P_M, P_χ, P_Q behave in the limit $x_3 \to 0$. It was assumed in reference [1] that then the dangerous irrelevant variable x_3 enters in the form of multiplicative singular powers of x_3, *e.g.*,

$$f_L(x_1, x_2, x_3) = x_3^{p_3}\tilde{f}_L(x_1 x_3^{p_1}, x_2 x_3^{p_2}). \tag{5}$$

This assumption was in the first place motivated by the fact that this is the mechanism that operates for the scaling in the bulk for $d > 4$ [44], and secondly by various phenomenological arguments. In particular, it was argued that standard thermodynamic fluctuation theory requires for $T < T_\mathrm{c}$ and sufficiently large L that the distribution function $P_L(M)$ of the magnetization per spin for M near the spontaneous magnetization $\pm M_\mathrm{b}$ is a sum of two Gaussians [1,2,12],

$$P_L(M) = \frac{L^{d/2}}{2\sqrt{2\pi\chi_\mathrm{b}}}\Big\{\exp\left[-(M-M_\mathrm{b})^2 L^d/2\chi_\mathrm{b}\right] + \exp\left[-(M+M_\mathrm{b})^2 L^d/2\chi_\mathrm{b}\right]\Big\}. \tag{6}$$

Using $M_\mathrm{b} = \hat{M}_\mathrm{b}|t|^\beta = \hat{M}_\mathrm{b}(-t)^{1/2}$ and $\chi_\mathrm{b} = \hat{\chi}'_\mathrm{b}|t|^{-\gamma} = \hat{\chi}'_\mathrm{b}(-t)^{-1}$ the arguments of the exponential functions have the form

$$\frac{1}{2}\left[(M/\hat{M}_\mathrm{b})|t|^{-1/2} \mp 1\right]^2 (L/\ell_\mathrm{T})^d, \tag{7}$$

with $\ell_\mathrm{T}^d = M_\mathrm{b}^{-2}\chi_\mathrm{b} = \hat{M}_\mathrm{b}^{-2}\hat{\chi}'_\mathrm{b}t^{-2}$. Taking moments of this distribution one hence expects that the scaling functions in equations (2–4) reduce to scaling functions of a single variable $(L/\ell_\mathrm{T})^{d/2} \propto tL^{d/2}$ or, keeping the amplitudes ξ_0 and ℓ_0 explicitly present, $tL^{d/2}\xi_0^{-2}\ell_0^{(4-d)/2}$, *i.e.*,

$$\langle|M|\rangle = L^{-d/4}\tilde{P}_M\left(tL^{d/2}\xi_0^{-2}\ell_0^{(4-d)/2}\right), \tag{8}$$

$$\chi = L^{d/2}\tilde{P}_\chi\left(tL^{d/2}\xi_0^{-2}\ell_0^{(4-d)/2}\right) \tag{9}$$

and

$$Q = \tilde{P}_Q\left(tL^{d/2}\xi_0^{-2}\ell_0^{(4-d)/2}\right). \tag{10}$$

Note that scale factors for the magnetization and the susceptibility have been absorbed in P_M (or $\tilde{P}_M$) and P_χ

(or $\tilde{P}_\chi$), respectively, while in ratios such as Q (and hence in P_Q and $\tilde{P}_Q$) such scale factors are divided out and fully universal functions remain.

These arguments as they were presented in references [1,2] did not tell anything about the explicit form of the scaling functions $\tilde{P}_M(x)$, $\tilde{P}_\chi(x)$ and $\tilde{P}_Q(x)$, however, and hence no prediction for the supposedly universal constant $\tilde{P}_Q(0)$ was made. In fact, making the (premature!) assumption that linear dimensions $L = 3$ to 7 lattice spacings are already large enough to obtain the limit $x_3 \propto (L/\ell_0)^{-1} \to 0$ in $d = 5$ dimensions, it was argued that at T_c there occurs a distribution of the scaled order parameter $P_L(\phi) \propto \exp(A\phi^2 - \phi^4)$, which implies a shift of T_c as $T_\mathrm{c}(L)/T_\mathrm{c}(\infty) - 1 \propto AL^{-d/2}$, if $T_\mathrm{c}(L)$ is defined as the temperature where $P_L(\phi)$ starts to develop a two-phase structure. However, the next step in the development, due to Brézin and Zinn-Justin [17], suggested that in the scaling limit $P_L(\phi) \propto \exp(-\phi^4)$ at T_c, since the shift of T_c as defined above should only exhibit a scaling with a higher power of L^{-1}, namely $T_\mathrm{c}(L)/T_\mathrm{c}(\infty) - 1 \propto L^{2-d}$, because it results from corrections to the scaling description given in equations (8–10). According to reference [17], the asymptotic behavior is simply given by the homogeneous order parameter M in the finite system,

$$P_L(M) = \exp\left[-L^d\left(\frac{1}{2}r_0M^2 + uM^4\right)\right], \qquad (11)$$

where $r_0 = a_0t$ changes sign at T_c, u is the dangerous irrelevant variable mentioned above, both a_0 and u being nonuniversal constants. From equation (11) it is straightforward to derive that [17]

$$\tilde{P}_Q(0) = 8\pi^2/\Gamma^4(1/4) \approx 0.456\,947. \qquad (12)$$

However, the statements of CD imply that the continuum model considered in [17] actually leads to a behavior differing from equation (11) and thus at this point also equation (12) seems without safe foundation. CD obtain, in the large-n limit of the n-vector model on the lattice rather than in the continuum, a result for the scaling function $P_\chi(x,y)$ (Eq. (3); $x = t(L/\xi_0)^2$, $y = (L/\ell_0)^{4-d}$) which is believed to be asymptotically exact, namely

$$P_\chi(x,y) = \frac{2}{J_0}\left[\delta(x,y) + \sqrt{[\delta(x,y)]^2 + 4y}\right]^{-1}, \qquad (13)$$

where J_0 is the interaction range of the ϕ^4 model on the d-dimensional hypercubic lattice (the lattice spacing being taken as unity here throughout),

$$J_0 = \frac{1}{dL^d}\sum_{i,j} J_{ij}|\mathbf{r}_i - \mathbf{r}_j|^2, \qquad (14)$$

and $\delta(x,y)$ is given by

$$\delta(x,y) = x - yI_1(J_0^{-1}P_\chi^{-1}), \qquad (15)$$

with the function $I_m(x)$, $m = 1, 2, \ldots$, being

$$I_m(x) = \frac{1}{(2\pi)^{2m}}\int_0^\infty \mathrm{d}y\, y^{m-1}\exp(-xy/4\pi^2) \times \left[\left(\frac{\pi}{y}\right)^{d/2} - \left(\sum_{p=-\infty}^{\infty} e^{-yp^2}\right)^d + 1\right]. \qquad (16)$$

In terms of the Hamiltonian of the n-vector model with n-component vectors ϕ_i on the lattice,

$$H = \sum_i\left[\frac{r_0}{2}\phi_i^2 + u_0(\phi_i^2)^2\right] + \sum_{i,j}\frac{J_{ij}}{2}(\phi_i - \phi_j)^2, \qquad (17)$$

the characteristic lengths ξ_0, ℓ_0 in equations (2–4) are given by

$$\xi_0^2 = \frac{J_0}{a_0}(1 + S_\mathrm{c}^\mathrm{b}), \qquad \ell_0^{d-4} = \frac{4u_0n}{J_0^2}\frac{1}{1 + S_\mathrm{c}^\mathrm{b}}, \qquad (18)$$

with $r_0 = r_{0\mathrm{c}} + a_0t$ and

$$S_\mathrm{c}^\mathrm{b} = u_0n\int \mathrm{d}\mathbf{k}\,[\delta J(\mathbf{k})]^{-2}, \qquad \delta J(\mathbf{k}) = J(\mathbf{0}) - J(\mathbf{k}), \qquad (19)$$

where $J(\mathbf{k}) \equiv L^{-d}\sum_{i,j} J_{ij}\exp[-i\mathbf{k}\cdot(\mathbf{r}_i - \mathbf{r}_j)]$. For the n-vector model with $n = 1$, which is supposed to belong to the Ising universality class, comparable results are obtained only to one-loop order in perturbation theory [31]. Although the results are not exact, their scaling structure is analogous to equations (13–16) and this structure is not expected to be changed by the higher-order terms of the loop expansion. Defining reduced moments

$$\theta_m(Y) = \frac{\int_0^\infty \mathrm{d}\phi\,\phi^m\exp\left[-\frac{1}{2}Y\phi^2 - \phi^4\right]}{\int_0^\infty \mathrm{d}\phi\,\exp\left[-\frac{1}{2}Y\phi^2 - \phi^4\right]} \qquad (20)$$

CD find [31,45]

$$P_\chi(x,y) = \frac{1}{J_0}\frac{\theta_2(Y(x,y))}{\sqrt{y + 36I_2(\bar{r})y^2}}, \qquad (21)$$

$$P_Q(x,y) = \frac{[\theta_2(Y(x,y))]^2}{\theta_4(Y(x,y))}, \qquad (22)$$

with

$$Y(x,y) = \frac{\left[x - 12yI_1(\bar{r}) - 144\theta_2(xy^{-1/2})I_2(\bar{r})y^{3/2}\right]}{\left[y + 36I_2(\bar{r})y^2\right]^{1/2}}, \qquad (23)$$

where $\bar{r} \equiv x + 12\theta_2(xy^{-1/2})y^{1/2}$. As should be clear from what has been said above, the results (21–23) should hold for sufficiently large L.

Armed with these results we are now in a better position to reconsider the question already posed in reference [1], namely to take the limit $y \to 0$. For this purpose we first consider the large-n limit, where we can rewrite equation (13) as

$$P_\chi(x,y) = \frac{1}{J_0\sqrt{y}}\left[\frac{\delta(x,y)}{2\sqrt{y}} + \sqrt{1 + [\delta(x,y)/(2\sqrt{y})]^2}\right]^{-1}. \qquad (24)$$

In the limit $y \to 0$ we see from equation (15) that $P_\chi(x, y)$ depends, apart from the prefactor, on x and y through the variable

$$\frac{\delta(x,y)}{2\sqrt{y}} \to \frac{x}{2\sqrt{y}} - \frac{1}{2}\sqrt{y} I_1(J_0^{-1}P_\chi^{-1}) \\ = \frac{1}{2} t L^{d/2} \xi_0^{-2} \ell_0^{(4-d)/2} - \frac{1}{2}(L/\ell_0)^{(4-d)/2} I_1(J_0^{-1}P_\chi^{-1}). \tag{25}$$

Thus we see that there exists a limit $t \to 0$, $L \to \infty$, $tL^{d/2}$ fixed, where the susceptibility scales exactly as postulated in equation (9), since then the correction term of order $(L/\ell_0)^{(4-d)/2}$ in equation (25) clearly is negligible ($J_0^{-1}P_\chi^{-1}$ tends toward zero in this limit, so the function I_1 approaches a finite constant). Contrary to statements made by CD themselves, *viz.* that the structure of equations (8–10) is incorrect for the ϕ^4 lattice model, we rather think that they have proven(!) the correctness of equation (11), in the limit specified above, at least for the large-n limit, and gratifyingly there is no contradiction at all between equations (13–19) and the ideas of reference [1] that led to equations (8–10). Of course, the strong merit of the CD treatment is that it yields not only the scaling structure but also the explicit scaling function and a full description of the corrections due to the dangerous irrelevant variable u_0.

We arrive at similar conclusions in the case $n = 1$, though one must recall that these results are only based on a one-loop order approximation. In the considered limit $y \to 0$ the quantity $Y(x, y)$ in equation (23) reduces to

$$Y(x,y) \to \frac{x}{\sqrt{y}}\left[1 - 18 I_2(\bar{r}) y\right] - 12 I_1(\bar{r})\sqrt{y} \\ = t L^{d/2} \xi_0^{-2} \ell_0^{(4-d)/2}\left[1 - 18 I_2(\bar{r})(L/\ell_0)^{4-d}\right] \\ - 12 I_1(\bar{r})(L/\ell_0)^{(4-d)/2}, \tag{26}$$

which is, apart from the additional $\mathcal{O}(L^{4-d})$ correction, fully analogous to equation (25). In the limit of interest ($t \to 0$, $L \to \infty$, $tL^{d/2}$ fixed), $\bar{r}$ vanishes and the functions I_1, I_2 take finite values, so we see again that equations (9, 10) hold. Moreover, one concludes that at the critical temperature $Y(0, y \to 0) \to 0$ and hence also equation (12) holds, as noted already by CD. It remains to be seen whether (12), which is less general than the scaling structure of equations (8–10), holds to all orders in the loop expansion.

In order to compare equations (20–23) to numerical Monte-Carlo data, it is clearly of interest to consider simple limiting cases of the susceptibility, where then the nonuniversal parameters ξ_0 and ℓ_0 can be extracted. Since accurate Monte-Carlo estimations of correlation lengths are much more difficult to perform than estimations of the susceptibility we note that in the large-n limit (Eqs. (13–19)) the bulk susceptibility is [29]

$$\chi_{\rm b} = -\frac{\partial^2 f_{\rm b}(t,h)}{\partial h^2} = \frac{\xi_{\rm b}^2}{J_0} = \frac{1 + S_{\rm c}^{\rm b}}{a_0 t}, \tag{27}$$

where $\xi_{\rm b} = \xi_0 t^{-\nu}$. The same result is obtained from equations (3, 13) using that, at fixed small t, $\delta(x, y) \approx x$ in the limit $L \to \infty$ and hence

$$P_\chi(x, y \to 0) \approx (J_0 x)^{-1} \Rightarrow \chi = L^2/[J_0(L/\xi_{\rm b})^2] = \chi_{\rm b}. \tag{28}$$

In contrast, at the critical temperature the result is

$$J_0\chi(T = T_{\rm c}) = L^{d/2}\ell_0^{(4-d)/2}. \tag{29}$$

Thus, one can determine both parameters of interest, ξ_0 and ℓ_0, from the behavior of χ in two simple limits. The same procedure can also be carried out in the $n = 1$ case, considering the limit $y \to 0$ at fixed small t,

$$\chi t = \frac{\xi_0^2}{J_0}\frac{x}{\sqrt{y + 36 I_2(\bar{r}) y^2}}\theta_2(Y(x,y)) \stackrel{y\to 0}{\longrightarrow} \frac{\xi_0^2}{J_0}, \tag{30}$$

while in the finite-size scaling limit ($x = 0$, y small) one obtains for $d = 5$

$$\chi = \frac{L^2}{J_0}\frac{1}{\sqrt{y}}\theta_2(0) = \frac{L^{d/2}}{J_0\sqrt{\ell_0}}\frac{\Gamma(\frac{3}{4})}{\Gamma(\frac{1}{4})}. \tag{31}$$

As we already noted, the interest of equations (20–23) is not only the combination of the scaling structure, equations (8–10), in the limit $t \to 0$, $L \to \infty$, $tL^{d/2} =$ const, but these equations also incorporate the effect of the corrections to the lowest-mode approximation, which we would recover if in equation (23) we had $Y(x, y) = xy^{-1/2}$.

3 Comparison of the Chen-Dohm predictions with simulation results for the d = 5 Ising model

In reference [8] only numerical data for the amplitude ratio Q have been considered, with $5 \le L \le 22$. In order to estimate the scaling parameter ℓ_0 we now analyze the corresponding data for the magnetic susceptibility. Thus, we apply a finite-size expansion similar to equation (3) in [8],

$$\chi(T, L) = L^{d/2}\left(p_0 + p_1\hat{t}L^{y_{\rm t}^*} + p_2\hat{t}^2 L^{2y_{\rm t}^*} \right.\\ \left. + q_1 L^{y_{\rm i}} + q_2 L^{2y_{\rm i}}\right), \tag{32}$$

where $\hat{t} = t + \alpha L^{y_{\rm i} - y_{\rm t}}$ and $y_{\rm t}^* = y_{\rm t} - y_{\rm i}/2$. So the term $\hat{t}L^{y_{\rm t}^*} = tL^{d/2} + \alpha L^{(4-d)/2}$ just corresponds to the scaling variable in equations (25, 26). The additional term in equation (26) was already mentioned in [8] as the "cross term" $\hat{t}L^{y_{\rm t}^* + y_{\rm i}}$; in contrast to the analysis of Q, it turns out to have a negligibly small coefficient in the analysis of the susceptibility. The leading power $L^{d/2}$ (Eq. (31)) has been confirmed numerically within less than one percent in reference [42]. In our analysis we have kept this power as well as the irrelevant exponent $y_{\rm i}$ fixed. This yielded a critical coupling $J/k_{\rm B}T_{\rm c} = 0.113\,9152(4)$, in excellent agreement with the value found in reference [8]

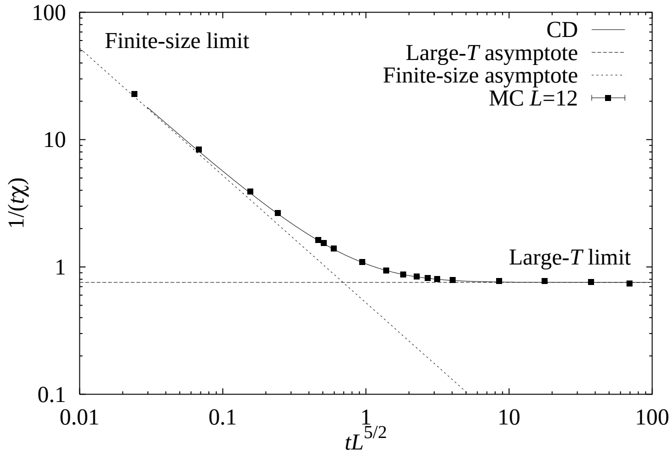

Fig. 1. Log-log plot of $1/(t\chi)$ *versus* $tL^{5/2}$, for the five-dimensional nearest-neighbor Ising model. Squares denote Monte-Carlo data as mentioned in the text, dashed lines represent equations (30, 31), respectively, with the parameters from equation (33). The finite-size asymptote included here refers to the limit $L \to \infty$ and has been estimated as described after equation (32).

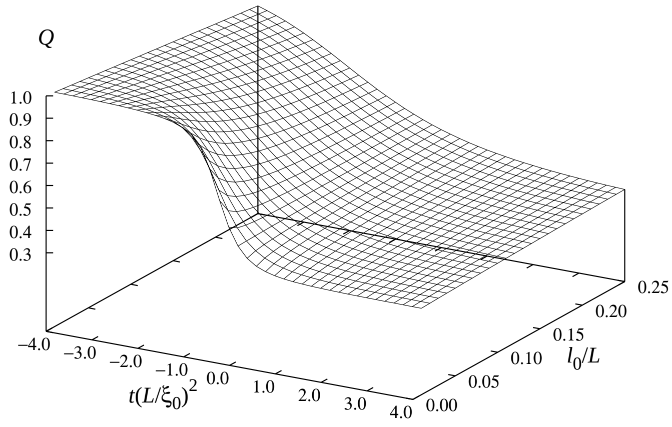

Fig. 2. Plot of the moment ratio $Q \equiv \langle M^2\rangle^2/\langle M^4\rangle$ for $d=5$ as a function of the two variables $x = tL^2/\xi_0^2$ and $y = (\ell_0/L)^{d-4}$, according to equations (20, 22, 23).

from keeping Q fixed at the zero-mode prediction (12), *viz.* $J/k_{\mathrm{B}}T_{\mathrm{c}} = 0.113\,9150(4)$ (numbers in parentheses denote the uncertainty in the last decimal places). Furthermore, we found $y_{\mathrm{t}}^* = 2.53(4)$, very close to $d/2$, and $p_0 = 1.86(7)$. The quality of the fit in terms of the χ^2 criterion was $\chi^2/\mathrm{DOF} = 1.06$. In order to improve the accuracy of our estimate for p_0, we have repeated the analysis with y_{t}^* fixed at $d/2$, finding $J/k_{\mathrm{B}}T_{\mathrm{c}} = 0.113\,9155(2)$ and $p_0 = 1.91(2)$ ($\chi^2/\mathrm{DOF} = 1.05$). All analyses were obtained with $5 \leq L \leq 22$; upon omitting the smallest system sizes, a very similar estimate for p_0 was obtained, with a minor increase in the uncertainty. For a more detailed analysis we refer to [41,42]. From our estimate for p_0 and equation (31) we find, using $J_0 = 2J/k_{\mathrm{B}}T$, $\ell_0 = 0.603(13)$. For the sake of clarity, it is stressed that this estimate for ℓ_0 thus pertains to the thermodynamic limit and is *not* a finite-size quantity.

It is also possible to extract ξ_0 from the Monte-Carlo data. However, here we use the series-expansion result from reference [46] for this purpose. Assuming the mean-field exponent $\gamma = 1$, it was found that asymptotically $\chi = A/(1 - v/v_{\mathrm{c}})$ with $A = 1.311(9)$ and $v = \tanh(J/k_{\mathrm{B}}T)$. Rewriting this in terms of the reduced temperature t, we have $\chi = A[\cosh(J/k_{\mathrm{B}}T_{\mathrm{c}})\sinh(J/k_{\mathrm{B}}T_{\mathrm{c}})/(J/k_{\mathrm{B}}T_{\mathrm{c}})]t^{-1} = 1.322t^{-1}$ and equation (30) shows that $\xi_0 = 0.549(2)$.

Figure 1 now shows the log-log plot of $(t\chi)^{-1}$ *versus* the scaling variable $tL^{d/2}$, using data for $T \geq T_{\mathrm{c}}$ only (in view of the very accurate estimates of the critical coupling, the errors due to the inaccuracy of T_{c} are not of major concern here). Available data for smaller system sizes have been omitted from this graph, because the rather strong deviations from scaling noted already in reference [2] would obscure its main purpose, namely to illustrate the use of the limits (30, 31) to extract ξ_0 and ℓ_0. Of course, due to the corrections to scaling included in equation (32) the Monte-Carlo data for $L = 12$ should not converge to the finite-size asymptote for $L \to \infty$, but to a slightly shifted straight line. However, on the scale of Figure 1 the finite-size asymptotes for $L = 12$ and $L \to \infty$ are indistinguishable. Because of their central interest we repeat our estimates

$$\ell_0 = 0.603(13), \quad \xi_0 = 0.549(2). \tag{33}$$

The amplitude $\xi_0^2\sqrt{\ell_0}$ which normalizes the scaling variable $tL^{d/2}$ (*cf.* Eq. (26)) becomes 0.234(4).

In the following graphs, also Monte-Carlo data from reference [2] ($L = 4$) and reference [3] ($L = 8, 12$) are included and it was found that all the Monte-Carlo data are, within their statistical errors, nicely compatible with each other. We have omitted the data of reference [3] for $L \geq 13$ here, since the rather irregular behavior found for the specific heat and the cumulant intersections for these system sizes indicates that these data suffer from statistical inaccuracies due to critical slowing down. Note that reference [3] used a single-spin-flip Metropolis algorithm, whereas in references [8,41,42] a single-cluster algorithm was applied. Available data from references [4,5] are restricted to temperatures very close to $T = T_{\mathrm{c}}$ and hence are unsuitable for our purposes.

We now focus on the quantity Q, equation (4), since the scaling behavior of this quantity has been so controversial. Figure 2 gives a plot of the CD function (22), keeping both x and y as separate variables. One can see that for x large and negative $Q = 1$ as it must be and for x large and positive $Q = 1/3$, irrespective of y. This simply reflects the trivial properties of the low- and high-temperature phases, respectively. For $|t(L/\xi_0)^2| < 1$, however, a clear y dependence is seen.

In Figure 3 we compare the various Monte-Carlo data to the CD function for Q as a function of tL^2 (*i.e.*, the variable proportional to x). Note that in these plots there are *no adjustable parameters* whatsoever, so the agreement is at first sight very remarkable. At second sight, however, one does observe that there are slight but systematic deviations between theory and simulation, which have

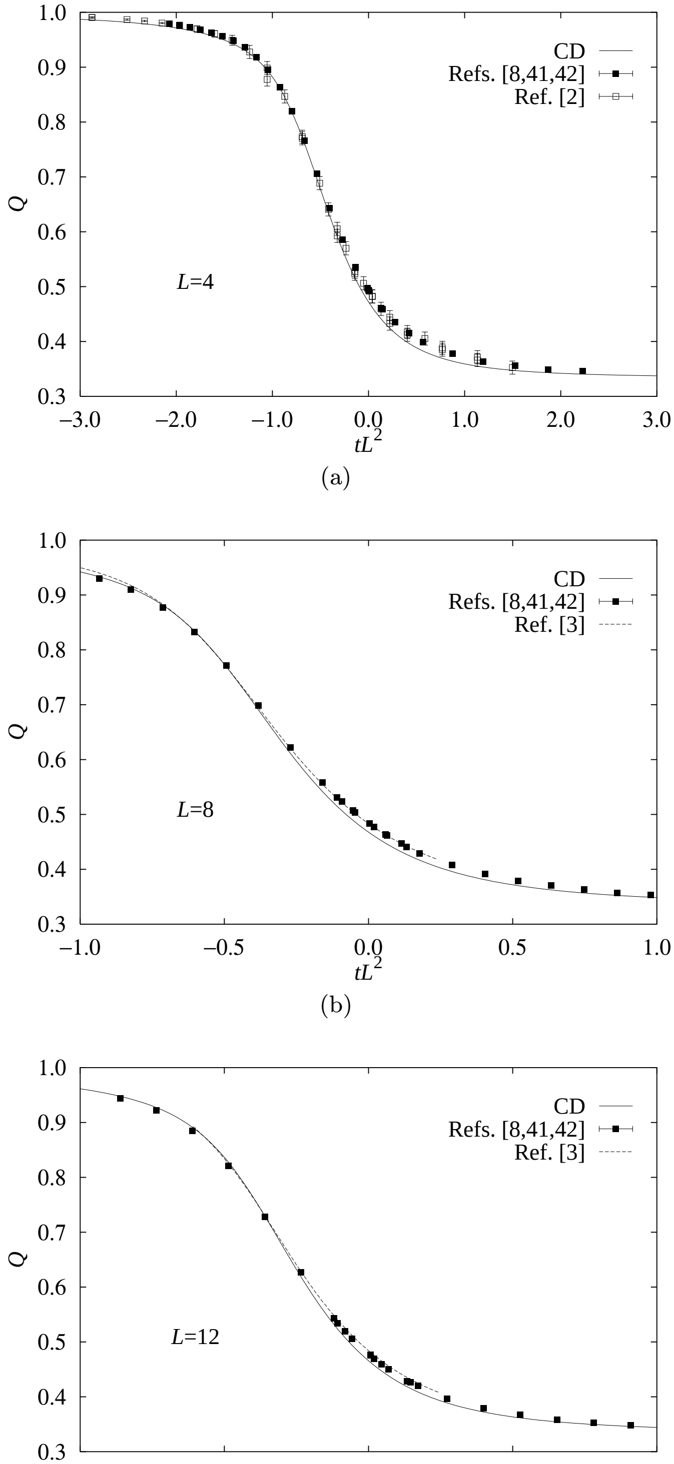

Fig. 3. Plot of Q *versus* tL^2 for (a) $L = 4$, (b) $L = 8$ and (c) $L = 12$. The full curves denote the predictions of reference [31]. Monte-Carlo data generated at specific temperatures, taken from references [2,8,41,42] are shown as open or full squares, respectively, while the histogram extrapolation data of reference [3] are shown as a broken curve.

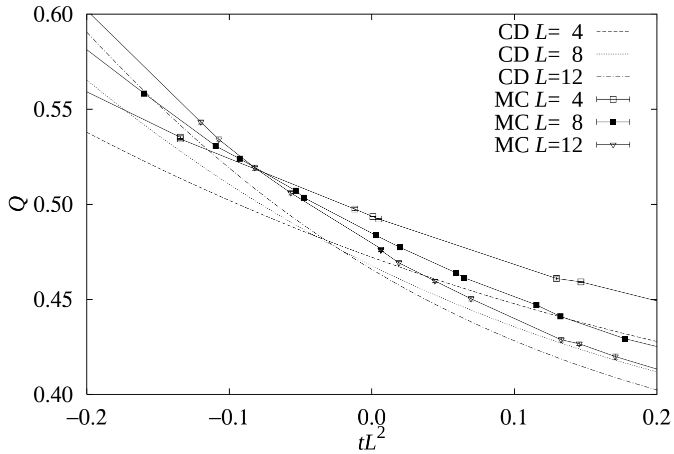

Fig. 4. Magnified plot of Q *versus* tL^2 near $tL^2 = 0$, *cf.* Figure 3, to demonstrate the occurrence of spurious cumulant intersections.

consequences for the intersection of the amplitude ratios for different system sizes. Figure 4 demonstrates that both the CD function and the Monte-Carlo data behave qualitatively similar: for a range of sizes ($4 \leq L \leq 12$) there is almost a common intersection point, but it occurs at a *negative* value of tL^2 and consequently the corresponding ordinate value $Q_{\rm int}$ is significantly larger than the predicted asymptotic value (12). While this spurious value of the CD function, for the range of system sizes considered here, is about $Q_{\rm int} \approx 0.48$, it lies around $Q_{\rm int} \approx 0.52$ for the Monte-Carlo data; Rickwardt *et al.* [3] quoted $Q_{\rm int} \approx 0.49(1)$, including data up to $L = 17$. The lesson to be learned from this graph is threefold: (i) one must not pay too much attention to the value of such a cumulant intersection if one does not have a sufficiently large range of linear dimensions at one's disposal; (ii) the CD function is a nice analytical example of a function that does produce a spurious "intersection", as pointed out already in reference [31]: although it looks so convincing on the graph, one knows that in the asymptotic limit the intersection occurs at $t = 0$ and yields $Q \approx 0.457$ (Eq. (12)); (iii) the CD function produces the same trend as the Monte-Carlo data only qualitatively, but not quantitatively.

What is the consequence of these results for the asymptotic scaling, equation (10)? This question is addressed in Figure 5, where the data from Figure 3 are replotted as a function of the scaling variable $tL^{d/2}$: it is seen that the data for $L = 4$ deviate from scaling in a systematic way, while for $L = 8, 12$ the data scale already rather nicely, although they are still a little bit set off in comparison to the theoretical scaling curves. Note that on these large scales one cannot distinguish the CD curve for $L = 12$ from the lowest-mode result! The general trend appears that in the neighborhood of $T = T_{\rm c}$ equation (22) yields a too small value for $Q(L)$.

In order to highlight the differences, we now amend the plot of Q at $T_{\rm c}$ as a function of L, which was shown in reference [8], by the prediction that would follow from

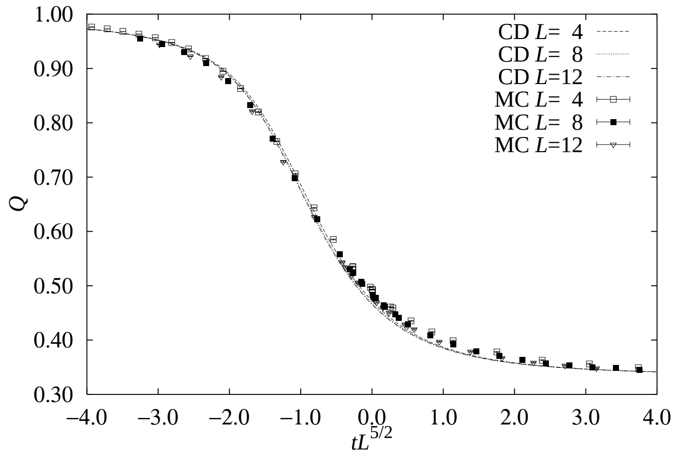

Fig. 5. Plot of Q as a function of $tL^{5/2}$, including both Monte-Carlo data for $L = 4, 8, 12$ and the CD functions. Note that the zero-mode curve, resulting from setting $Y = xy^{-1/2}$ in equations (20, 22, 23), practically coincides with the CD curve for $L = 12$ already, since ℓ_0 (Eq. (33)) is so small.

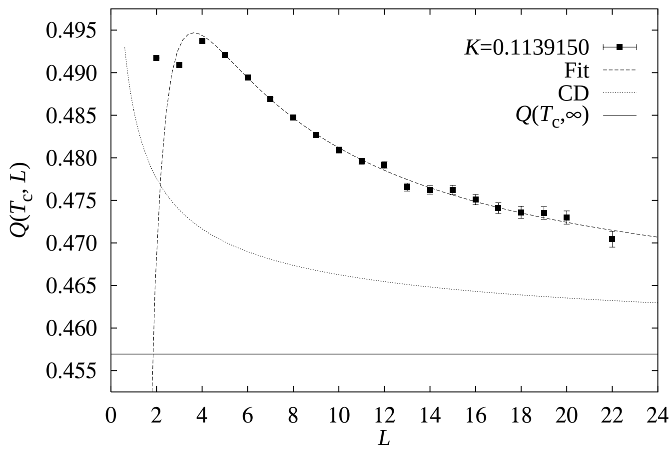

Fig. 6. Plot of $Q(T_c, L)$ *versus* L. Data points are the Monte-Carlo results from reference [8], including statistical errors. The broken curve is the empirical fit, as described in reference [8], while the horizontal line denotes the asymptotic result of equation (12). The CD prediction is shown as a dotted line.

CD (see Fig. 6): one indeed observes that the result of CD underestimates the differences between $Q(T_c, L)$ and $Q(T_c, \infty)$ distinctly – it basically yields a $1/\sqrt{L}$ correction, while the additional $1/L$ term resulting from CD is very small, unlike the rather pronounced $1/L$ correction that was found in the the empirical fit of reference [8]. Another, more tentative, way to quantify the differences is by adjusting ℓ_0 such that the CD curve yields a reasonable description of the numerical data. It turns out that a value as high as $\ell_0 \approx 3.2$ (instead of the estimated value 0.603 ± 0.013) is required to find some agreement in the region $12 \leq L \leq 22$. It clearly must be waited for a loop expansion to second order – which will yield additional $1/L$ corrections of so far unknown magnitude – before one can draw final conclusions about the agreement between theory and simulation (or lack thereof).

While in the comparison of the temperature dependence of Q as predicted by CD theory to the simulation results we have seen most of the disagreement for $t > 0$, Figure 7 shows that much more drastic deviations between theory and simulation occur for χ in the regime $t < 0$. The fact that for $t > 0$ there is perfect agreement for $L = 12$ is no surprise, of course, since these data have been of central relevance for the fit in Figure 1 that yielded ξ_0 and ℓ_0. It is clear that perhaps a better overall fit of the data is reached if one would fit ℓ_0 to describe the behavior of χ for tL^2 large and negative, but then the behavior for $t > 0$ would deteriorate. Let us note in passing that the term "susceptibility" is just used for convenience here: below T_c the real (reduced) susceptibility is of course given by $L^d(\langle M^2 \rangle - \langle |M|^2 \rangle)$.

Figure 8 shows then a plot of $\chi L^{-5/2}$ *versus* $tL^{5/2}$, comparing Monte-Carlo data for $L = 4$ and $L = 12$ [8] with corresponding predictions of the CD theory and the "zero-mode" curve. Again systematic deviations between CD theory and simulations are apparent: while the theory [31] converges to the zero-mode result from above, the Monte-Carlo results fall clearly *below* the zero-mode result and nearly coincide with it for $L = 12$. This coincidence can be understood from a closer consideration of $\chi(T_c)L^{-5/2}$ *versus* L (Fig. 9): after a rapid increase from below to a value already close to the asymptotic value, this quantity flattens around $L = 12$ and then slowly approaches (not necessarily in a monotonic way) its limiting value. In the whole region shown, the CD curve *qualitatively disagrees* with the data – this disagreement clearly cannot be remedied by a different adjustment of the parameters, because a monotonic decrease (close to a $1/\sqrt{L}$ behavior) is an intrinsic feature of equations (20–23) and also occurs in the large-n limit (Eq. (24)). The deviation at $L = 22$ cannot be explained from a mis-adjustment of ℓ_0, since both curves approach the same limiting value for $L \to \infty$, where all finite-size corrections must vanish. Thus, if ℓ_0 would have been chosen such that the CD curve coincides with the Monte-Carlo result for $L = 22$, a mismatch would have occurred at $L \to \infty$, which is clearly impossible.

Of course, discrepancies between finite-size data for very small linear dimensions (such as $L = 4$ and $L = 8$) and the CD theory (Eqs. (21–23)), which only fully captures the leading zero-mode result and the first correction terms (of order $L^{-1/2}$) to it, would not be an argument against the usefulness of the theory. However, Figures 6 and 9 clearly reveal that even for $L = 22$ one is still far from the regime where the CD theory satisfactorily describes the MC data.

4 Concluding remarks

In this paper Monte-Carlo results for five-dimensional Ising lattices have been reanalyzed and compared to recent theoretical predictions obtained by Chen and Dohm, in an attempt to clarify a somewhat controversial discussion. Our results can be summarized as follows.

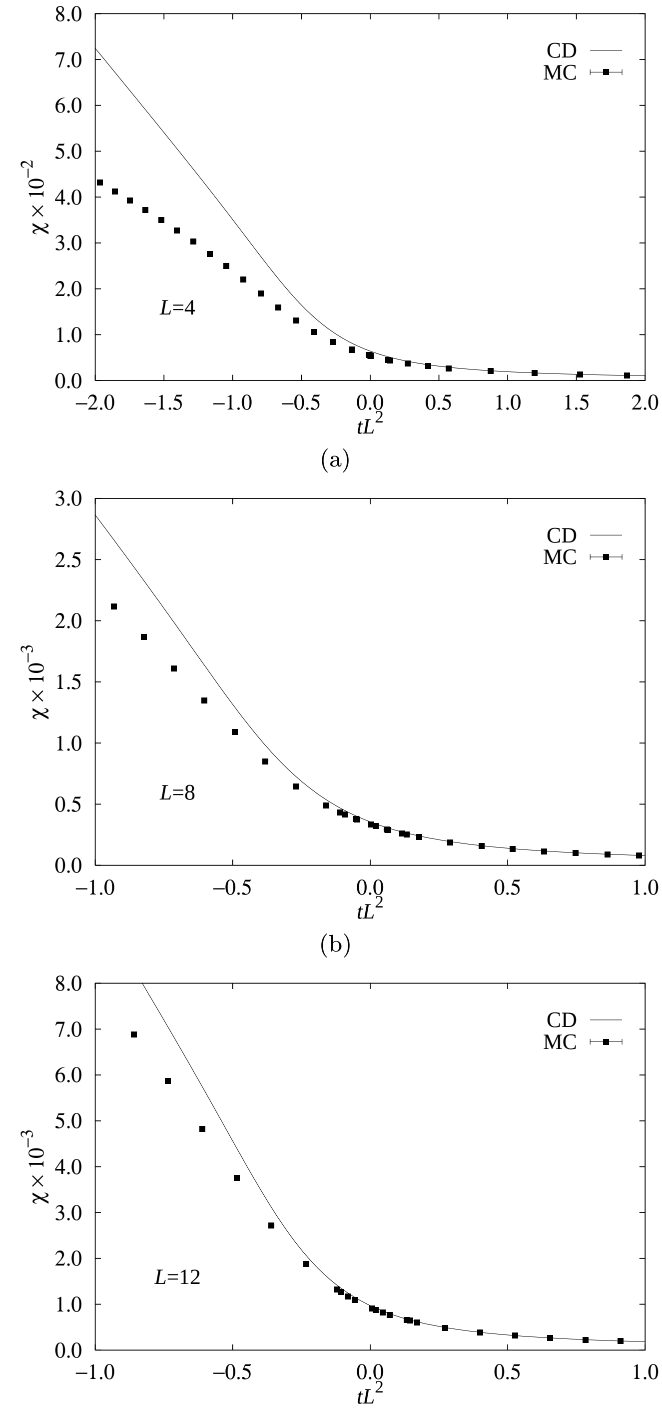

Fig. 7. Plot of χ *versus* tL^2 for (a) $L = 4$, (b) $L = 8$ and (c) $L = 12$. The full curves denote the predictions of reference [31], equation (21), while the squares are Monte-Carlo data of references [8,41,42].

(i) The CD theory reduces in the limit $t \to 0$, $L \to \infty$, $tL^{d/2}$ fixed, to the scaling structure proposed originally by Binder *et al.* [1] and explicitly illustrates the mechanism of multiplicative "renormalization" of variables by a dangerous irrelevant variable. In addition, it yields both the

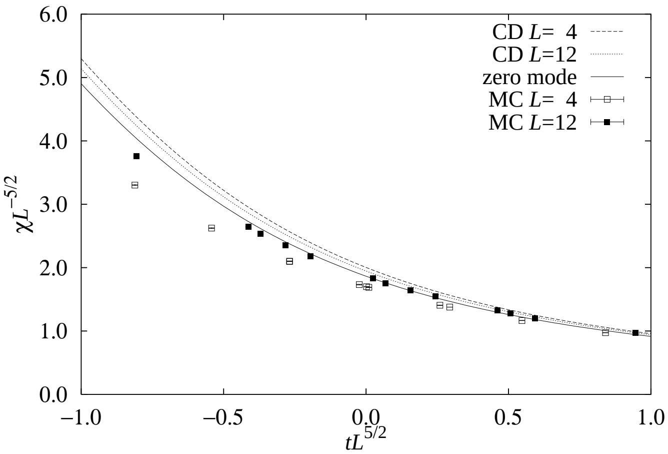

Fig. 8. Plot of $\chi L^{-5/2}$ *versus* $tL^{5/2}$ including Monte-Carlo data for $L = 4$ and $L = 12$. Broken curves show corresponding CD predictions, full curve is the zero-mode result.

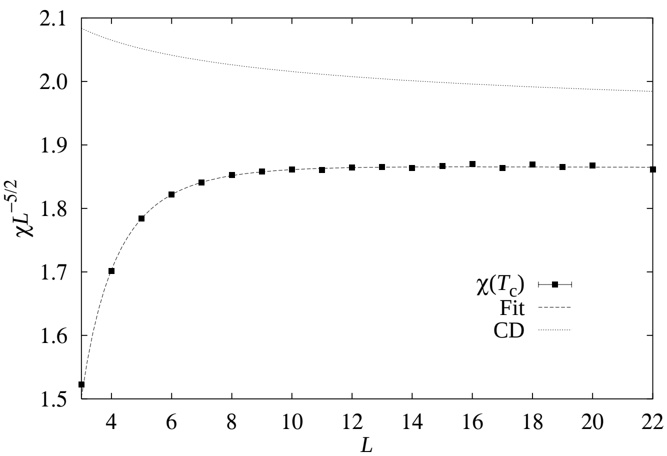

Fig. 9. Plot of $\chi(T_c)L^{-5/2}$ *versus* L (where $J/k_B T_c = 0.113\,9150$). The dashed curve is a fit to equation (32) as described in the text. The dotted curve is the CD result (21).

asymptotic scaling functions of various moments of the order parameter distribution as a function of the variable $tL^{d/2}$ and the leading corrections to it, which are of order $L^{(4-d)/2}$. However, the comparison with the Monte-Carlo data indicates that strong subleading corrections (of order $1/L$ for $d = 5$) are present as well, which are not predicted by the CD theory, and one would need much larger L than accessible here ($L_{\max} = 22$) in order that these subleading corrections are visible. So a quantitative agreement between theory and simulation is still far out of reach!

(ii) The question must be asked to what extent the ϕ^4 model on a lattice for $d > 4$ yields the same behavior as the Ising model. Of course, one can take the parameters $r_0 \to -\infty$, $u_0 \to \infty$ in equation (17) in such a proportion that the model precisely reduces to the Ising model (for a discussion see, *e.g.*, Ref. [47]). At this point, we have not attempted to deal with this problem.

(iii) The CD theory yields a nice illustrative example how one can be misled by apparent cumulant intersections which converge to the exact result extremely slowly as $L \to \infty$. It is rather likely that this is the reason for the difficulties noted in the Monte-Carlo studies in references [1–3]. Both the CD theory and the simulations give clear evidence that for a full understanding of the problem a variation of parameters over a broad range is desirable, including the behavior both above and below T_c, as well as at T_c. Corrections to the leading scaling behavior need careful consideration, which was already one of the central messages of references [6,8,27].

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