Finite-size scaling of the correlation length above the upper critical dimension in the five-dimensional Ising model

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We show numerically that correlation length at the critical point in the five-dimensional Ising model varies with system size L as $L^{5/4}$, rather than proportional to L, as in standard finite-size scaling (FSS) theory. Our results confirm a hypothesis that FSS expressions in dimension d greater than the upper critical dimension of 4 should have L replaced by $L^{d/4}$ for cubic samples with periodic boundary conditions. We also investigate numerically the logarithmic corrections to FSS in $d=4$.

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I. INTRODUCTION

Finite-size scaling[1,2] (FSS) has been extremely useful in extrapolating numerical results on finite systems in the vicinity of a critical point to the thermodynamic limit, in order to get information on critical singularities. The basic hypothesis of FSS is that the linear size of the system L enters in the ratio L/ξ_∞ where ξ_∞ is the correlation length of the infinite system (which we will call the "bulk" correlation length for convenience) and which diverges as the critical temperature T_c is approached as

$$\xi_\infty \approx c_0 t^{-\nu}, \tag{1}$$

where

$$t \equiv \frac{T-T_c}{T_c} \tag{2}$$

measures the deviation from criticality. Here c_0 is a *nonuniversal* "metric factor"[3] and we use the symbol $\approx$ to signify "asymptotically equal to." Hence, if a quantity X diverges in the bulk as $t^{-y_x \nu}$, the FSS form for the behavior of X is

$$\frac{X}{X_0} \approx L^{y_x} P^{\pm}\left(\frac{L}{\xi_\infty}\right) \approx L^{y_x}\widetilde{X}(c_1 L^{1/\nu} t), \tag{3}$$

where X_0 and c_1 are nonuniversal scale factors, and $\pm$ refers to $t \gtrless 0$. The scaling functions $P^{\pm}$ and $\widetilde{X}$ are *universal*.[3] In the last expression in Eq. (3), we have taken the argument of the function $P^{\pm}$ in the first expression to the power $1/\nu$, in order that temperature appears linearly. This has the advantage that a *single* smooth function $\widetilde{X}$, applies *both* above and below T_c, whereas *two* functions $P^{\pm}$ are needed in the first expression in Eq. (3).

It is often convenient to consider *dimensionless* quantities, because these are expected to have $y_x=0$. Two commonly studied examples are (i) the "Binder ratio"[4]

$$g \equiv \frac{1}{2}\left(3 - \frac{\langle m^4\rangle}{\langle m^2\rangle^2}\right) \approx W^{\pm}\left(\frac{L}{\xi_\infty}\right) \approx \widetilde{g}(c_1 L^{1/\nu} t), \tag{4}$$

where m is the order parameter, and (ii) the ratio of the correlation length *of the finite system* ξ_L to the system size[3,5,6]

$$\frac{\xi_L}{L} \approx U^{\pm}\left(\frac{L}{\xi_\infty}\right) \approx \widetilde{\xi}(c_1 L^{1/\nu} t). \tag{5}$$

The definition of ξ_L is not unique (though any reasonable definition will give the same scaling form). We shall give one definition, which is often used in numerical work, in the next section. Again, the scaling functions, $W^{\pm}$, $\widetilde{g}$, $U^{\pm}$ and $\widetilde{\xi}$, are universal.

Note from Eqs. (4) and (5) that, for dimensionless quantities like g and ξ_L/L, data for different sizes *intersect at the critical temperature*. Hence, dimensionless quantities are very convenient because they locate the critical temperature in a simple way, from the crossing point, without needing to know the values of other quantities such as exponents. Furthermore, since the scaling functions $\widetilde{g}(x)$ and $\widetilde{\xi}(x)$ are *universal* the values of g and ξ_L/L at the crossing point (i.e., at T_c) are also universal.

Finite size scaling, as represented here by Eqs. (3)–(5), is expected to be valid in the limit $L\to\infty$, $t\to 0$, with $L^{1/\nu}t$ arbitrary. Originally proposed on phenomenological grounds, a justification for FSS was later provided by Brézin[7] using renormalization group (RG) arguments, at least for the case of systems without disorder (which is the only case we discuss here). However, Brézin[7] also noted that FSS breaks down at the "upper critical dimension"[8] $d_u=4$. One can understand this intuitively since, for $d>d_u$ critical exponents are given by d-independent mean field values, e.g., $\nu=1/2$, and the corresponding field theory is a free theory (i.e., the fluctuations are Gaussian) since the effective coupling constant vanishes at long length scales. This coupling constant is irrelevant in the RG sense, but singularities occur when it tends to zero, so that it cannot simply be set to its "fixed point" value of zero. Singularities arising from this dangerous irrelevant variable lead to a breakdown of scaling relations involving the dimensionality, which are known as "hyperscaling relations." An example is $d\nu=2-\alpha$, where α, the specific heat exponent, is equal to 0 for $d>4$. Standard FSS implies hyperscaling, so that violation of hyperscaling means that there must also be a breakdown of the standard FSS expressions in Eqs. (3)–(5) for $d>4$.

Nonetheless, since the bulk behavior for $d>4$ is trivial, one might imagine that, in this limit, the size dependence can be also be expressed in fairly simple way and this turns out to be the case. A natural hypothesis[9,10] for cubic samples with periodic boundary conditions is that, for $d>4$, FSS formulae can still be applied but with the system size L replaced by a *larger* length[11]

$$\ell = A_1 L^{d/4}, \tag{6}$$

where A_1 is nonuniversal.

This hypothesis makes FSS consistent with mean field exponents (which are independent of d and violate hyperscaling) for $d>4$. We shall see that physically ℓ is *the correlation length at the critical point*. With this replacement, Eqs. (3)–(5) become (remember $d>4$ here)

$$\frac{X}{X_0} \approx \ell^{y_x} P^{\pm}\left(\frac{\ell}{\xi_\infty}\right) \approx L^{dy_x/4}\widetilde{X}(c_2 L^{d/2} t), \tag{7}$$

$$g \approx W^{\pm}\left(\frac{\ell}{\xi_\infty}\right) \approx \widetilde{g}(c_2 L^{d/2} t), \tag{8}$$

$$\frac{\xi_L}{l} \approx U^{\pm}\left(\frac{\ell}{\xi_\infty}\right), \quad \text{i.e.,} \quad \frac{\xi_L}{L^{d/4}} \approx A_1 \widetilde{\xi}(c_2 L^{d/2} t), \tag{9}$$

with c_2 nonuniversal, where we have noted that $\nu=1/2$ for $d>4$. As before, the scaling functions are universal, so that the value of g at the crossing point at T_c is universal. Furthermore, this universal value has been calculated.[7,12] We see that, at criticality, ξ_L is of order $L^{d/4}$, which is much greater than L for large sizes, a result which, at first, seems surprising. The value of $\xi_L/L^{d/4}$ at criticality, however, is *nonuniversal* because of the factor of A_1 in Eq. (9). This factor occurs because ℓ has dimensions of length, so that, for Eq. (6) to be dimensionally correct, A_1 must be proportional to $a^{1-d/4}$, where a is a microscopic length scale; e.g., the lattice spacing. Quantities involving microscopic length scales are not universal, so that A_1 is not universal.

There has been extensive discussion[13–18] as to whether Eq. (8) applies to the five-dimensional Ising model in the limits $L\to\infty$, $t\to 0$. Apparently it does,[14,18] although there appear to be several corrections to FSS that conspire to give a "crossing" for small sizes at a value of g that differs from the calculated universal[12] value.

As noted above, a surprising feature of Eq. (9) is that the correlation length of the finite system at the critical point is greater than the system size. To our knowledge there does not appear to have been any direct verification of this prediction for $d>4$ by numerical simulations. In this paper, we confirm the prediction in Eq. (9) by Monte Carlo simulations on the five-dimensional Ising model. We also carry out similar simulations for the four-dimensional Ising model, for which logarithmic corrections to standard FSS are expected.[7]

In Sec. II we describe the model and some aspects of the simulations. The results in five dimensions are presented in Sec. III, and the results in four dimension are presented in Sec. IV. We summarize our results in Sec. V.

II. THE MODEL

The Hamiltonian is given by

$$\mathcal{H} = -J\sum_{\langle i,j\rangle} S_i S_j, \tag{10}$$

where the Ising spins take values $S_i=\pm 1$, and the sites i are on a hypercubic lattice in d dimensions of size $N=L^d$. We take $d=4$ and 5, and apply periodic boundary conditions. The sum is over nearest neighbor pairs of sites, and from now on we set $J=1$.

The magnetization per spin is given by

$$m = \frac{1}{N}\sum_{i=1}^{N} S_i, \tag{11}$$

and the Binder ratio is then given in terms of moments of m by Eq. (4). The correlation length of the finite system, is given by the following finite difference expression:[6]

$$\xi_L = \frac{1}{2\sin(k_{\min}/2)}\sqrt{\frac{C(\mathbf{k}_{\min})}{C(0)} - 1}, \tag{12}$$

where

$$C(\mathbf{k}) = \frac{1}{N}\sum_{i,j}\langle S_i S_j\rangle \exp[i\mathbf{k}\cdot(\mathbf{R}_i - \mathbf{R}_j)] \tag{13}$$

is the Fourier transform of the spin-spin correlation function, and $\mathbf{k}_{\min}=(2\pi/L)(1,0,0)$ is the smallest nonzero wave vector on the lattice. Above T_c and for $L\to\infty$, Eq. (12) gives the usual second moment definition of the correlation length.

We perform Monte Carlo simulations using the Wolff[19] cluster algorithm to reduce the effects of critical slowing down.

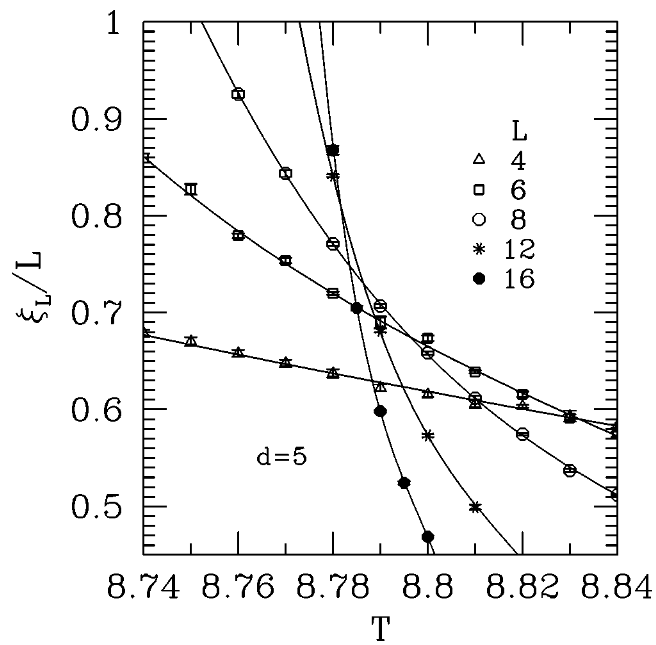

FIG. 1. Data for ξ_L/L in $d=5$. Clearly the data do not intersect at a common point, as would be expected if the conventional FSS expression [Eq. (5)] applied.

III. RESULTS IN FIVE DIMENSIONS

Data for ξ_L/L are shown in Fig. 1 for sizes $4\leqslant L\leqslant 16$.

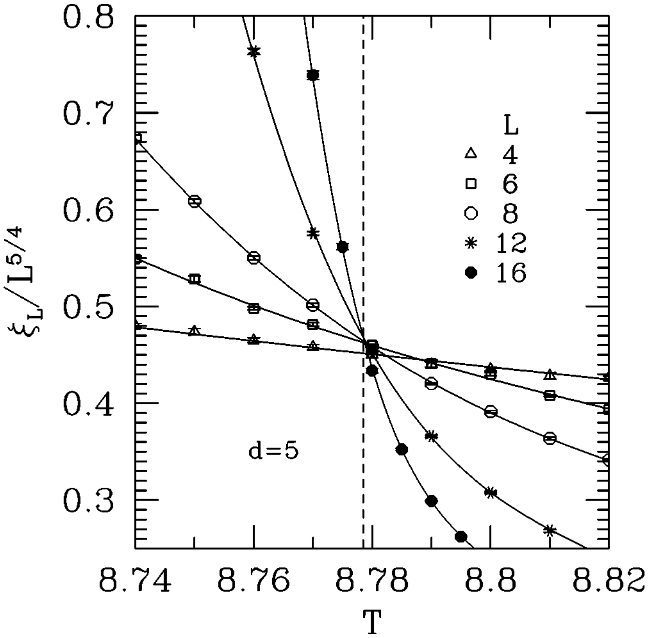

FIG. 2. Data for $\xi_L/L^{5/4}$ in $d=5$. Clearly the data intersect close to a common point, as expected for the modified FSS expression in Eq. (9). The vertical line is at $T=8.7785$, which is our best estimate for T_c.

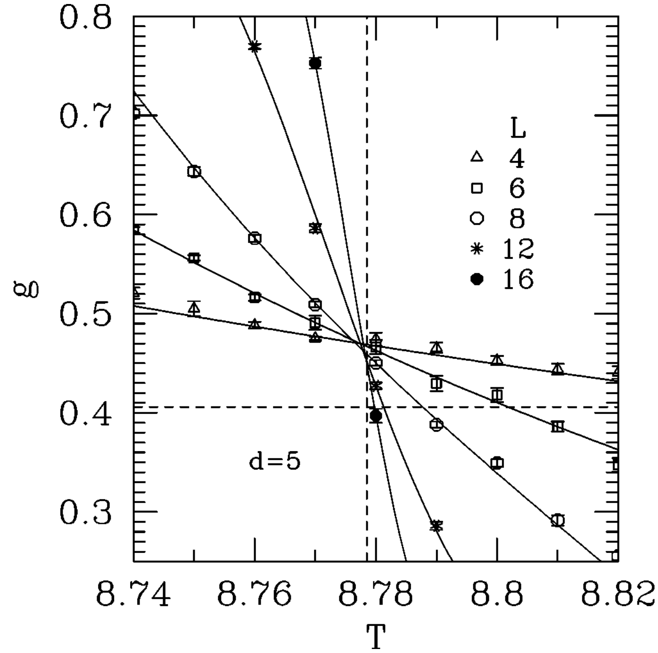

FIG. 4. Data for the Binder ratio in $d=5$. The vertical dashed line corresponds to $T=8.7785$, which is our best estimate of T_c from the correlation length data, see Fig. 3. The horizontal dashed line corresponds to $g=0.4058\ldots$, the predicted (see Refs. 7 and 12) universal value.

According to standard FSS [Eq. (5)], the data would intersect at a common point, which is clearly not the case. However, according to the modified FSS expression in Eq. (9), data for $\xi_L/L^{5/4}$ should intersect at a common point, and Fig. 2 shows that this works reasonably well. Figure 2 therefore provides convincing evidence that the correlation length at the critical point varies as $L^{5/4}$ in five dimensions, rather than being proportional to L, as would be expected in standard FSS.

A scaling plot of the data in Fig. 2 according to the second expression in Eq. (9) is shown in Fig. 3. Note that in addition to the vertical axis being scaled by $L^{5/4}$, rather than L as in standard FSS, $T-T_c$ is scaled by $L^{5/2}$, rather than $L^{1/\nu}(=L^2)$ as

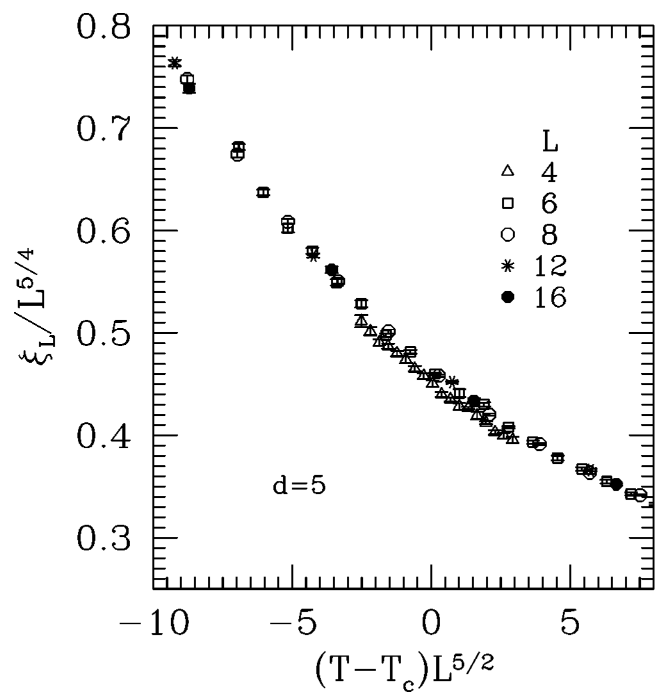

FIG. 3. A scaling plot for the data in Fig. 2 according to the second expression in Eq. (9) with $T_c=8.7785$.

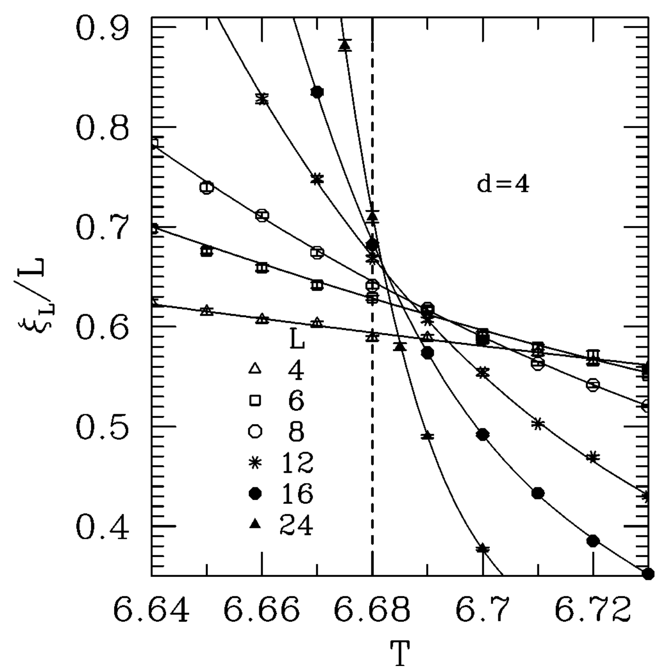

FIG. 5. Data for ξ_L/L in $d=4$. According to conventional FSS [Eq. (5)], the data should have a common intersection. This is clearly not the case.

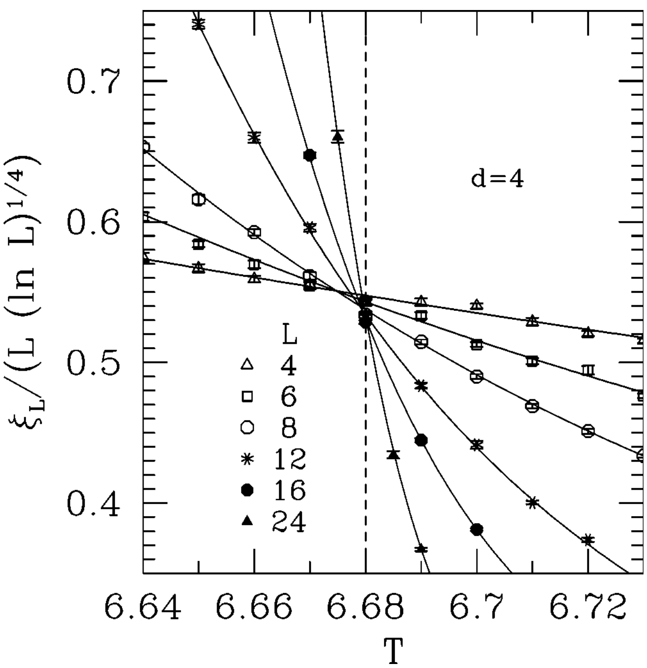

FIG. 6. Data for $\xi_L/L(\ln L)^{1/4}$ in $d=4$. The data intersect at close to a common point.

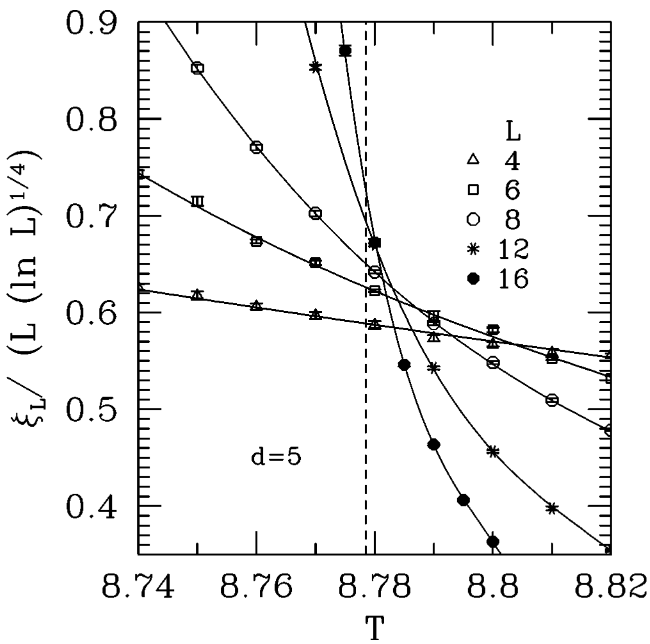

FIG. 7. Data for $\xi_L/L(\ln L)^{1/4}$ in $d=5$. Clearly the data do not intersect at a commont point, indicating that the assumption of logarithmic corrections to FSS does not work in $d=5$, although it is correct at $d=4$ (see Fig. 6).

in standard FSS. Apart from $L=4$, for which the data are consistently too low presumably because of corrections to FSS, the data scale well with $T_c=8.7785$. By considering different choices for T_c we estimate that $T_c=8.7785(5)$, consistent with the more accurate result 8.778 44(2) in Ref. 18.

For completeness, we also show results for the Binder ratio in Fig. 4. As found in other work,[13,15–18] the data for small sizes intersect at a value of g larger than the predicted[7,12] universal value of 0.4058… . The data for larger sizes have intersections at somewhat smaller values and presumably[18] would reach the universal value for $L\rightarrow\infty$.

IV. RESULTS IN FOUR DIMENSIONS

In four dimensions, Brézin[7] argued that $\xi_L \propto L(\log L)^{1/4}$ at criticality, so that we expect that FSS expressions should be modified by the replacement

$$L \rightarrow \ell = A_2 L(\ln L)^{1/4}, \quad (d=4). \tag{14}$$

In Fig. 5, we show a plot for ξ_L/L (i.e., without the logarithmic factor). Clearly the data do not show a common intersection. However, including the logarithmic factor, the plot in Fig. 6 shows a good intersection with only small corrections to FSS. The factor $\ln L$ can be replaced by $\ln(L/L_0)$ where L_0 is a microscopic scale, and with an appropriate choice of L_0 we get sharper intersections. However, $\ln(L/L_0)=(\ln L)(1+\ln L_0/\ln L)$, so that including L_0 corresponds to an *additive* correction to FSS (which vanishes only logarithmically). It is difficult to separate this from other corrections to FSS, and so we do not feel we can give a reliable estimate for L_0.

We also consider the possibility that logarithmic corrections to FSS might also apply in $d=5$, rather than the power law correction in Eq. (6). However, the data for $\xi_L/L(\ln L)^{1/4}$ in Fig. 7 clearly does not show a common intersection. Similarly, we find that a plot of $\xi_L/L \ln L$ also does not show a common intersection. Hence, we feel that our data rules out logarithmic corrections to FSS in $d=5$, but supports the modification in Eq. (6).

V. CONCLUSIONS

We have demonstrated that the FSS behavior of the correlation length (for a cubic sample with periodic boundary conditions) in five dimensions follows Eq. (9), which is the expected modification of FSS for the case $d>4$. This provides confirmation that the standard FSS expressions, e.g., Eqs. (3)–(5), can be simply modified above $d=4$ by the replacement[11] $L\rightarrow \ell \propto L^{d/4}$, which gives Eqs. (7)–(9). This had been verified before for the Binder ratio, but not, to our knowledge, for the correlation length. It is interesting that the correlation length at the critical point is of order ℓ and hence much bigger than the system size L. This is possible because the long wavelength fluctuations are non-interacting near criticality for $d>4$. We also demonstrated the expected logarithmic modification to FSS of the correlation length for d precisely equal to 4.

It is also interesting to ask what are the corresponding results with $d>4$ for other geometries and boundary conditions. For the "strip" geometry, where the sample is infinite in one direction and of size L in the others, Brézin[7] showed that the correlation length at the critical point varies as $L^{(d-1)/3}$ (which is reasonable since FSS is done only with respect to the $d-1$ finite dimensions). It is then natural to expect that FSS will then work with L replaced throughout by $L^{(d-1)/3}$.

For free boundary conditions, it seems obvious that even for $d>4$ the behavior of the system will be affected when ξ_L becomes of order L, rather than only change when ξ_L becomes of order the much larger length ℓ. Hence we expect that the standard FSS expressions, Eqs. (3)–(5) would apply with $\nu=1/2$. The ratio ξ_∞/ℓ may also enter but, since $\ell \gg L$ for large L, such terms would presumably be corrections to the scaling terms which involve ξ_∞/L. Since FSS for models with free boundary conditions in $d>4$ is poorly understood, it would be interesting to investigate such models in some detail.

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[11] Erik Luijten (private communication) has pointed out that this prescription needs clarification in the presence of a magnetic field h. Standard FSS scaling functions then have a second argument, hL^σ, and the issue is what value to take for σ before the transformation $L\to\ell$ is made. If hyperscaling is satisfied then σ is equal to both $y_h\equiv(d+2-\eta)/2$ and $\Delta/\nu=(\beta+\gamma)/\nu$. However, if hyperscaling is not satisfied, it is the latter expression that must be taken in order to get the correct behavior of bulk thermodynamic quantities. For $d>4$, we have $(\beta+\gamma)/\nu=3$ and, with the replacement $L\to\ell$, the field enters the scaling functions in the combination $hL^{3d/4}$, in agreement with earlier work (see Refs. 13 and 14).

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