Finite-size tests of hyperscaling

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The possible form of hyperscaling violations in finite-size scaling theory is discussed. The implications for recent tests in Monte Carlo simulations of the $d=3$ Ising model are examined, and new results for the $d=5$ Ising model are presented.

Recently two extensive Monte Carlo calculations[1,2] have been carried out which test the validity of hyperscaling in the three-dimensional Ising model. In the calculation by Freedman and Baker,[1] they "observe a systematic downward trend by more than twice the statistical error for a quantity which should be constant if hyperscaling is satisfied," while Barber, Pearson, Toussaint, and Richardson[2] conclude that their results require "the anomalous dimension to be small, and are consistent with hyperscaling." The purpose of this paper is to resolve this apparent conflict by showing that these two collaborations evaluated different anomalous exponents, and that the exponent evaluated by Barber *et al.*, which they erroneously identified with Fisher's anomalous dimension,[3] actually vanishes on theoretical grounds. New Monte Carlo results are also presented for the five-dimensional Ising model which confirm the theoretical predictions for hyperscaling violation in this case.

To start, we investigate the consequence of the existence of a "dangerous irrelevant variable" on the finite-size scaling form of the free energy, and on the hyperscaling relations for critical exponents. We then show that consistency conditions require that the anomalous exponent introduced by Barber *et al.*[2] must be zero. Finally, we discuss the finite-size scaling form of the renormalized coupling constant for the Ising model,[4] and the results of a Monte Carlo simulation for the dimensionality $d=5$.

According to the renormalization-group derivations[5,6] of finite-size scaling, the singular part of the free energy f_L and the correlation length[7] ξ_L have the form

$$f_L = L^{-d} f(tL^{y_T}, hL^{y_H}, uL^{y_U}) , \quad (1)$$

$$\xi_L = L\xi(tL^{y_T}, hL^{y_H}, uL^{y_U}) , \quad (2)$$

where t is the reduced temperature $t=(T-T_c)/T_c$ (T_c is the transition temperature of the infinite system), h is the magnetic field, and u is an irrelevant variable, while $y_T>0$, $y_H>0$, and $y_U<0$ are renormalization-group exponents. We use equality signs to indicate here asymptotic scaling relations. If the free-energy scaling function $f(x,y,z)$ is singular in the limit $z\to 0$, then u is called a dangerous irrelevant variable.[3,6] For simplicity we assume here that the correlation scaling function $\xi(x,y,z)$ is regular in this limit, but later we consider the possibility that it is singular. We assume that for small z,

$$f(x,y,z) = z^{p_1}\bar{f}(xz^{p_2}, yz^{p_3}) . \quad (3)$$

The choice of this particular pattern, multiplicative singular powers of z, is motivated by the known[3] mechanism for the *bulk* scaling at $d>d_c=4$. Equation (3) implies

$$f_L = L^{-d^*} F(tL^{y_T^*}, hL^{y_H^*}) , \quad (4)$$

where scale factors have been absorbed in t and h, and $d^* = d - p_1 y_U$, $y_T^* = y_T + p_2 y_U$, and $y_H^* = y_H + p_3 y_U$ are the effective exponents. Note that the anomalous exponent introduced by Barber *et al.*[2] corresponds to $d-d^*$, while Fisher's exponent[3] ω^* is given by

$$\omega^* = d - d^*/(y_T^* \nu) . \quad (5)$$

These two exponents would be the same if $y_T^*\nu=1$, which was implicitly assumed by Barber *et al.*,[2] but has not been proven. We will show instead that $d^*=d$ for cubic or similarly shaped systems,[6] as usually employed in Monte Carlo simulations.[1,2]

The existence of the limit $L\to\infty$ of f_L corresponding to the bulk free energy f_∞ implies that for $x\to\pm\infty$ and $y\,|x|^{-\Delta}$ fixed,

$$F(x,y) = |x|^{d^*/y_T^*} Y_\pm(y\,|x|^{-\Delta}) , \quad (6)$$

where $\Delta = y_H^*/y_T^*$, and $Y_\pm$ is the scaling function for $t \gtrless 0$. Likewise the existence of the bulk correlation length ξ_∞ in this limit leads to the asymptotic form

$$\xi(x,y,0) = |x|^{-\nu} X_\pm (y|x|^{-\Delta'}) , \tag{7}$$

where

$$\nu = 1/y_T \text{ and } \Delta' = y_H/y_T , \tag{8}$$

and we assumed for simplicity that the scaling function ξ in Eq. (2) is nonsingular as $z \to 0$. Taking suitable derivatives of the free energy, one finds the following scaling relations $\alpha = 2 - d^*/y_T^*$, $\beta = d^*/y_T^* - \Delta$, and $\gamma = 2\Delta - d^*/y_T^*$, where α, β, and γ are the thermodynamic exponents for the specific heat, magnetization, and susceptibility, respectively. Consequently y_T^* and y_H^* can be written as

$$y_T^* = d^*/(\gamma + 2\beta) , \tag{9}$$

$$y_H^* = d^*(\gamma+\beta)/(\gamma+2\beta) . \tag{10}$$

Hyperscaling violations occur if y_T^* and/or Δ differ from the exponents $y_T (=1/\nu)$ and $\Delta' (= y_H/y_T)$ appearing in the scaling form of the correlation length. However, we will show that even in this case one must have $d^* = d$.

We now give three arguments which support $d^* = d$. First, consider the finite-size magnetization m_L and susceptibility χ_L:

$$m_L = \langle s \rangle_L , \tag{11}$$

$$\chi_L = L^d (\langle s^2 \rangle_L - \langle s \rangle_L^2) , \tag{12}$$

where $s = (1/L^d) \sum s_i$, s_i is the spin at the ith site, and $\langle\ \rangle_L$ denotes the thermal average. According to Eq. (4), m_L and χ_L have the scaling form

$$m_L = \frac{\partial f_L}{\partial h} = L^{y_H^* - d^*} V(tL^{y_T^*}, hL^{y_H^*}) , \tag{13}$$

$$\chi_L = \frac{\partial^2 f_L}{\partial h^2} = L^{2y_H^* - d^*} W(tL^{y_T^*}, hL^{y_H^*}) , \tag{14}$$

where the scaling functions V and W are obtained from F.

For the bulk magnetization, m_b, as well as the susceptibility, χ_b, special care must be taken in order of the limits $L \to \infty$ and $h \to 0^\pm$ below the critical temperature. Taking first the limit $L \to \infty$, and afterwards the limit $h \to 0^\pm$, one obtains the conventional bulk values,

$$m_b = a|t|^\beta \text{ and } \chi_b = b|t|^{-\gamma} \text{ as } T \to T_c^- , \tag{15}$$

so that, by Eq. (12),

$$\langle s^2 \rangle_L = m_b^2 + L^{-d}\chi_b \quad (t<0,\ L\to\infty) . \tag{16}$$

However, if we first set $h=0$ and then take the limit $L \to \infty$, then $\langle s \rangle_L \equiv 0$ but we expect (see Refs. 4 and 6 for details)

$$\lim_{L\to\infty} [\langle s^2 \rangle_{L,h=0}] = m_b^2 \tag{17}$$

[in fact, Eq. (16) applies in this limit as well[4,6]]. By Eqs. (12) and (17), the zero-field susceptibility behaves according to

$$\chi_L \propto L^d |t|^{2\beta} \text{ as } T \to T_c^- . \tag{18}$$

To obtain this result from the scaling form, Eq. (14), we must require[6]

$$\lim_{x\to\pm\infty} W(x,0) \propto |x|^{2\beta} \tag{19}$$

and

$$d^* = 2(y_H^* + \beta y_T^*) - d . \tag{20}$$

Substituting Eqs. (9) and (10) in Eq. (20), we obtain the relation

$$d^* = d , \tag{21}$$

which also implies $p_1 = 0$ in Eq. (3).

Second, we show that this condition also follows from the finite-size scaling form of f_L at the ferromagnetic phase boundary due to the existence of a discontinuity fixed point.[8] In this case the finite-size magnetization m_L below the critical temperature takes the form[6]

$$m_L = m_b \tanh(m_b h L^d) \tag{22}$$

for $L \gg \xi_b$, and $|h| \ll (m_b \xi_b)^{-1} L^{1-d}$, where ξ_b is the bulk correlation length, and m_b is the bulk magnetization, Eq. (15). Hence, χ_L is given by

$$\chi_L = L^d m_b^2 \cosh^{-2}(m_b h L^d) . \tag{23}$$

For $h=0$, χ_L reduces to Eq. (18) when $T \to T_c^-$, and therefore implies $d^* = d$, Eq. (21).

Finally, we consider the finite-size scaling properties of the zero-field probability distribution $P(s)$ of the magnetization below the critical temperature. Binder[4] has shown that for large L and s near $\pm m_b$, $P_L(s)$ can be written approximately in the form

$$P_L(s) = \frac{L^{d/2}}{2(2\pi\chi_b)^{1/2}} \left(e^{-(s-m_b)^2 L^d / 2\chi_b} + e^{-(s+m_b)^2 L^d/2\chi_b} \right) . \tag{24}$$

Hence the arguments of the exponential functions have the form

$$(s|t|^{-\beta} + a)^2 \frac{(|t| L^{y_T^*})^{\gamma+2\beta}}{2b} ,$$

which demonstrates the occurrence of the scaling combination $|t| L^{y_T^*}$ in $P_L(s)$, where $y_T^* = d/(\gamma+2\beta)$. Likewise, by including a magnetic field h, the arguments of the exponential become $(s \pm m_b - \chi_b h)^2 L^d / 2\chi_b$ and the term linear in h can be written as

$$(b|t|L^{d/(\gamma+2\beta)})^{-(\gamma+\beta)} h L^{y_H^*} .$$

This shows the dependence of $P_L(s)$ on the scaling variable $L^{y_H^*}$, where $y_H^* = d(\gamma+\beta)/(\gamma+2\beta)$. These expressions for y_T^* and y_H^* are precisely Eqs. (9) and (10), but with $d^* = d$. If we assume that no other scaling variables occur, the scaling form Eq. (4) follows, with $d^* = d$.

Next, we discuss some recent Monte Carlo calculations[1,2] which test possible hyperscaling violation in the

$d=3$ Ising model. These calculations evaluated the $h=0$ finite-size renormalized coupling g_L introduced by Binder,[4]

$$g_L=\frac{\langle s^4\rangle_L}{\langle s^2\rangle_L^2}-3=\left[\frac{\chi_L^{(4)}}{L^d\chi_L^2}\right]_{h=0}, \qquad (25)$$

where χ_L is given by Eq. (14), and

$$\chi_L^{(4)}=\frac{\partial^4 f_L}{\partial h^4}\approx L^{4y_H^*-d^*}W^{(4)}(tL^{y_T^*}) . \qquad (26)$$

Substituting Eqs. (14) and (28) in Eq. (27), we find that for $t=0$,

$$g_L=L^{d^*-d}G(tL^{y_T^*}) , \qquad (27)$$

where G is a scaling function. Since $d^*=d$, it follows that g_L is a constant (nonzero in general) at $T=T_c$.

The finite-size scaling analysis of the Monte Carlo data by Barber *et al.*[2] implies that indeed $d-d^*=0$, with an error of ± 0.04 due to the uncertainty in their determination of the critical temperature. This was interpreted by them as evidence for the validity of hyperscaling, but we have shown here that $d^*=d$ even when hyperscaling is violated.

For $t>0$ and $L\rightarrow\infty$, χ_L and $\chi_L^{(4)}$ take their bulk values $\chi_L\propto t^{-\gamma}$ and $\chi_L^{(4)}\propto t^{-\gamma-2\Delta}$ so that

$$g_L\propto(t^{d^*/y_T^*}L^d)^{-1} \quad \text{for } L\gg t^{-1/y_T^*} , \qquad (28)$$

where we have used $\gamma-2\Delta=-d^*/y_T^*$. Baker and Freedman[1] evaluated g_L for values of $t>0$ such that the correlation length $\xi_L=cL$, where c is a constant. After some algebra, this yields

$$g_L\propto L^{-\omega^*} , \qquad (29)$$

where ω^*, Eq. (5), is Fisher's anomalous dimension,[3] and is positive. For lattices of dimensions $L=3$ to 60 they find $\omega^*\simeq 0.2$. Note, however, that their result depends on the assumption, Eq. (6), that the scaling function ξ in Eq. (2) is not singular as $uL^{y_U}\rightarrow 0$.

We now briefly turn our attention to the possibility that $\xi(x,y,z)$ is singular in the limit $z\rightarrow 0$. In analogy with Eq. (3) we assume that

$$\xi(x,y,z)=z^{q_1}\overline{\xi}(xz^{q_2},yz^{q_3}) , \qquad (30)$$

which implies

$$\xi_L\sim L^{1+q_1y_U}Z(tL^{y_T^{**}},hL^{y_H^{**}}) , \qquad (31)$$

where $y_T^{**}=y_T+q_2y_U$ and $y_H^{**}=y_H+q_3y_U$. Likewise in the limit $x\rightarrow\pm\infty$ and $y\,|x|^{-\Delta^{**}}$ fixed,

$$Z(x,y)\rightarrow|x|^{-\nu}\widetilde{Z}_\pm(y\,|x|^{-\Delta^{**}}) , \qquad (32)$$

where $\nu=(1+q_1y_U)/y_T^{**}$ and $\Delta^{**}=y_H^{**}/y_T^{**}$. Since the finite-size correlation length ξ_L is bounded by L, we require $q_1y_U\le 0$. Even if one adopts a plausible assumption that for $t=h=0$, the correlation length increases up to the linear dimensions of the lattice, which implies that $q_1=0$ and $\nu=1/y_T^{**}$, y_T^{**} need not be equal to y_T leading to a new possible source for hyperscaling violation.

Finally, we comment on the effect of boundary conditions on our analysis. The predictions presented here are unchanged in the thermodynamic limit ($L\rightarrow\infty$) if the reduced temperature t in Eq. (4) is replaced by a "shifted" variable t_L, where

$$t_L=[T-T_c(L)]/T_c , \qquad (33)$$

in which $T_c(L)$ is a "pseudo T_c" for the finite system. This could, for example, be defined as the temperature where the probability distribution of the magnetization starts to develop a two-peak structure. One then defines a shift exponent ψ by

$$[T_c(L)-T_c]/T_c=AL^{-1/\psi} , \qquad (34)$$

where A is a constant. For systems with a surface it is expected that $\psi=\nu$, because properties of the finite system should differ from their bulk values when ξ_L approaches the system size. In this case the shift in T_c is greater than the range of the finite-size rounding if hyperscaling is violated, because $y_T^*>\frac{1}{2}$. However, we shall argue below that $\psi=1/y_T^*$ for periodic boundary conditions.

A well-known example which violates hyperscaling is the Ising model (more generally the n-component vector model) for $d>4$, where critical exponents stick at their mean field values. It is straightforward to show[6] that the free energy of a finite system scales as in Eq. (4) with $y_T^*=d/2$, $y_H^*=d/4$ compared with $y_T=1/\nu=2$, and $y_H=(d+2)/2$. However, these[6] renormalization-group arguments do not give information on the size of the shift in T_c, for which an explicit calculation must be performed. This is possible for the n-component model with periodic boundary conditions in the limit $n\rightarrow\infty$. By a straightforward extension of the work of Brézin[9] one can evaluate the scaling function $W(x,0)$ for the susceptibility, and see that the scaling form of Eq. (4) is valid, so the coefficient of the $L^{-1/\nu}$ term in Eq. (34) must vanish for this model. We observe that this is a general result for periodic boundary conditions *provided that* $tL^{y_T^*}$ *is the only temperature variable which enters thermodynamic scaling*, and then $\psi=1/y_T^*$ follows by a standard argument.[10]

We have tested our claim that $d^*=d$ by Monte Carlo simulations on the five-dimensional Ising model on a cubic lattice with nearest-neighbor interaction, J, for sizes between $L=3$ and 7. Figure 1 shows that the data for g_L intersect at $T/J\simeq 8.77$, $g_L\simeq -1.00$. A nonzero value of g_L is just what is expected from Eq. (27) with $d^*=d$. Furthermore, the temperature agrees precisely with the estimate of T_c from high-temperature series by Fisher and Gaunt.[11] In Fig. 2 we show that the data scale well with the predicted exponent $y_T^*=\frac{5}{2}$ instead of $y_T=1/\nu=2$. It is possible to evaluate the scaling function $G(x)$ in Eq. (27) exactly for $d>4$ because, in the critical region, the probability distribution for the magnetization per spin s has the mean-field form

$$P_L(s)\propto\exp[-L^d(ct_Ls^2+us^4)] , \qquad (35)$$

where c and u are constants. By the substitution $\phi=(uL^d)^{1/4}s$, one finds that

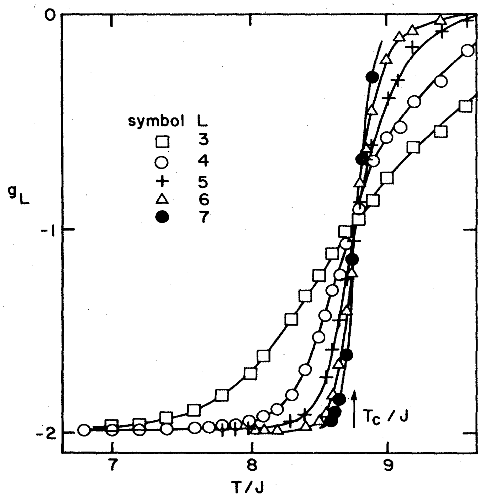

FIG. 1. Monte Carlo results for g_L as a function of T/J for sizes $L=3$ to 7, where 16 000 iterations per spin have been performed for each data point. The arrow marks the value $T_c/J=8.77$ from Ref. 11.

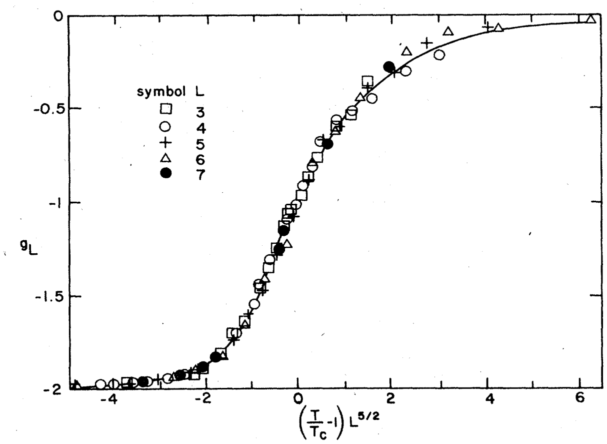

FIG. 2. The data for g_L shown in Fig. 1 plotted vs the scaling variable $(T/T_c-1)L^{5/2}$, where $T_c=8.77J$. The solid line is obtained from the mean-field form of the free energy, as described in the text.

$$G(x)=\frac{\langle\phi^4\rangle}{\langle\phi^2\rangle^2}-3\ , \tag{36}$$

where the averages are obtained by integrating ϕ from $-\infty$ to $+\infty$ with the weight

$$P_L(\phi)\propto\exp[-a(x-b)\phi^2-\phi^4]\ , \tag{37}$$

where $a=c/u^{1/2}$ and $ab=A$ is the coefficient of the shift relation, Eq. (34) (with $\psi^{-1}=y_T^*=d/2$). The solid curve in Fig. 2 is obtained from Eqs. (36) and (37) with $b=0.37$, $a=0.56$, and fits the data very well.

To conclude, we propose that the free energy of a finite system with periodic boundary conditions scales as in Eq. (4) with y_T^* and y_H^* given by Eqs. (9) and (10) and $d^*=d$. For other boundary conditions, where the system has a surface, it is probably necessary to use both $tL^{y_T^*}$ and $tL^{1/\nu}$ for a complete asymptotic description. When hyperscaling is violated it is not possible to determine the correlation length exponent ν from the free energy, and its derivatives, and it is necessary to carry out a *separate* calculation, using either renormalization-group techniques or explicitly looking at the spatial dependence of the correlations.

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[7]For a finite system of linear dimension L some care must be taken in the definition of the correlation length, particularly for temperatures T below the critical temperature T_c. For periodic boundary conditions we adopt the relation

$$2d\xi_L^2=\sum_{i,j}(\vec{r}_i-\vec{r}_j)^2(\langle s_is_j\rangle-c_L)\Big/\sum_{i,j}(\langle s_is_j\rangle-c_L)\ ,$$

where $\vec{r}_i$ is the position of lattice site i,

$$c_L=\frac{1}{L^d}\sum_i\langle s_is_{i'}\rangle\ ,$$

and i' is the site with $\vec{r}_{i'}=\vec{r}_i+\frac{1}{2}\ (1,1,\ldots,1)L$. Note that for $L\to\infty$, $c_L\to m_b^2$, where m_b is the bulk magnetization, so

$\xi_L^2 \rightarrow \xi_b^2$, the square of the bulk correlation length, defined as the second moment of the connected correlation function $\langle s_i s_j \rangle - \langle s_i \rangle \langle s_j \rangle$.

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