What is the Dimension from Scaling of Finite Systems?

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(Received 10 August 1992)

Finite-size scaling allows the extraction of a dimension from scaling d_s, as well as critical exponents for systems with a second-order phase transition. The calculation of d_s allows comparisons to be made with other expansions in dimension, in which d_s plays the role of the physical dimension. This is demonstrated by a numerical transfer-matrix study of the pure ferromagnetic Ising model in two and three dimensions, as well as for quenched random bonds in the two-dimensional Ising ferromagnet.

PACS numbers: 05.50.+q, 05.70.Jk, 64.60.Fr, 75.10.Hk

Numerical studies of critical phenomena must be performed using Monte Carlo methods on finite lattices [1], or on systems which are infinite in one dimension by the numerical transfer-matrix method [2]. However, in both cases the systems which can be studied do not have any critical behavior, since phase transitions in short-ranged models can occur only in the limit where at least two dimensions are taken to infinity. Nevertheless, the infinite-lattice behavior of phase transitions can be obtained by studying the finite-size scaling (FSS) behavior of systems amenable to computer simulations [3–5].

Another useful methodology in the study of phase transitions are expansions in dimension. For the short-ranged Ising model there are Wilson-Fisher expansions about the upper critical dimension (expansions in $d=4-\epsilon$) [6, 7] as well as asymptotic expansions about the lower critical dimension (expansions in $d=1+\epsilon$) [8–12].

It has been the accepted belief that FSS of model systems could only be compared with expansions in dimension at the physical dimension. The only exception to this was the study of fractal lattices [13] (where it has been shown that the fractal dimension is the physical dimension only in the limit in which the fractal becomes translationally invariant [14]) and in a recent interpolation procedure [15]. In this Letter we show that the calculation of a dimension from scaling d_s for finite systems enables one to make contact with dimensional expansions. In particular, we postulate that with the use of nonperiodic boundary conditions it is possible to vary d_s, and that d_s plays the role of the physical dimension d of the system. Although in the limit of large systems $d_s \rightarrow d$, it is possible to use d_s to obtain results for critical exponents *near* the physical dimension d. We will demonstrate this approach through a numerical transfer matrix study of the ferromagnetic Ising model on square and simple-cubic lattices. However, for reasons sketched below it is anticipated that similar application of FSS to compare with dimensional expansions should be valid for other models.

The Ising model studied consists of spins $s=\pm 1$ located at the sites of a hypercubic lattice. The isotropic ferromagnetic nearest-neighbor coupling constant is J and the magnetic field is H. The partition function for a lattice with N spins in each $d-1$ dimensional layer and M layers is given in the normal fashion by [2, 16, 17] $Z = \mathrm{Tr}((\underline{D}_H\, \underline{D}_{d-1}\, \underline{A})^M)$. Periodic boundary conditions have been imposed in the transfer direction. The $2^N \times 2^N$ matrix $\underline{A}$ is a direct (Kronecker) product of N identical 2×2 matrices with elements $\langle s_i|\underline{a}|s_j\rangle = \exp(Js_is_j/k_BT)$, where k_B is Boltzmann's constant and T is the temperature. The matrix $\underline{A}$ contains interactions between spins in adjoining layers. The other two $2^N \times 2^N$ matrices can be chosen to be diagonal. The matrix $\underline{D}_H$ contains interactions of the spins with a magnetic field, and is the direct product of N 2×2 diagonal matrices $\underline{h}$ with elements $\langle s_i|\underline{h}|s_i\rangle = \exp(Hs_i/k_BT)$. The matrix $\underline{D}_{d-1}$ contains all interactions between the spins within a given $d-1$ dimensional layer. The elements of this matrix depend on the dimension of the lattice within the layer as well as the boundary conditions imposed in this layer. We will use boundary conditions in which the bonds at the boundary have strength gJ. Hence $g=1$ yields periodic boundary conditions, $g=0$ free boundary conditions, and $g=-1$ antiperiodic boundary conditions. For $d=2$ the lattice is $L\times M$ with $N=L$ and there is only one bond per layer with a strength gJ. For $d=3$ the lattice is $L\times L\times M$ so $N=L^2$ and each layer has $2L$ bonds with strength gJ.

In the limit $M\rightarrow\infty$ the longitudinal correlation length is given by $\xi = 1/\ln|\lambda_0/\lambda_1|$, where λ_0 (λ_1) is the largest (next-largest) eigenvalue of the transfer matrix. Near the critical temperature T_c, the correlation length diverges as $\xi \approx t^{-\nu}$ with reduced temperature $t = |(T-T_c)/T_c|$ and $y_T = 1/\nu$. The FSS expression for ξ is given by [2–4]

$$\xi(T,H,N) = N^{1/(d_s-1)}\, \mathcal{F}\big(tN^{y_T/(d_s-1)}, HN^{y_H/(d_s-1)}\big). \tag{1}$$

This would be traditional FSS if one set $d_s = d$, where d is the dimension of the underlying lattice. However, we will determine d_s by FSS. In order to do this, define

$$\Omega_{ij}(T) = \ln\big[\xi(T,N_i)/\xi(T,N_j)\big]/\ln(N_i/N_j). \tag{2}$$

If T_c were known exactly, $\Omega_{ij}(T_c)$ could be viewed as a finite-size estimate for $1/(d_s-1)$. By using three lattice sizes and locating the finite temperature minimum of

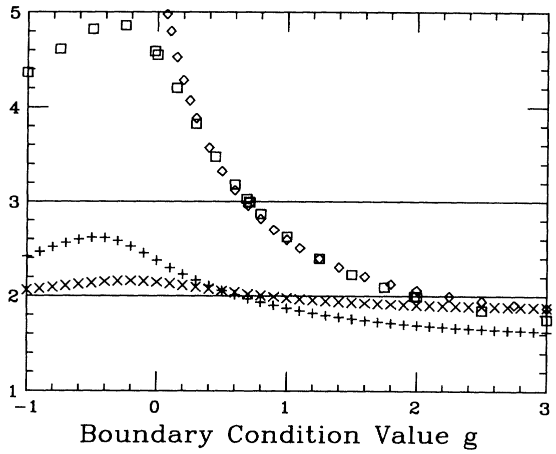

FIG. 1. The dimension from scaling d_s as a function of the strength of the bonds on the boundary. For the $d = 2$ Ising ferromagnet three $L\times\infty$ lattices of size L, $L+1$, and $L+2$ were used with $L = 4$ (+) and 10 (×). For the $d = 3$ Ising ferromagnet $L\times L\times\infty$ lattices were used with the three sizes L, $L+1$, and $L+2$ with $L = 2$ (◇) and 3 (□).

$$R^2 = (\Omega_{12} - \Omega_{13})^2 + (\Omega_{12} - \Omega_{23})^2 + (\Omega_{13} - \Omega_{23})^2, \quad (3)$$

it is possible to obtain finite-size estimates for both T_c and $1/(d_s–1)$. This possibility was mentioned in Ref. [18], but has not been further investigated.

In Fig. 1 d_s obtained from FSS of numerical transfer matrix data is shown for the $d = 2$ and $d = 3$ Ising ferromagnetic as a function of the boundary strength g. Since the bulk critical exponents do not depend on g, as N increases d_s approaches d for a wider range of g values. However, we see that for moderate L in $d = 2$ the range of d_s is rather large for moderate values of g. In $d = 3$ the exact diagonalization must be performed on matrices of size 2^{L^2} which at present allows only four attainable lattice sizes with $L \leq 5$. (For $L = 5$ this required the calculation of the two largest eigenvalues of a nonsparse real symmetric matrix with vectors of size 3.4×10^7. This was done through a program written in FORTRAN/PARIS on a Thinking Machines Corporation CM-2 with 2^{16} one-bit processors and 2 Gbytes of main computer memory.) Figure 1 shows that for the simple-cubic lattice the accessible range of lattice sizes gives d_s values which extend over a wide range.

The critical exponents can now be obtained in the usual fashion [2]. Differentiating Eq. (1) with respect to T and evaluating it at $H = 0$ and the finite-size estimate for T_c gives

$$\frac{y_T + 1}{d_s - 1} = \ln\left[\frac{\partial\xi(T,N_i)/\partial T}{\partial\xi(T,N_j)/\partial T}\right] \Big/ \ln(N_i/N_j). \quad (4)$$

Dividing Eq. (4) by $1/(d_s - 1)$ gives an estimate for y_T.

In Fig. 2 the critical exponent y_T obtained from Eq. (4) is plotted for the square lattice [Fig. 2(a)] and the simple-cubic lattice [Fig. 2(b)] as a function of d_s. Also

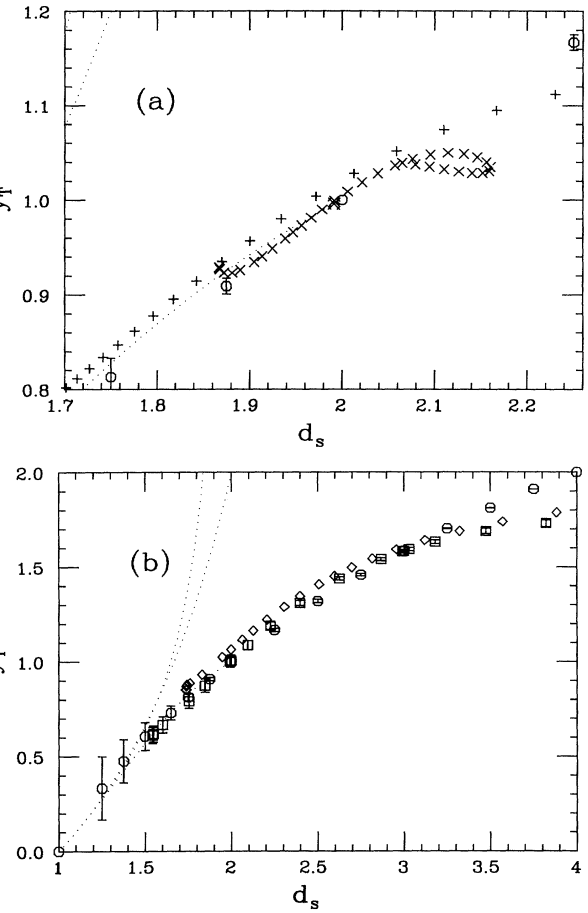

FIG. 2. The critical exponent y_T is plotted as a function of the dimension from scaling, d_s, for the (a) $d = 2$ and (b) $d = 3$ Ising ferromagnet. The symbols for the finite-size scaling study are the same as in Fig. 1. Also shown are results of the asymptotic expansion for the near-planar interface model in $d = 1 + \epsilon$ (dotted lines) [8, 9] and resummed expansions in $d = 4 - \epsilon$ (○ with error bars) [7].

plotted in Fig. 2 are the highest three orders of asymptotic expansions for y_T in $d = 1 + \epsilon$ [8, 9] and resummed expansions in $d = 4 - \epsilon$ [7]. These graphs show that the association of d_s with d is warranted near the physical dimension. Figure 2 also illustrates what constitutes the definition of "near" in these models. The error estimates shown in Fig. 2(b) for $L = 3$, were obtained by using each pair of lattices in Eq. (4). It is also seen that it is easier to extend d_s downward in dimension by making g large (see Fig. 1) than upward in dimension. This is a consequence of the fact that to try to extend d_s upward in dimension means that one needs to pass through free boundary conditions ($g = 0$), and for $d = 2$ this involves introducing an interface into the model [19]. The scaling for the square-lattice model has been shown to be different for values $g < 0$ [20, 21]. In fact, Fig. 1 shows that for $g < 0$ d_s starts to decrease again, leading to the loop seen in Fig. 2(a).

The magnetic exponent y_H can be found in a similar fashion by differentiating Eq. (1) twice with respect to H (Fig. 3). Figure 3 demonstrates that for d_s near d the FSS results agree with the results from expansions in dimension. This means that whenever d_s is "near" d both y_T and y_H agree with the expansions in dimension.

Do the critical exponents change with the addition of quenched random defects? Harris [22] predicted that the answer is yes only if the critical exponent (α) of the specific heat of the pure model is greater than zero. For the $d = 2$ Ising model $\alpha = 0$, so this is a marginal situation [23]. However, using the hyperscaling relation $d\nu = 2 - \alpha$ (or through more general arguments [24]) it is shown that the critical exponents should change with the addition of disorder whenever the pure model has $y_T > d/2$. Thus disorder should change the critical exponents for the Ising model for $d > 2$ but not for $d < 2$. The use of d_s allows one to check this prediction. Because of the difficulty with obtaining reasonable values for ξ from three lattice sizes, the Ising model on a square lattice with quenched random ferromagnetic bonds with strengths J_1 and J_2 was studied. This model is self-dual when the two bond strengths occur with equal probability [25]. Consequently, only two lattice sizes at the infinite-lattice value for T_c are required to obtain d_s from Eq. (2). The lattices used were $L \times M$ with $M = 10^7$, and were analyzed to obtain y_T from Eq. (4). The values of L used were between 2 and 10. Periodic boundary conditions (which give $d_s < d$) and antiperiodic boundary conditions (which give $d_s > d$) were used. As seen from Fig. 4 the critical exponents change with the addition of disorder to values with $y_T < d/2$ as predicted [24] for $d_s > 2$, while the critical exponents remain unchanged to within error estimates for $L > 2$ for $d_s < 2$. Note that the value for the J_1,J_2 model with the largest value of d_s used $L = 2$, and consequently this point should not be expected to fit smoothly on $d = 4 - \epsilon$ expansions for the Ising model with quenched disorder [26].

A natural question is why d_s behaves like d. The FSS expressions in Eq. (1) can be derived by renormalization group (RG) arguments with $1/L$ as an additional relevant scaling field [2]. In the infinite-dimensional space of interaction parameters for real-space RG rescaling there are separate fixed points associated with the physical di-

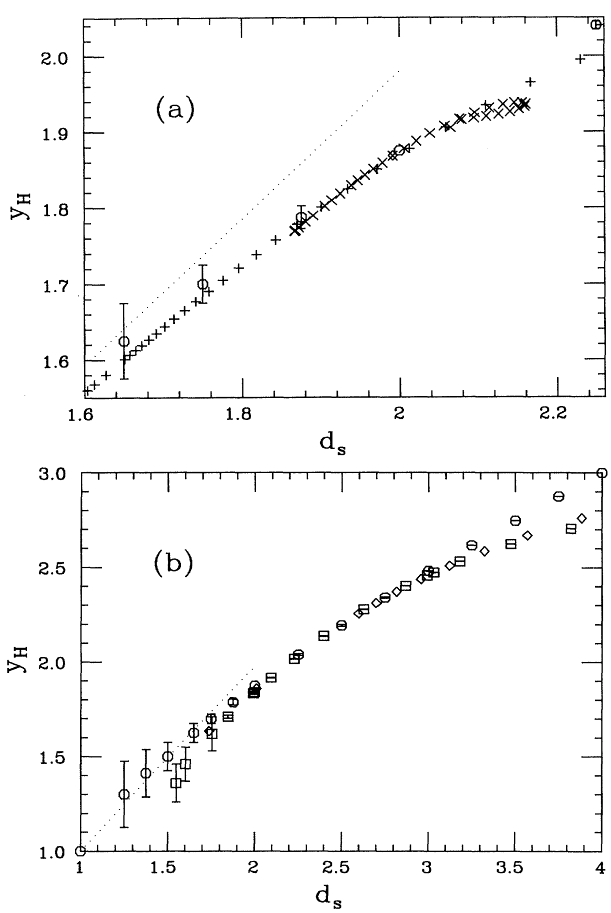

FIG. 3. The magnetic critical exponent y_H is shown as a function of the dimension from scaling d_s (a) for the $d = 2$ Ising ferromagnet and (b) for the $d = 3$ Ising ferromagnet. The symbols are the same as in Fig. 2. The dotted line is the result for the droplet model in $d = 1 + \epsilon$ dimensions [10].

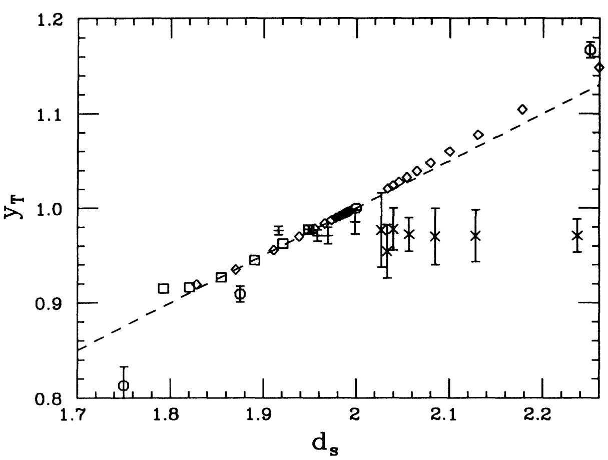

FIG. 4. The critical exponent y_T is shown as a function of the dimension from scaling d_s near d=2. Resummed expansions in d=4$-\epsilon$ are shown (○ with error bars) [7]. Results for the pure $d = 2$ Ising ferromagnet are shown (◇) using periodic boundary conditions ($d_s < 2$) and antiperiodic boundary conditions ($d_s > 2$). Results for the d=2 Ising ferromagnet with quenched random ferromagnetic bonds of strength J_1 and J_2 chosen with equal probabilities are shown for periodic (+) and antiperiodic (×) boundary conditions for various L values. Also shown are boundary conditions with bond strengths gJ (g>1) using L values 4 and 5 (□). The dashed line is the Harris criterion [22, 24] $y_T = d/2$. This demonstrates that with quenched disorder the critical exponents change for d>2, in agreement with the Harris criterion.

mensions 2 and 3. However, these fixed points are on a *line segment of fixed points* for general d between the upper and lower critical dimension. Consequently, whenever one is near the linear regime of the fixed point for the d-dimensional model, one should also be near the linear regime for the model in $d+\kappa$ dimensions for small κ. Since both d_s and the critical exponents are estimated from the same region in this space of couplings, d_s should be associated with the critical exponents obtained from the FSS.

An alternative explanation for the results in noninteger dimensions near the physical dimension may be to view the FSS as that of a system during a dimensional crossover (from d-dimensional behavior to one-dimensional behavior). Recently O'Connor and Stephens [27] have shown that the RG that interpolates between different dimensions has effective exponents appropriate for the system in noninteger dimensions. Which, if either, of these explanations is correct and how applicable this method is to other models remains for future investigations.

We have postulated that FSS scaling for systems with second-order phase transitions should allow one to obtain results for universal quantities for dimensions *near* the physical dimension. This allows direct comparisons between computer studies of critical phenomena and of expansions in dimension. We have shown that this is the case for the ferromagnetic nearest-neighbor Ising model on square and simple-cubic lattices, where results for both y_T and y_H agree with expansions in $d = 4 - \epsilon$ [7] and $d = 1 + \epsilon$ [8–10]. This method can also be applied to systems with quenched random disorder.

The author wishes to thank A. Aharony, V. Privman, P. A. Rikvold, J. Viñals, and R. K. P. Zia for useful discussions. The author also thanks P. E. Oppenheimer for discussions about PARIS programming of the CM-2. This research was supported in part by the Florida State University Supercomputer Computations Research Institute which is partially funded through Contract No. DE-FC05-85ER25000 by the U.S. Department of Energy.

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