

PHYSICAL REVIEW LETTERS

VOLUME 76

4 MARCH 1996

NUMBER 10

Finite-Size Scaling and Universality above the Upper Critical Dimensionality

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(Received 8 November 1995)

According to renormalization theory, Ising systems above their upper critical dimensionality $d_u = 4$ have classical critical behavior and the ratio of magnetization moments $Q = \langle m^2 \rangle^2 / \langle m^4 \rangle$ has the universal value 0.456947... However, Monte Carlo simulations of $d = 5$ Ising models have been reported which yield strikingly different results, suggesting that the renormalization scenario is incorrect. We investigate this issue by simulation of a more general model in which $d_u < 4$, and a careful analysis of the corrections to scaling. Our results are in perfect agreement with the renormalization theory and provide an explanation of the discrepancy mentioned.

PACS numbers: 05.70.Jk, 64.60.Ak, 64.60.Fr, 75.10.Hk

One of the most important contributions to the modern theory of critical phenomena is Wilson's renormalization theory (see Ref. [1] for an early review). This theory explains the existence of a so-called *upper critical dimensionality* d_u . It predicts that systems with a dimensionality $d > d_u$ exhibit classical exponents and violate hyperscaling, whereas systems with a lower dimensionality behave nonclassically. For Ising-like systems with short-range interactions, $d_u = 4$. In recent years, a controversy has arisen about the value of the "renormalized coupling constant" or "Binder cumulant" [2] for $d > d_u$. On the one hand, a renormalization calculation for hypercubic systems with periodic boundary conditions [3] predicts that the Binder cumulant assumes a universal value for $d \geq d_u$. On the other hand, Monte Carlo simulations of the five-dimensional Ising model [4–6] yielded significantly different results. Since the renormalization theory forms the basis of our present-day understanding of phase transitions and critical phenomena, it is of fundamental interest to examine any discrepancies and inconsistencies with this theory. Furthermore, there exist several models with a lower value of d_u [5,7] where the above-mentioned issue may be of experimental interest as well.

In this Letter, we answer the question concerning the value of the Binder cumulant. One of the key issues is the shift of the "critical temperature" in finite systems. We rederive this shift, which was already calculated in

Ref. [3], from basic renormalization equations and show that the result agrees with the shifts observed in Refs. [4–6]. Furthermore, we determine the Binder cumulant in the context of a more general Ising-like model with algebraically decaying interactions. This model is subject to the same renormalization equations as the aforementioned $d = 5$ Ising model, and effectively reduces to the nearest-neighbor model when the interactions decay fast enough. For slow decay, the upper critical dimensionality decreases below 4 and we have thus been able to investigate the question concerning the universality of the Binder cumulant in the classical region by means of Monte Carlo simulations of low-dimensional models. This enabled us to examine a much larger range of system sizes than in the five-dimensional case. High statistical accuracies were obtained by using a novel Monte Carlo algorithm for systems with long-range interactions and we could resolve various corrections to scaling that are present. The results turn out to be in complete agreement with the renormalization predictions.

We formulate our analysis in terms of the dimensionless amplitude ratio $Q = \langle m^2 \rangle^2 / \langle m^4 \rangle$, where m is the magnetization. This ratio is related to the fourth-order cumulant introduced by Binder [2]. In Ref. [3], it is predicted that in hypercubic short-range Ising-like systems with periodic boundary conditions and $d \geq 4$ this quantity takes at the critical temperature T_c the universal

value $8\pi^2/\Gamma^4(\frac{1}{2}) = 0.456947\dots$, which is simply the value of Q in the mean-field model [8]. In contrast, the Monte Carlo simulations in Refs. [5,6] yield the values $Q \approx 0.50$ and $0.489(6)$, respectively. In Ref. [6], this discrepancy is explained by a size-dependent shift of the “effective critical temperature” $T_c(L)$ (defined by, e.g., the maximum in the specific heat)

$$T_c(L) = T_c - AL^{-d/2}, \quad (1)$$

which was obtained in Refs. [4,5] from scaling arguments. L denotes the linear system size.

In order to examine this issue we will first outline the theoretical framework for scaling above d_u . As was shown by Brézin [9], conventional finite-size scaling breaks down for $d \geq d_u$. This is an example of Fisher’s mechanism of *dangerous irrelevant variables* (see, e.g., Refs. [10,11]). To examine the consequences of this mechanism for the finite-size scaling behavior, we briefly review the renormalization transformation for Ising-like models. Near criticality, one can represent the Hamiltonian for these models by one of the Landau-Ginzburg-Wilson type,

$$\mathcal{H}(\phi)/k_B T = \int_V d^d x \left\{ \frac{1}{2}(\nabla\phi)^2 - h\phi + \frac{1}{2}r_0\phi^2 + u\phi^4 \right\}. \quad (2)$$

h is the magnetic field, r_0 is a temperaturelike parameter, and the term proportional to u keeps ϕ finite when $r_0 \leq 0$. Under a spatial rescaling with a factor $b = e^l$ the renormalization equations are, to first order in r_0 and u , given in differential form by (see, e.g., Ref. [12])

$$\frac{dr_0}{dl} = y_t r_0 + \alpha u, \quad (3a)$$

$$\frac{du}{dl} = y_i u, \quad (3b)$$

in which y_t and y_i are the renormalization exponents of the temperature field and the irrelevant field u , respectively, and α is a constant depending on the dimensionality d . Upon integration, these equations yield, to first order in u ,

$$r'_0(b) = b^{y_t}[(r_0 - \tilde{\alpha}u) + \tilde{\alpha}ub^{y_i - y_t}], \quad (4a)$$

$$u'(b) = b^{y_i}u, \quad (4b)$$

where $\tilde{\alpha}$ is a constant. This shows that the reduced temperature $t \equiv (T - T_c)/T_c$ is proportional to $r_0 - \tilde{\alpha}u$. Correspondingly, the free energy density f scales as

$$f(t, h, u, 1/L) = b^{-d} f(b^{y_t}[t + \tilde{\alpha}ub^{y_i - y_t}], b^{y_h}h, b^{y_i}u, b/L) + g, \quad (5)$$

where we have included a finite-size field L^{-1} and g denotes the analytic part of the transformation. The first

term on the right hand side (RHS) can be abbreviated as $b^{-d}f(t', h', u', b/L)$. For $d \geq 4$, the critical behavior is determined by the Gaussian fixed point $(t^*, u^*) = (0, 0)$. However, for $T \leq T_c$, the free energy is singular at $u = 0$. Hence u is a dangerous irrelevant variable. The finite-size scaling properties of thermodynamic quantities can be obtained by renormalizing the system to size 1, i.e., setting $b = L$. The number of degrees of freedom then reduces to 1 and the free energy to

$$f(t', h', u', 1) = \ln \int_{-\infty}^{+\infty} d\phi \times \exp \left[h'\phi - \frac{1}{2}r'_0(L)\phi^2 - u'(L)\phi^4 \right]. \quad (6)$$

The substitution $\phi' = \phi/u'^{1/4}$ leads to

$$f(t', h', u', 1) = \tilde{f}(\tilde{t}, \tilde{h}), \quad (7)$$

with $\tilde{t} = t'/u'^{1/2}$ and $\tilde{h} = h'/u'^{1/4}$. Upon renormalization, the analytic part g of the transformation also contributes to the singular dependence of the free energy on t ; see, e.g., Ref. [12]. We absorb this contribution in the function \tilde{f} . Setting $b = L$ and combining Eqs. (5) and (7) yields

$$f\left(t, h, u, \frac{1}{L}\right) = L^{-d} \tilde{f}\left(L^{y_t - y_i/2} \frac{1}{u^{1/2}} [t + \tilde{\alpha}uL^{y_i - y_t}], L^{y_h - y_i/4} \frac{h}{u^{1/4}}\right). \quad (8)$$

For $d \geq 4$, $y_t = 2$, $y_h = 1 + d/2$, and $y_i = 4 - d$. The first argument on the RHS is the scaled temperature

$$\tilde{t} = L^{d/2} \frac{1}{\sqrt{u}} (t + \tilde{\alpha}uL^{2-d}). \quad (9)$$

Interpreting the term $\tilde{\alpha}uL^{2-d}$ as a shift in the effective critical temperature for a finite system, we recover the result of Ref. [3].

Let us now use the above derivation to examine the shift and rounding of critical singularities in finite systems. Observables can be calculated from the free energy by differentiating with respect to a suitable parameter. Ignoring the analytic part of the free energy, we can express the thermodynamic quantities in terms of *universal* functions of the two arguments that appear in the RHS of Eq. (8). For example, the specific heat can be written as the product of a power of the rescaling factor and a *universal* function of the scaled fields. Let the maximum of this function occur at $\tilde{t} = c$ (c a constant). Then, the specific heat maximum occurs at a temperature which differs, in leading orders of L , from the critical temperature by

$$\Delta t = c\sqrt{u}L^{-d/2} - \tilde{\alpha}uL^{2-d}. \quad (10)$$

The leading L dependence of Eq. (10) agrees with Eq. (1). However, on the basis of Eq. (1) it is argued in Refs. [4–6] that the term between brackets in Eq. (9) could be replaced by $t + aL^{-d/2}$, where a is a nonuniversal constant. If this argument were correct, it would have serious consequences for the renormalization scenario: There must be a contribution of a new type between the square brackets in Eq. (4a), proportional to $b^{-d/2}$. There is no renormalization mechanism known to us which would yield such a term. Furthermore, in leading orders of L Eq. (9) must be replaced by

$$\tilde{t} = L^{d/2} \frac{1}{\sqrt{u}} (t + aL^{-d/2}) \propto L^{d/2} t + a, \quad (11)$$

and in general critical-point values of finite-size scaling functions become dependent on a : They are no longer universal. We illustrate this for the ratio Q . Since the magnetization moments can be expressed in derivatives of the free energy with respect to the magnetic field, the renormalization theory predicts

$$Q_L(T) = \tilde{Q}(\tilde{t}L^{y_i^*}) + q_1 L^{d-2y_h^*} + \dots \quad (12)$$

Here \tilde{Q} is a universal function, t stands for the argument between brackets in Eq. (9), and we have introduced the exponents $y_i^* \equiv y_i - y_i/2$ and $y_h^* \equiv y_h - y_i/4$. The additional term $q_1 L^{d-2y_h^*} = q_1 L^{-d/2}$ arises from the analytic part of the free energy. Now suppose that Eq. (11) is correct instead of Eq. (9). Then the argument of \tilde{Q} is nonuniversal at the critical point and so is $Q = \lim_{L \rightarrow \infty} Q_L(T_c)$. The value calculated in Ref. [3] is then just the particular value of Q for the mean-field model.

Can we reconcile the renormalization scenario with the Monte Carlo results obtained until now? The evidence for an effective critical temperature as in Eq. (1) is based upon the locations of the maxima in the susceptibility and the specific heat, and those of the inflection points of the absolute magnetization and the renormalized coupling constant $g_L \equiv -3 + 1/Q_L$. However, we have seen above that Eq. (9) is fully compatible with a deviation $\Delta t \approx L^{-d/2}$ [see Eq. (10)]. Therefore, the observed shifts do not provide evidence for the term proportional to a in Eq. (11), and we look for a different source of the discrepancy between the renormalization and Monte Carlo results for Q . Equation (8) shows that there are several corrections to scaling which may well account for this. When Eq. (12) is expanded in $\tilde{t}L^{y_i^*}$, the term proportional to \tilde{a} yields a term $q_2 L^{2-d/2}$. Furthermore, when we include a nonlinear contribution in u in (3), factors u in Eq. (8) are replaced by $u(1 + \gamma u L^{y_i})$ and we find an additional term $q_3 L^{4-d}$. Higher powers of these corrections may also be taken into account in the analysis, as well as the term $q_1 L^{-d/2}$ in (12). However, the determination of these corrections would require accurate data for a large range of system sizes L , and the high dimensionality of the $d = 5$ Ising model presents here

a major obstacle. The results presented in Refs. [4,5] were based on $3 \leq L \leq 7$ and therefore the results were by no means conclusive. Reference [6] used the range $5 \leq L \leq 17$. Given these limited ranges of system sizes, it seems uncertain whether all important corrections have been resolved. Thus the Monte Carlo evidence against the renormalization result of Ref. [3] is not compelling.

Here we follow a different approach to test the renormalization predictions. In Ref. [7], Fisher, Ma, and Nickel investigated the renormalization behavior of $O(n)$ models with ferromagnetic long-range interactions decaying as $r^{-(d+\sigma)}$ ($\sigma > 0$). The Fourier transform of the Landau-Ginzburg-Wilson Hamiltonian is quite similar to that of Eq. (2); only the term proportional to k^2 is replaced by a term proportional to k^σ . Thus the renormalization equations have the same form as for short-range interactions; only the exponents and the coefficient α in Eq. (3) assume different values. For $0 < \sigma \leq d/2$ ($d \leq 4$), the Gaussian fixed point is stable and the critical exponents have fixed, classical values (and hence hyperscaling is violated). The upper critical dimensionality is thus $d_u = 2\sigma$. In Fig. 1, the regions of classical and nonclassical behavior are shown as a function of d and σ . Introducing a parameter $\varepsilon = 2\sigma - d$, we note that the classical exponents apply for $\varepsilon < 0$, just as in the short-range case, where $\varepsilon = 4 - d$. In the limit $\sigma \downarrow 0$, each spin interacts equally with every other spin, so that we can identify this case with the mean-field model. Thus there is an analogy between the (short-range) Ising model with $4 \leq d < \infty$ and the long-range model with $0 < \sigma \leq d/2$. If the amplitude ratio Q has a nonuniversal value, we may therefore expect that this manifests itself in the long-range case as well.

In general, the study of models with long-range interactions is notoriously difficult, due to the large number of interactions that have to be taken into account. How-

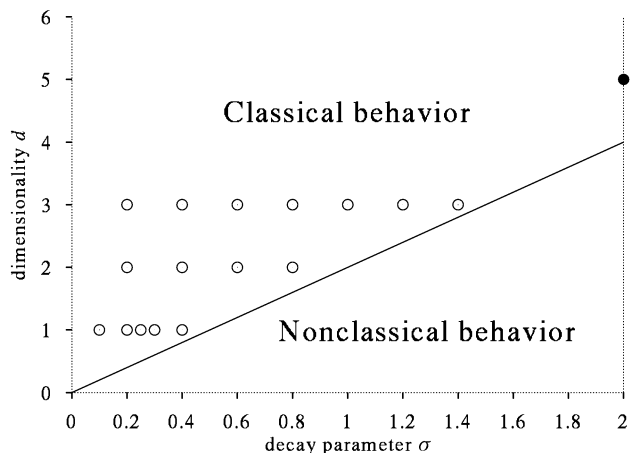


FIG. 1. Dimensionality vs decay parameter σ for various models. Short-range models are described by $\sigma = 2$. The open circles indicate the models investigated in this article, and the black circle marks that of Refs. [4–6].

ever, a novel Monte Carlo algorithm [8] of the Wolff cluster type [13] is available that suppresses critical slowing down and, in spite of the fact that each spin interacts with every other spin, consumes a time per spin independent of the system size. Thus we could simulate models with algebraically decaying interactions in one, two, and three dimensions and obtain accuracies that were not feasible up until now (cf. Ref. [14], and references therein). For $d = 1$, the interaction was taken exactly $Kr^{-(d+\sigma)}$, whereas for $d = 2$ and 3, the interaction was slightly modified with irrelevant contributions decaying as higher powers of r^{-1} [8]. To account for the periodic boundary conditions, the actual spin-spin couplings are equal to the sum over all periodic images. We have studied linear system sizes $10 \leq L \leq 150\,000$ for $d = 1$, $4 \leq L \leq 240$ for $d = 2$, and $4 \leq L \leq 64$ for $d = 3$, generating between 10^6 and 4×10^6 Wolff clusters per simulation. The ranges of system sizes are larger than in Refs. [4–6], and more intermediate values of L are available. These facts, as well as the high statistical accuracy of the Monte Carlo results, allowed us to resolve the leading finite-size corrections in the Q_L .

The finite-size scaling analysis was based on the Taylor expansion of the renormalization prediction for Q_L near criticality:

$$Q_L(T) = Q + p_1 t L^{y_t^*} + p_2 t^2 L^{2y_t^*} + p_3 t^3 L^{3y_t^*} + \dots \\ + q_1 L^{d-2y_h^*} + \dots + q_3 L^{y_i} + \dots \quad (13)$$

The coefficients p_i and q_i are nonuniversal and the renormalization exponents are $y_t = \sigma$, $y_h = (d + \sigma)/2$, and $y_i = 2\sigma - d$. The corresponding values $y_t^* = d/2$ and $y_h^* = 3d/4$ coincide with those in the short-range case. In addition to the corrections to scaling in Eq. (13) we have

TABLE I. The ratio Q and critical coupling K_c for systems with long-range interactions in one, two, and three dimensions, for several values of the parameter σ in the range $0 < \sigma \leq d/2$. The numbers between parentheses represent the errors in the last decimal places.

d	σ	Q	K_c
1	0.1	0.4584(14)	0.047618(2)
1	0.2	0.4573(28)	0.092234(5)
1	0.25	0.4564(22)	0.114137(6)
1	0.3	0.4590(45)	0.136106(9)
1	0.4	0.4569(34)	0.181150(10)
2	0.2	0.4573(10)	0.028533(3)
2	0.4	0.4565(17)	0.051824(4)
2	0.6	0.4546(52)	0.071358(8)
2	0.8	0.4570(55)	0.088089(7)
3	0.2	0.4557(18)	0.0144344(14)
3	0.4	0.45686(8)	0.0262927(15)
3	0.6	0.4554(17)	0.036045(3)
3	0.8	0.4562(13)	0.044034(2)
3	1.0	0.4580(25)	0.050517(3)
3	1.2	0.4556(26)	0.055678(2)
3	1.4	0.460(9)	0.059669(3)

also included higher powers of $q_3 L^{y_i}$, which become important especially when σ is close to $d/2$. In fact, omitting these corrections yielded estimates for Q close to those obtained in Refs. [5,6], although the residuals strongly indicated the presence of additional corrections. This confirms the assumption that the discrepancy between the $d = 5$ Monte Carlo results and the renormalization calculation is caused by corrections to scaling. Furthermore, the coefficient $\tilde{\alpha}$ in Eq. (9) is very small in all cases, in accordance with the fact that this correction term could not be resolved in Ref. [6]. An extensive analysis of the data will be presented elsewhere. We have fixed all exponents at the theoretical values, in order to minimize the uncertainty in Q . The results presented in Table I show that the agreement between the renormalization prediction for Q and the Monte Carlo data is excellent.

It could, for the purpose of comparison, be of some interest to make a correspondence between systems with short-range interactions in $d > 4$ dimensions and d' -dimensional systems with long-range interactions decaying as $r^{-(d'+\sigma)}$. Such a correspondence is possible by expressing the various finite-size scaling relations in terms of the number of particles N instead of the linear system size L . Then the dependence of the thermal and magnetic exponents on the dimensionality is absorbed in the parameter $N = L^d$ (or $L^{d'}$) and the renormalization predictions for both models differ only in the (modified) irrelevant exponents, $(4-d)/d$ and $(2\sigma-d')/d'$, respectively. For both models, these exponents vary between 0 and -1 in the classical range, and the matching condition appears as $\frac{\sigma}{d} = \frac{2}{d}$. Hence, we may compare the $d = 5$ (short-range) Ising model with the $\sigma = \frac{2}{5}d'$ long-range model, i.e., $\sigma = 0.4, 0.8$, and 1.2 for $d' = 1, 2$, and 3 , respectively. In this sense the present work approaches the nonclassical regime even closer than Refs. [4–6].

Finally, we remark that models with long-range interactions provide an effective way to explore scaling properties above the upper critical dimensionality. For example, the approach adopted in this Letter may be generalized to planar, Heisenberg, and q -state Potts models, including percolation problems. For $\sigma < 2$, d_u is reduced by a factor $\sigma/2$ in the case of long-range interactions.

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