# Corrections to finite-size-scaling laws and convergence of transfer-matrix methods

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We examine the finite-size-scaling laws relating the values of a quantity in a (hypercubic) box of size L, or on a bar of transverse size L (i.e., of cross section  $L^{D-1}$ ), to the same quantity in the infinite-volume limit. A field-theoretical argument shows that the corrections to these laws are governed by the bulk correction-to-scaling exponent  $\omega$  (also denoted  $\Delta_1/\nu$  or  $-y_3$ ). The data of transfer-matrix methods, like those of the phenomenological renormalization, have therefore generally the same asymptotic convergence exponent  $\omega$ . It is shown explicitly in some examples that other convergence laws may occur. The large-N limit of the  $O(N)$  spin model allows for a more refined quantitative study: dependence of corrections to finite-size scaling upon the details of interactions, range of values of L for which the convergence is asymptotic, and nonuniversality of apparent critical exponents in the mean-field case  $(D > D<sub>c</sub>)$ .

### I. INTRODUCTION

Numerical studies of statistical-mechanical models very often imply the extrapolation of data concerning finite or partially finite systems to the infinite-volume (or thermodynamical) limit. Three of the most powerful numerical approaches to the study of critical phenomena suffer from this extrapolation problem, namely the Monte Carlo method, the Monte Carlo renormalization-group method, and the transfer-matrix method. In the following we shall consider essentially the last approach, which exhibits purely systematic finite-size effects in nonrandom models, while Monte Carlo results always have both systematic and statistical errors, and moreover may have intrinsic problems due to metastability or critica1 slowing down.

The transfer-matrix method (see Refs. <sup>1</sup>—<sup>3</sup> for recent reviews) originated with Nightingale.<sup>4</sup> It consists of solving exactly the model under investigation on a lattice which is a bar of finite section  $L^{D-1}$  and infinite length in the last direction. The transfer-matrix formalism is particularly well adapted to this geometry. The exact knowledge of the largest two eigenvalues of the transfer operator is usually sufficient to determine every quantity of interest, such as the free energy  $F_L(\beta)$  (and its derivatives: specific heat, magnetization, entropy, susceptibility), as well as the correlation length  $\xi_L(\beta)$ , characterizing the exponential falloff of correlations in the infinite direction of the bar.

The only questionable point in the transfer-matrix method is the convergence of the values  $Q_L(\beta)$  of any observable on a bar of transverse size  $L$  (i.e., of cross section  $L^{D-1}$  to the thermodynamical value  $Q(\beta)$ . Let us restrict ourselves to periodic boundary conditions: Most applications of the transfer-matrix approach use this type of condition. Moreover, other boundary specifications may introduce nontrivial surface effects. For  $\beta \neq \beta_c$ ,  $Q_L (\beta)$  is expected to converge exponentially towards  $Q(\beta)$  whenever  $\xi(\beta)$  and  $Q(\beta)$  are finite.<sup>5</sup> More interesting is the vicinity of the critical point  $\beta_c$ , where the bulk correlation length  $\xi(\beta)$  diverges. Fisher proposed the following scaling behavior when L and  $\xi(\beta)$  are both large but comparable: $5,6$ 

$$
Q_L(\beta) = Q(\beta) F_Q(L/\xi(\beta)) , \qquad (1)
$$

where  $F_Q$  is a universal scaling function. This finite-size scaling hypothesis was extended<sup>7</sup> to the area of critical dynamics.

One very interesting choice for  $Q$  is the correlation length itself. Consider the following transformation:

$$
T_{L,L'}: \beta \rightarrow \beta'
$$
 such that  $\frac{\xi_L(\beta)}{L} = \frac{\xi_{L'}(\beta')}{L'}$  (2)

for two fixed sizes  $L$  and  $L'$ . Then Fisher's relation implies that the fixed point  $\beta_{L,L'}$  of the transformation  $T_{L,L'}$ is an estimate of  $\beta_c$  for large L and L':

$$
\frac{\xi_L(\beta_{L,L'})}{L} = \frac{\xi_{L'}(\beta_{L,L'})}{L'} \implies \beta_{L,L'} \underset{L,L' \to \infty}{\longrightarrow} \beta_c , \qquad (3)
$$

and that the linearization of  $T_{L,L'}$  around  $\beta_{L,L'}$  gives an estimate  $v_{L,L}$  of the critical index  $v$ :

$$
1 + \frac{1}{v_{L,L'}} = \frac{\ln[(d\xi_{L'}/d\beta)/(d\xi_{L}/d\beta)_{\beta=\beta_{L,L'}}]}{\ln(L'/L)}.
$$
 (4)

The map  $T_{L,L'}$  can be viewed as a real-space renormalization-group transformation, usually called "phenomenological renormalization." It involves only one variable  $(\beta)$  in a natural way, without any artificial truncation (except the finiteness of  $L, L'$ ).

This phenomenological renormalization has been applied to a very large variety of models, mostly in two dimensions (see Refs. <sup>1</sup>—3, and references therein). In most cases, this method leads to very stable and accurate results (even for reasonable sizes  $L$ ). The Hamiltonian version, where the infinite direction is continuous and the finite transverse ones are kept discrete, has also been extensively used. $8-10$  Models with quenched disorder, where the relevant quantities are the Liapunov exponents of a product of a large number of random matrices, have also been investigated through the transfer-matrix--plusinvestigated through the transfer-man-<br>phenomenological-renormalization method.<sup>11,12</sup>

Finite-size scaling has been considered for a long time as a reasonable heuristic assumption. $4-7$  It has been shown by Brézin<sup>13</sup> that the field-theoretical approach naturally implies the invariance of the size L under the renormalization-group flow. This essential. property is not sufficient to ensure the validity of finite-size scaling, since some regularity properties of the scaling functions around the infrared stable fixed point are needed. These conditions are not fulfilled when the fixed point is trivial (mean-field theory). Finite-size scaling is therefore valid for dimensionalities  $D < D_c$ , where  $D_c$  is the upper critical dimension.

A question of great practical importance is the convergence towards the thermodynamical values of the finite-L estimates such as  $\beta_{L,L}$ ,  $v_{L,L}$ , or other critical indices. It has been recently argued<sup>14</sup> that this convergence is asymptotically governed by the bulk leading-correction-toscaling exponent  $\omega$  (also denoted  $\Delta_1/v$  or  $-y_3$ ). Since  $\omega$ is rather large for most two-dimensional systems, the phenomenological-renormalization approach converges much more rapidly than other types of analysis,  $1<sup>5</sup>$  which may involve smaller leading-corrections-to-scaling exponents.

The contents of the present paper are as follows: In Sec. II, we present a simple general field-theoretical approach to the corrections to finite-size scaling, which confirms the results of Privman and Fisher,<sup>14</sup> and generalize them to other extrapolation methods, including those quoted in Ref. 15. In Sec. III we consider the example of the  $O(N)$  ( $N = \infty$ ) spin model in arbitrary dimension  $(D \ge 2)$ . Since this model is soluble on a bar as well as in the infinite space, we can compare theoretical predictions and numerical data, study the dependence of the correction amplitudes upon the details of the interactions, and see how the small-L results obey the asymptotic correction laws. Our results are extended to the marginal case  $D = D<sub>c</sub> = 4$ . For  $D > D<sub>c</sub>$ , the phenomenologicalrenormalization predictions depend upon the particular choice of renormalization, and therefore generally do not give the correct mean-field values for critical indices.

## II. GENERAL APPROACH TO CORRECTIONS TO FINITE-SIZE SCALING

### A. Field-theoretical argument

In this section we shall repeat briefly Brézin's proof<sup>13</sup> of the validity of Fisher's finite-size scaling hypothesis, and show how it can be extended to incorporate the leading nonanalytic corrections, governed by the exponent  $\omega$ , just as for the bulk quantities. We shall follow throughout this section the notation and the method exposed in Ref. 16.

Consider a  $(\vec{\phi}^2)^2$  field theory on a hypercubic lattice in D dimensions. The associated partition function reads

$$
Z = \int \left[ \prod_x d\phi_x \right] \exp \left[ \frac{1}{2} \sum_{x,\mu} \nabla_{\mu} \vec{\phi}_x \cdot \nabla_{\mu} \vec{\phi}_x + \sum_x \left[ \frac{m_0^2}{2} \vec{\phi}_x^2 + \frac{g_0}{4!} (\vec{\phi}_x^2)^2 \right] \right].
$$
 (5)

In renormalization theory, all the divergences appearing as the lattice spacing  $a$  goes to zero can be absorbed in a finite number of counterterms, as long as the theory is renormalizable [i.e., for  $D \le D_c$  with  $D_c = 4$  in the case of  $(\vec{\phi}^2)^2$ . Brezin has shown that the counterterms of the infinite-volume theory are sufficient to make the physical quantities finite in an arbitrary geometry with periodic boundary conditions. In other words, the size  $L$  of a (hypercubic) box with  $L^D$  sites, or the transverse size L of a par of section  $L^{D-1}$  is not renormalized.

The irreducible Green's functions  $\Gamma_L^{(N)}$  obey therefore the same renormalization-group equations as their thermodynamical (infinite-volume) values  $\Gamma^{(N)}$ :

$$
\Gamma_L^{(N)}(t,g,\mu) = \exp\left(-\frac{N}{2} \int_1^{\lambda} dx \frac{1}{x} \eta(g(x))\right)
$$

$$
\times \Gamma_L^{(N)}(t(\lambda), g(\lambda), \lambda \mu) .
$$
 (6)

Consider the ratio

$$
\varphi_L(t,g,\mu) = \frac{\Gamma_L^{(N)}(t,g,\mu)}{\Gamma^{(N)}(t,g,\mu)}.
$$
\n(7)

It follows directly from (6) that  $\varphi_L$  is an invariant of the renormalization-group flow:

$$
\varphi_L(t,g,\mu) = \varphi_L(t(\lambda),g(\lambda),\lambda\mu) \tag{8}
$$

obtain

Using dimensional analysis and choosing 
$$
\lambda = 1/L\mu
$$
, we obtain  
\n
$$
\varphi_L(t,g,\mu) = \psi \left[ L^2 t \left[ \frac{1}{L\mu} \right], g \left[ \frac{1}{L\mu} \right] \right].
$$
\n(9)

Assume now that  $L$  is very large in lattice spacing units:  $L \gg a$  or  $L\mu \gg 1$ . Then  $g(1/L\mu)$  goes to the stable fixed point  $g^* = g(0)$ , and the running temperature  $t(1/L\mu)$  is such that

$$
L^{2}t\left(\frac{1}{L\mu}\right)\sim tL^{1/\nu}\sim\left(\frac{L}{\xi(\beta)}\right)^{1/\nu}.
$$
 (10)

Equation (9) can therefore be equivalently rewritten as

$$
Q_L(\beta) = Q(\beta)\varphi_Q(tL^{1/\nu})
$$
\n(11)

or

$$
Q_L(\beta) = Q(\beta) F_Q(L/\xi(\beta)) \tag{12}
$$

or

$$
Q_L(\beta) = L^{\tau/\nu} f_Q(tL^{1/\nu}) \tag{13}
$$

That proves the validity of Fisher's relation for any multiplicatively renormalizable quantity Q with critical exponent  $\tau$  [Q( $\beta$ ) ~ ( $\beta - \beta_c$ )<sup>- $\tau$ </sup>].

Consider now the corrections to Eq.  $(11)$  when L and  $\xi(\beta)$  are both large but finite. The most convenient way to deal with such effects is to introduce a g-dependent normalization of the temperature  $t(g)$  and an expansion formalization of the temperature  $\ell(\mathbf{g})$  and an expansion<br>of the  $\Gamma_L^{(N)}$  in a power series of  $(g - g^*)$  (see Chap. 8 of Ref. 16). We define the leading correction  $D_L^{(N)}(t,\mu)$  by

$$
\Gamma_L^{(N)}(t,g,\mu) = \exp\left(\frac{N}{2} \int_{g^*}^g dg' \frac{\eta(g') - \eta}{W(g')}\right)
$$
  
 
$$
\times \Gamma_L^{(N)}(t(g), g^*, \mu)
$$
  
 
$$
\times [1 + (g - g^*)D_L^{(N)}(t(g), \mu) + \cdots]. \qquad (14)
$$

This quantity satisfies the following renormalizationgroup equation:

$$
\left[\mu \frac{\partial}{\partial \mu} + \omega - \left[\frac{1}{\nu} - 2\right] t \frac{\partial}{\partial t} \right] D_L^{(N)}(t, \mu) = 0 ,
$$
 (15)

where  $\omega = \beta'(g^*)$  is the usual bulk correction-to-scaling exponent. The general solution of (15) reads

$$
D_L^{(N)}(t,\mu) = \lambda^{\omega} D_L^{(N)}(t(\lambda),\lambda \mu) \tag{16}
$$

Using dimensional analysis we obtain

$$
D_L^{(N)}(t,\mu) = \lambda^{\omega} D_{L\lambda\mu}^{(N)}(t(\lambda)/\lambda^2\mu^2) \tag{17}
$$

Choosing  $\lambda = 1/L\mu \ll 1$  and using (10), we have finally

$$
D_L^{(N)}(t,\mu) = (L\mu)^{-\omega} D_1^{(N)}(tL^{1/\nu}) . \qquad (18)
$$

The field-theoretical approach predicts therefore the following general form of the finite-size scaling relation, including the leading correction term

$$
Q_L(\beta) = L^{\tau/\nu} [f_Q(tL^{1/\nu}) + L^{-\omega} f_Q^{(1)}(tL^{1/\nu}) + \cdots ] \qquad (19)
$$

for a multiplicatively renormalizable quantity.

For quantities which obey an inhomogeneous renormalization-group equation, (19) has to be modi-<br>fied.<sup>13,17</sup> For the specific heat, our prediction reads fied.<sup>13,17</sup> For the specific heat, our prediction reads

$$
C_L(t) = C_{\text{reg}}(t) + L^{\alpha/\nu} [f_c(tL^{1/\nu}) + L^{-\omega} f_c^{(1)}(tL^{1/\nu}) + \cdots],
$$
\n(20)

where  $C_{reg}(t)$  is the regular part of the bulk  $C(t)$ ;  $C_{sg}(t) = C(t) - C_{reg}(t)$  usually exhibits a power-law singularity in  $|t|$ 

In order to make our argument as simple as possible, we have considered only the temperature variable. The extension to a nonzero magnetic field, and to other quantities such as correlation functions, is straightforward.<sup>16</sup> The scaling functions  $f_{Q},\varphi_{Q},\ldots$  become functions of re-

duced variables:  
\n
$$
f(tL^{1/\nu}, tM^{-1/\beta}, tp_i^{-1/\nu}),
$$
\n(21)

where  $M$  is the magnetization and  $p_i$  the external momenta. Equations (19) and (20) are the main result of this section.

Let us discuss now the nature of other corrections to

scaling. Consider only the temperature dependence for simplicity.

It is known from the beginning of the renormalization group approach to critical phenomena' renormalization-<br><sup>8, 19</sup> that t is an analytic function of  $\beta$  near  $\beta_c$ .

Let us normalize  $t$  such that

$$
-t = (\beta - \beta_c) + \sigma(\beta - \beta_c)^2 + \cdots
$$
 (22)

On the other hand, since a bar of size  $L$  is in fact one dimensional,  $Q_L(\beta)$  is *analytic* in  $\beta$ , and therefore the  $f_Q^{(i)}$ are analytic in their arguments. That is generally not the case of  $F_Q$  or  $\varphi_Q$  in other formulations, (12) and (13). If one uses, for practical reasons, a convenient variable such as

as  

$$
\widetilde{t} = \beta - \beta_c, \text{ or } (T - T_c)/T_c, \text{ or } e^{2\beta J} - e^{2\beta_c J}, \dots,
$$
 (23)

the insertion of (23) into (19) and (20) leads to corrections the insertion of (23) into (19) and (20) leads to corrections<br>of the type  $L^{-1/\nu}$ ,  $L^{-2/\nu}$ ,.... These have been pointed  $out<sup>14,20</sup>$  and called nonlinear scaling fields effects, i.e., nonuniversal reparametrization effects. We shall show in the following that they are not apparent in most of the practical applications of Eqs. (19) and (20).

Besides these rather trivial corrections, there are other ones, of the form  $L^{-\omega_i}$ , due to further irrelevant operators. In the limit  $D \rightarrow 4$  we can affirm they are much maller than  $L^{-\omega}$ , since we have, in  $D=4-\epsilon$ ,

$$
\omega = \epsilon + O(\epsilon^2) \tag{24a}
$$

$$
\omega_i = 2n_i + O(\epsilon), \quad n_i = 1, 2, \dots,
$$
 (24b)

where  $\omega_i$  correspond to operators  $\mathcal{O}_i$  of (canonical) dimension  $\delta_i = 4+2n_i$ .  $n = 1$  contains for instance

$$
\mathscr{O}_1 = (\vec{\phi}^2)^3, \quad \mathscr{O}_2 = \vec{\phi}^2 (\partial_\mu \vec{\phi})^2, \dots \tag{25}
$$

For models which cannot be described by a field theory, we do not have any *a priori* estimate of  $\omega$ , nor the  $\omega_i$ 's.

The comparison between theory and experiment in fluids (see Ref. 21, and references therein) encounters the very same problems of reparametrization effects, and of irrelevant operators. Since arbitrary crossed products of rrelevant operators. Since arbitrary crossed products of  $L^{-\omega_i}$  terms may appear, the general correction term in ' terms may appear, the general correction term in the variable  $t$  in Eqs. (19) and (20) is

$$
L^{-\left(N_0\omega+\sum_i N_i\omega_i\right)} \quad \text{with} \quad N_0, N_i=0,1,\ldots.
$$

For practical purposes, one has to keep in mind that usual variables such as  $\beta$  are analytic in t, but not equal to t.

### B. Application to the phenomenological renormalization

We can deduce from Eqs.  $(19)$  and  $(20)$  the asymptotic convergence laws of the data obtained by different analyses of the transfer-matrix approach. Consider first the phenomenological-renormalization transform (2). Equation  $(19)$  for the correlation length reads

$$
\frac{\xi_L(\beta)}{L} = f(tL^{1/\nu}) + L^{-\omega} f_1(tL^{1/\nu}) + \cdots
$$
 (26)

The relation between (26) and the convergence of  $\beta_{L,L'}$ and  $v_{L,L'}$  has been studied by Derrida and de Seze.<sup>1</sup> Let us summarize their notation:

$$
\xi_L(\beta_c) = A_0 L (1 + A_1 L^{-\omega} + \cdots)
$$
  
[with  $A_0 = f(0)$ ;  $A_1 = f_1(0) / f(0)$ ],  

$$
\frac{d\xi_L}{d\beta}\Big|_{\beta = \beta_c} = B_0 L^{1 + 1/\nu} (1 + B_1 L^{-\omega} + \cdots)
$$
(27)

[with 
$$
B_0 = -f'(0)
$$
;  $B_1 = f'_1(0)/f'(0)$ ],  
\n
$$
\frac{d^2 \xi_L}{d\beta^2} \bigg|_{\beta = \beta_c} = C_0 L^{1+2/\nu} (1 + C_1 L^{-\omega} + C_2 L^{-1/\nu} + \cdots)
$$
\n[with  $C_0 = f''(0)$ ;  $C_1 = f''_1(0)/f''(0)$ ;  $C_2 = -2\sigma f'(0)$ 

 $f''(0)$ ]. The term  $C_2L^{-1/\nu}$ , which is of no interest in the fol-

lowing, is an explicit example of a reparametrization correction.

The authors of Ref. <sup>1</sup> deduce from (27) that the quantities  $\beta_{L,L'}$  and  $v_{L,L'}$  converge towards  $\beta_c$  and  $\nu$  (in the limit  $L, L' \rightarrow \infty$  with  $L' = \lambda L$  and  $0 < \lambda \le 1$  fixed) as

$$
\beta_{L,L'} - \beta_c \sim \delta_{\beta} L^{-\omega - 1/\nu},
$$
  
\n
$$
v_{L,L'} - v \sim \delta_{\gamma} L^{-\omega}.
$$
 (28)

In the very current case  $L' = L - 1$  or  $L - 2$  (i.e.,  $\lambda \rightarrow 1$ ), the amplitudes  $\delta$  read

$$
\delta_{\beta} = \omega v \frac{A_0 A_1}{B_0} = -\omega v \frac{f_1(0)}{f'(0)},
$$
  
\n
$$
\delta_v = \omega v^2 \left[ B_1 - \frac{A_0 C_0 A_1}{B_0^2} \right]
$$
  
\n
$$
= \omega v^2 \frac{f'(0) f'_1(0) - f''(0) f_1(0)}{f'(0)^2}.
$$

This method can be generalized to renormalization from a size L to a size L' with  $l \ll L' \ll L$ , such as  $L' \sim cL^{\sigma}$ (with  $0 < \sigma < 1$ ). In that case, it is easy to realize that the difference between  $\beta_{L,L'}$  and  $\beta_c$  reads

$$
\beta_{L,L'} - \beta_c \sim \delta_{\beta}(L')^{-\omega}L^{-1/\nu} \sim \text{const} \times L^{-(1/\nu + \sigma \omega)}
$$
  
with (29a)

$$
\delta_{\beta} = \frac{A_0 A_1}{B_0} \; .
$$

while the estimate for  $\nu$  converges as

$$
v_{L,L'} - v \sim \delta_v \frac{(L')^{-\omega}}{\ln(L/L')}
$$

with

$$
\delta_{\mathbf{v}} = -\mathbf{v}^2 \left[ B_1 - \frac{A_0 C_0 A_1}{B_0^2} \right].
$$

In the extreme case where L' is kept *finite* while  $L \rightarrow \infty$ , the convergence of  $\beta_{L,L'}$  towards  $\beta_c$  is in  $L^{-1/\nu}$ , while the convergence of  $v_{L,L'}$  towards v is in (lnL)

### C. Application to other quantities

Consider now the convergence of other analysis methods suggested in Ref. 15. Take the susceptibility  $\chi$ as a prototype of a multiplicativity renormalizable observable. We have therefore

$$
\chi_L(\beta) = L^{\gamma/\nu} [f(tL^{1/\nu}) + L^{-\omega} f_1(tL^{1/\nu}) + \cdots]. \tag{30}
$$

A way of extracting  $2-\eta=\gamma/\nu$  (and therefore  $\gamma$  if  $\nu$  is known) is to look at the maxima  $\chi_L^*$  of the curves  $\chi_L(\beta)$ , occurring for values  $t_L^*$  of t. Taking the first derivative of Eq. (30) leads to

$$
t_L^* L^{1/\nu} = x_0 + L^{-\omega} x_1 + \cdots , \qquad (31)
$$

where  $x_0$  is the solution of  $f'(x)=0$  (assume it is unique, i.e.,  $X_L$  has only one maximum for large enough L) and

$$
x_1 = -\frac{f_1'(x_0)}{f''(x_0)}.
$$
 (32)

Defining estimates of  $\gamma/\nu$  by

$$
\left[\frac{\gamma}{\nu}\right]_{L,L'} = \frac{\ln(\chi_L^*/\chi_{L'}^*)}{\ln(L/L')} \,,\tag{33}
$$

we obtain from Eqs. (30)–(32), in the limit  $L, L' \rightarrow \infty$ ,

$$
\left[\frac{\gamma}{\nu}\right]_{L,L'} - \frac{\gamma}{\nu} \sim \delta_{\gamma} L^{-\omega} \,,\tag{34}
$$

where  $\delta_{\gamma}$  reads, in the case  $L'/L = \lambda \rightarrow 1$ ,

$$
\delta_{\gamma} = -\omega \frac{f_1(x_0)}{f(x_0)} \tag{35}
$$

The same method, when applied to the specific heat, may be governed by another convergence exponent. Let us look for the values  $t_L^*$  at which the curves  $C_L(t)$  have their maxima  $C_L^*$ . The equation to be solved is [see Eq. (20)]

$$
f'_{c}(t_L^* L^{1/\nu}) + L^{-\omega} f_c^{(1)'}(t_L^* L^{1/\nu}) + L^{-\alpha/\nu} C_{reg}(t^*) + \cdots = 0.
$$

It is therefore clear that the convergence exponent of It is therefore clear that the convergence exponent of  $L^*L^{1/\nu}$  towards  $y_0$  such that  $f'_c(y_0)=0$ , and of  $(\alpha/\nu)_{L,L'}$ towards  $\alpha/\nu = 2/\nu - D$ , is the smaller between  $\alpha/\nu$  and  $\omega$ . In the example of the three-dimensional Ising model  $(\alpha/\nu=0.2 < \omega=0.8)$ ,  $\alpha/\nu$  is clearly dominant.

Assume  $\alpha/\nu < \omega$ . We then have

$$
t_L^* L^{1/\nu} = y_0 + L^{-\alpha/\nu} y_1 + \cdots, \qquad (36)
$$

with

$$
y_1 = -\frac{C'_{\text{reg}}(0)}{f'_c''(y_0)}
$$
(37)

and

(29b)

$$
\left[\frac{\alpha}{\nu}\right]_{L,L'} - \frac{\alpha}{\nu} \sim \delta_{\alpha} L^{-\alpha/\nu} \tag{38}
$$

with the same notation as for  $\gamma$ , and with

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$$
\delta_{\alpha} = -\frac{\alpha}{\nu} \frac{C_{\text{reg}}(0)}{f_c(y_0)} \qquad (39) \qquad t_L^* L^{1/\nu} = z_0 + z_1 L^{-1/\nu} + \cdots
$$

when  $L'/L = \lambda \rightarrow 1$ .

Although finite-size scaling for the specific heat has been extensively used, the large difference in asymptotic convergence laws for specific heat  $(L^{-\alpha/\nu})$  and susceptibility ( $L^{-\omega}$ ) has not been noticed in numerical works, as far as we know, even when  $\alpha \ll \omega \nu$ .

There exist other extrapolation methods, much less currently used, which break explicitly the scale invariance or the reparametrization invariance of the theory. The two following examples will clarify what we mean by these breakings.

The first case one can imagine is a situation where one cannot a priori attach the data  $Q_L$  to the size L or  $L - 1$ . This ambiguity may occur when comparing results with periodic and free boundary conditions. Let us make a model of this case by defining a modified phenomenological-renormalization equation:

$$
\frac{\xi_L(\beta)}{L-b} = \frac{\xi_{L'}(\beta')}{L'-b} , \qquad (40)
$$

where  $b$  is some unknown but constant boundary effect. Equation (26) implies that the fixed point  $\beta_{L,L}$  of the map (40) is given (in the variable  $t$ ) by

$$
t_{L,L'} = \frac{A_0}{B_0} \frac{A_1 (L^{-\omega} - L'^{-\omega}) + b(L^{-1} - L'^{-1}) + \cdots}{L^{1/\nu} - L'^{1/\nu}} \tag{41}
$$

Assume  $\omega > 1$ . Then  $\beta_{L,L'}$  and the associated estimate  $v_{L,L'}$  will converge towards  $\beta_c$  and v as

$$
\beta_{L,L'} - \beta_c \sim \delta_{\beta} L^{-(1/\nu)-1},
$$
  
\n
$$
v_{L,L'} - v \sim \delta_{\nu} L^{-1},
$$
\n(42)

with amplitudes  $\delta$  which become, in the limit  $L/L'=\lambda\rightarrow 1$ .

$$
\delta_{\beta} = -bv \frac{A_0}{B_0} = bv \frac{f(0)}{f'(0)},
$$
  
\n
$$
\delta_{\nu} = -bv^2 \frac{A_0 C_0}{B_0} = bv^2 \frac{f(0) f''(0)}{f'(0)^2}.
$$
\n(43)

Another case where convergence may not be governed by the bulk exponent  $\omega$  is the extrapolation of a nonreparametrization invariant quantity, such as an inflection *point.* Indeed, the maximum of a curve  $f(t)$  is invariant in replacing  $t \rightarrow t(t)$ , but the inflection point is not. Let us return to our example of the susceptibility, and look at the point  $t_L^*$  where  $d^2X_L/d\beta^2=0$ . Equation (30) leads to [ $\sigma$ . is as in Eq.  $(22)$ ]

$$
f''(t_L^* L^{1/\nu}) + L^{-\omega} f_1''(t_L^* L^{1/\nu}) - \sigma L^{-1/\nu} f'(t_L^* L^{1/\nu}) = 0.
$$
\n(44)

Assume  $1/\nu < \omega$ . Then  $1/\nu$  becomes the leading convergence exponent

$$
t_L^* L^{1/\nu} = z_0 + z_1 L^{-1/\nu} + \cdots \t{,}
$$
\t(45)

with

$$
f''(z_0) = 0,
$$
  
\n
$$
z_1 = \sigma \frac{f'(z_0)}{f'''(z_0)}.
$$
\n(46)

The corresponding  $(\gamma/v)_{L,L'}$  defined as in Eq. (33) converge as

$$
\left|\frac{\gamma}{\nu}\right|_{L,L'} - \frac{\gamma}{\nu} \sim \delta_{\gamma} L^{-1/\nu},\tag{47}
$$

and  $\delta_{\gamma}$  reads, in the limit  $L'/L = \lambda \rightarrow 1$ ,

$$
\delta_{\gamma} = -\frac{\sigma}{\nu} \frac{f'(z_0)^2}{f'''(z_0)} \ . \tag{48}
$$

We have certainly not exhausted all possible examples of convergence of transfer-matrix data to their therrnodynamical limit. Our main result is the introduction of corrections to finite-size scaling in Fisher's relation. These are governed by the bulk exponent  $\omega$ . Most of the applications of finite-size scaling exhibit therefore the same convergence exponent. We have nevertheless listed some cases where a special effect, existence of a regular background, ambiguity on the definition of the size, use of coordinate-dependent properties, or renormalization from L to  $L' \ll L$ , may lead to another asymptotic convergence exponent, such as  $1/v$ , 1,  $\alpha/v$  or even 0. In particular, the exponent  $1/v$  is less frequent than suggested in (Ref. 15). Other situations we have not yet explored are certainly understandable through the basic equations derived in this section.

### III. EXAMPLE OF THE O(N) ( $N \rightarrow \infty$ ) SPIN MODEL

In this section we reply to, in the particular case of a soluble model, some of the questions left unanswered in Sec. II: How large are the correction amplitudes  $\delta$ ; what range of values of L is really governed by the exponent  $\omega$ ?

### A. Exact solution for arbitrary  $D > 2$

This section is essentially a continuation of Brézin's work<sup>13</sup> on the large-N limit. Consider the  $O(N)$  spin model on a. D-dimensional hypercubic lattice with arbitrary finite-range ferromagnetic translationally invariant couplings  $K_{ij} = K(i - j)$ ,

$$
H = -\frac{N}{2} \sum_{i,j} K_{ij} \vec{S}_i \cdot \vec{S}_j , \qquad (49)
$$

and the constraint  $\vec{S}_{i}^{2}=1$  at each site. It is known since the work of Stanley<sup>22</sup> that this model considerably simplifies in the large- $N$  limit. Consider its partition function

$$
Z = \int \left[ \prod_i d^N S_i \right] \left[ \prod_i \delta(\vec{S}_i^2 - 1) \right] \exp \left[ \frac{N\beta}{2} \sum_{i,j} K_{ij} \vec{S}_i \cdot \vec{S}_j \right].
$$
\n(50)

By introducing a Fourier representation of the  $\delta$  function, we obtain a Gaussian integral over  $\vec{S}_i$ , leading to

$$
Z = \int \left[ \prod_{i} d\alpha_{i} \right] \exp \left[ N \left[ \sum_{i} \alpha_{i} - \frac{1}{2} \text{Tr} \ln(2\alpha - \beta K) + \text{const} \right] \right], \tag{51}
$$

where the operator  $\alpha$  has matrix elements  $\alpha_{ij} = \alpha_i \delta_{ij}$ .

The large- $N$  limit is dominated by the saddle point with lowest effective action. In the infinite volume, as well as on a bar with periodic boundary conditions, this saddle point is constant:

$$
\alpha_i = \alpha_c \quad \text{for all } i
$$

with

$$
\left\langle 0 \left| \frac{1}{2\alpha_c - \beta K} \right| 0 \right\rangle = 1 . \tag{52}
$$

The situation with any other type of boundary condition is much more complicated.<sup>17</sup> Let us introduce the notation

$$
\widetilde{K}(q) = \sum_{n} K(n)e^{-iq_{\mu}n_{\mu}},
$$
\n
$$
K(q) = \widetilde{K}(0) - \widetilde{K}(q).
$$
\n(53)

We shall restrict ourselves to isotropic ferromagnetic models, and *normalize*  $\beta$  such that

$$
K(q) = q^2 + O(q_\mu^4) \tag{54}
$$

The usual nearest-neighbor model corresponds to

$$
K(q) = 2 \sum_{\mu} (1 - \cos q_{\mu}).
$$
 (55)

The solution of Eq. (52) reads as the following.

(1) Infinite volume:  $\alpha_c = (\beta/2)[m^2 + \tilde{K}(0)]$  with

$$
\beta = \int d\tilde{q} \frac{1}{m^2 + K(q)} \,, \tag{56}
$$

where  $\int d\tilde{q}$  is the normalized measure on the Brillouin zone.

(2) Bar with transverse size L:  $\alpha_c = (\beta/2)[m_L^2 + \tilde{K}(0)]$ with

$$
\beta = \int \frac{dq_{||}}{2\pi} \sum_{q_{\perp}} \frac{1}{m_{L}^{2} + K(q)} , \qquad (57)
$$

$$
\sum_{q_1} = \frac{1}{L^{D-1}} \sum_{0 \le n_\mu \le L-1}
$$

where  $q_{\mu} = (2\pi/L)n_{\mu}$  for each direction  $(1 \leq \mu \leq D - 1)$ .

When they are small, the quantities m and  $m<sub>L</sub>$  can be identified with the inverse correlation lengths  $\xi^{-1}$  and  $\xi_L^{-1}$ , respectively. The difference between  $m^{-1}$  and the genuine correlation length [defined as the nearest complex zero of  $m^2 + K(q)$ ] has a relative weight  $\xi^{-2}$ . Other  $D > 2$ )

$$
\beta_c = \int d\tilde{q} \frac{1}{K(q)} = \left\langle 0 \left| \frac{1}{K} \right| 0 \right\rangle . \tag{58}
$$

We define the scaling variables

$$
x = \frac{L}{\xi}, \ \ y = \frac{\xi_L}{\xi}, \ \ z = \frac{y}{x} = \frac{\xi_L}{L}
$$
 (59)

and hence

$$
\xi^{-1} = m = \frac{x}{L}, \quad \xi_L^{-1} = m_L = \frac{x}{yL} = \frac{1}{zL}.
$$

The domain of interest of finite-size scaling is therefore  $L\rightarrow\infty$  at fixed x.

Equation (57) can be transformed (by using Poisson summation formula) into

$$
\beta = \sum_{n_1} I(n_1) \text{ with } I(n_1) = \int d\tilde{q} \frac{e^{iq_1 n_1 L}}{m_L^2 + K(q)} , \qquad (60)
$$

where  $n_1$  describes  $\mathbb{Z}^{D-1}$ . The term  $n_1=0$  is just the infinite-volume temperature corresponding to mass  $m<sub>L</sub>$ .

We obtain therefore, by subtracting (56) from (60),

(61) 
$$
t(m_L) - t(m) = S(m_L),
$$

where

$$
t(m) = \beta_c - \beta = m^2 \int d\tilde{q} \frac{1}{[m^2 + K(q)]K(q)}
$$
(62)

and

$$
S(m_L) = \sum_{n_1(\neq 0)} I(n_1) \ . \tag{63}
$$

Let us first estimate  $S(m<sub>L</sub>)$  in our domain of interest.  $I(n_+)$  can be rewritten as

$$
I(n_1) = \int d\alpha \, e^{-\alpha m_L^2} \prod_{\mu} \left[ \int \frac{dq_{\mu}}{2\pi} e^{iq_{\mu}n_{\mu}L - \alpha q_{\mu}^2} [1 + O(q_{\mu}^4)] \right].
$$

The leading term gives after integration

$$
S(m_L) = (4\pi)^{-D/2} L^{2-D} F_0(z) , \qquad (64)
$$

with  $z$  as in (59) and

where  
\n
$$
F_p(z) = \int_0^\infty t^{p-D/2} e^{-t/z^2} g(t) dt,
$$
\n
$$
\sum_{q_1} = \frac{1}{L^{D-1}} \sum_{0 \le n_\mu \le L-1} g(t) = \left[ \sum_{n \in \mathbb{Z}} e^{-n^2/4t} \right]^{D-1} - 1.
$$
\n(65)  
\nwhere  $a_\mu = (2\pi/L) n_\mu$  for each direction  $(1 < \mu < D - 1)$ 

Equations (64) and (65) give a well-defined continuation of the asymptotic large- $L$  behavior of Eq. (63) to noninteger values of D. The following asymptotic behaviors of the functions  $F_p$  will be useful throughout this section:

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$$
F_p(z) \sim \begin{cases} (4\pi)^{(D-1)/2} \Gamma(p+\frac{1}{2}) z^{2p+1} [1+O(z^{-(D-1)})] & \text{as } z \to \infty ,\\ 2^{(D+1)/2-p} \pi^{1/2} (D-1) z^{p+3/2-D/2} e^{-1/z} [1+O(z)] & \text{as } z \to 0 . \end{cases}
$$
(66)

The nonuniversal  $O(q_\mu^4)$  terms give corrections to (65) which have a relative weight  $L^{-2}$ . They will be negligible throughout the following [see remark after Eq. (57)].

Consider now the small-m behavior of  $t(m)$ , and define for that purpose its Mellin transform:

$$
M(s) = \int_0^\infty dm \, m^{s-1} t(m) \,. \tag{67}
$$

It is easy to check that  $M(s)$  is defined through (67) for  $Res > 2-D$  and  $-2 < Res < 0$  (these domains intersect for  $D > 2$ ), and that it is related by

$$
M(s) = -\frac{\pi}{2\sin(s\pi/2)}J(s)
$$
 (68)

to the following transform of the couplings:

$$
J(s) = \int d\tilde{q} K(q)^{s/2 - 1} = \langle 0 | K^{s/2 - 1} | 0 \rangle .
$$
 (69)

Since  $K_{ij}$  is a finite-range operator,  $K(q)$  is an analytic even function of each  $q_{\mu}$ . The poles of  $J(s)$  are therefore located at  $s = 2 - D - 2n$   $(n = 0, 1, 2, ...)$ . The corresponding residues are not explicitly computable, except the first one:

$$
Res(J, 2-D) = \frac{2(4\pi)^{-D/2}}{\Gamma(\frac{1}{2}D)}.
$$
 (70)

The analytic continuation of  $M$  has therefore a double series of poles:

$$
s = -2, -4, -6, \ldots,
$$
  

$$
s = 2-D, -D, -2-D, \ldots.
$$

In order to pursue our study of finite-size scaling, we have to deal successively with three cases:  $2 < D < 4$ ,  $D = 4$ , and  $D > 4$ .

### B. The normal case  $(2 < D < 4)$

In order to study the leading correction to finite-size scaling, let us take into account the first two terms in the scaling, let us take into account the rifst two terms in the expansion of  $t(m)$  for small m. These are given by the poles of M at  $s = 2-D$  and  $s = -2$ :

$$
t(m) = -(4\pi)^{-D/2} \Gamma(1 - \frac{1}{2}D)m^{D-2}
$$
  
+
$$
J(-2)m^{2} + O(m^{D}).
$$
 (71)

Equation (71) gives in particular the well-known values of the exponents  $\omega$  and  $\nu$  in the large-N limit:

$$
v = \frac{1}{D-2}
$$
,  $\omega = 4-D$  for  $2 < D < 4$ .

If we consider only the leading term in (71), we can rewrite Eq. (61) in terms of the scaling variables:  $x = L/\xi$ and  $y = \xi_L / \xi = xz$ , namely

$$
\Gamma(1 - \frac{1}{2}D)(x^{D-2} - z^{2-D}) = F_0(z) . \tag{72}
$$

This relation is precisely Fisher's finite-size scaling equation for the correlation length. As expected, it is universal ( $F_0$  does not depend on  $K_{ij}$  at all).

The limits of Eq. (72) when x goes to 0 and  $\infty$  deserve some special interest. The behavior of  $y(x)$  for large x has been recently analyzed<sup>23</sup> for arbitrary models, including lattice gauge theories, in terms of integral equations involving elastic diffusion amplitudes. In the present case, we have the following behavior:

$$
1 - y \sim \frac{D - 1}{\Gamma(2 - \frac{1}{2}D)} \pi^{1/2} (x/2)^{(1 - D)/2} e^{-x} . \tag{73}
$$

This relation can be continued to  $D = 2$ . In order to compare the O( $\infty$ ) models to other ones in  $D = 2$ ,  $^{23}$  and  $D = 2$ and  $D = 3$  for the O( $\infty$ ) model, we give in Table I the values of  $y = \xi_L / \xi$  corresponding to some particular values of  $x$ , in two and three dimensions. (That question is meaningless in  $D > 4$ : see Secs. III C and III D). (See also Figs. 2 and 3.)

The  $x \rightarrow 0$  limit of Eq. (72) gives a universal amplitude A (denoted  $A_0$  in Sec. II) such that

$$
\xi_L(\beta_c) \sim AL \quad \text{for } L \gg 1 \; . \tag{74}
$$

The universality of  $A$  is a consequence of the universality of Fisher's scaling function.<sup>5,6,24</sup>

A is the solution of

|  $\pi \epsilon$ 

$$
-\Gamma(1-\tfrac{1}{2}D) = A^{D-2}F_0(A) \tag{75}
$$

A is clearly universal (independent of  $K_{ij}$  and of any reparametrization of  $\beta$ ). When  $D \rightarrow 2$  or 4, A diverges according to

$$
A \sim \begin{cases} (4\pi^2 \epsilon)^{-1/3} & \text{for } D = 4 - \epsilon \;, \\ \frac{1}{\pi \epsilon} & \text{for } D = 2 + \epsilon \;. \end{cases}
$$
 (76a)

Figure <sup>1</sup> shows a plot of A versus dimension D.

The quantity  $A$  has been the subject of some interest in wo dimensions,  $1,25,26$  where it is related for a very large variety of isotropic systems to the critical exponent  $\eta$ :

$$
A\eta = \frac{1}{\pi} \tag{77}
$$

TABLE I. Values of  $y = \xi_L / \xi$  corresponding to some particular values of  $x = L/\xi$  for the O( $\infty$ ) model in two and three dimensions.





FIG. 1. Universal amplitude A such that  $\xi_L(\beta_c) \sim AL$  as a function of the dimensionality D.

This equation has been generalized to anisotropic systems,  $^{26}$  and to the Hamiltonian formalism<sup>27,28</sup> in  $1 + 1$  dimensions.

The existence of this universal relation between  $A$  and  $\eta$  has been recently related<sup>29</sup> to conformal invariance of two-dimensional critical theories. It is therefore not very surprising that, for  $D > 2$  where the conformal invariance is much less restrictive,  $A$  is not simply related to critical exponents. Equation (75) suggests that the relation between  $A$  and other universal quantities such as amplitude ratios, if any, is far from being as simple as (77).

In two dimensions, Eqs. (71) and (72) become, respectively,

$$
t(m) = -\frac{1}{2\pi} \ln \frac{m}{\Lambda_0} + O(m^2 \ln m) , \qquad (78)
$$

where  $\Lambda_0$  is a model-dependent constant ( $\Lambda_0$ =5.6568 in the nearest-neighbor model) and

$$
F_0(z) = -2\ln y \tag{79}
$$

The small- $x$  behavior of  $y$  is therefore

$$
y \sim -\frac{1}{\pi} x \ln x \tag{80}
$$

In other words, although finite-size scaling is valid [the function  $y(x)$  does exist], we do not have (74) at  $\beta = \beta_c = \infty$ . Figures 2 and 3 show plots of the function  $y(x)$  in two and three dimensions.

Let us now include the leading correction term to the finite-size scaling relation (72):

$$
\Gamma(1-\frac{1}{2}D)(x^{D-2}-z^{2-D})
$$
  
 
$$
+(4\pi)^{D/2}J(-2)L^{-\omega}(z^{-2}-x^{2})=F_{0}(z).
$$
 (81)

The correction term is in  $L^{-\omega}(\omega=4-D)$ , as expected from Sec. II. It is of course nonuniversal, but depends on



FIG. 2. Finite-size scaling relation between  $x = L/\xi$  and  $y = \xi_L / \xi$  in two dimensions.

the couplings  $K_{ij}$  through one number:  $J(-2)$ . Moreover, as  $D\rightarrow 4$ ,  $J(-2)$  becomes universal, in the sense that we obtain

$$
J(-2) \sim -\frac{1}{8\pi^2 \epsilon} \quad \text{in } D = 4 - \epsilon \tag{82}
$$

independently of the  $K_{ij}$  and the normalization (54) of  $\beta$ .

As  $D \rightarrow 2$ ,  $J(-2)$  is dominated by the residue of J at  $s = -D$ . Its dependence upon  $K_{ij}$  is therefore explicitly tractable. Assume we have only on-axis couplings, such that

$$
K(q) = q^2 + \lambda \sum_{\mu} q_{\mu}^4 + O(q_{\mu}^6)
$$
 (83)

[notice that the ordinary nearest-neighbor couplings (55) lead to  $\lambda = -\frac{1}{12}$ . We have then



FIG. 3. Finite-size scaling relation between  $x = L/\xi$  and  $y = \frac{\xi_L}{\xi}$  in three dimensions. The slope at the origin is  $A = 0.661395...$ 

$$
J(-2) \sim -\frac{3\lambda}{4\pi\epsilon} \quad \text{for } D = 2 + \epsilon \; . \tag{84}
$$

Whenever  $\lambda$  is negative,  $J(-2)$  vanishes at least once in the interval  $2 < D < 4$ . In the nearest-neighbor case,  $J(-2)=0$  for  $D=3.322178...$ 

In three dimensions, there exists no easy way to predict even the sign of  $J(-2)$ . Therefore, we have investigated numerically  $J(-2)$  in the case of on-axis couplings  $K_1 > 0$  between nearest neighbors and  $K_2$  between sites at distance 2 along each axis. Let r denote the ratio  $K_2/K_1$ . The absolute normalization of  $K_1, K_2$  being fixed by Eq. (54), every nonuniversal quantity is a function of  $r$ . In order to keep a ferromagnetic model, we have to take  $r > -\frac{1}{4}$ . Figures 4 and 5 show the variations of  $\beta_c$  and  $J(-2)$  versus r. Notice that  $J(-2)$  vanishes for a very small value of  $r (r \sim -0.041)$ .

The most interesting application of (81) is the prediction of the convergence amplitudes  $\delta_{\beta}, \delta_{\nu}$  defined in Sec. III8, and the comparison with actual results of the phenomenological-renormalization-group transform (2)— (4) in three dimensions.

By expanding the solution  $z(x)$  of Eq. (81) around  $z(0) = A$  in a double series in t [see Eq. (62)] and  $L^{-\omega}$ , we can compute the various coefficients of Eq. (27) as a function of the universal quantity  $J(-2)$  [ $\beta$  is as in (54)]:

$$
A_1 = \frac{(4\pi)^{D/2}J(-2)}{\Delta(A)},
$$
  
\n
$$
B_0 = \frac{(4\pi)^{D/2}A^3}{\Delta(A)},
$$
  
\n
$$
B_1 = \frac{(4\pi)^{D/2}J(-2)}{A^2\Delta(A)^2}
$$
  
\n
$$
\times [2A^2F_1(A) - 4F_2(A)
$$
  
\n
$$
-(D-2)(D-3)\Gamma(1-\frac{1}{2}D)A^{6-D}],
$$
 (85)

$$
C_0 = \frac{(4\pi)^D A^3}{\Delta(A)^3}
$$
  
×[6A<sup>2</sup>F<sub>1</sub>(A) - 4F<sub>2</sub>(A)

$$
-(D-1)(D-2)\Gamma(1-\tfrac{1}{2}D)A^{6-D}\,,
$$

with the notation (66) and

$$
\Delta(A) = 2F_1(A) - (D-2)\Gamma(1 - \frac{1}{2}D)A^{4-D}.
$$
 (86)

We have therefore  

$$
\beta_{L,L-1} - \beta_c \sim \delta_{\beta} L^{-\omega - 1/\nu}
$$

with

$$
\delta_{\beta} = \frac{4 - D}{D - 2} \frac{J(-2)}{A^2} ,
$$
\n(87)

$$
v_{L,L-1} - v \sim \delta_v L^{-\omega}
$$



FIG. 4. Critical temperature  $\beta_c$  as a function of the ratio r of second-neighbor to nearest-neighbor interactions, in three dimensions.

with

$$
\delta_v = -2 \frac{4-D}{(D-2)^2} \frac{(4\pi)^{D/2} J(-2)}{\Delta(A)}
$$

When  $D$  goes to 4, we have the following universal behavior:

$$
\delta_{\beta} \sim -\frac{1}{4} \left[ \frac{\epsilon}{2\pi} \right]^{1/3}, \ \delta_{\nu} \sim \frac{\epsilon}{6} \ \text{for} \ D = 4 - \epsilon \ .
$$
 (88)

When D goes to 2,  $\delta_{\beta}/\beta_c$  and  $\delta_{\nu}/\nu$  vanish in a nonuniversal way. In the case of on-axis couplings [see Eqs. (83) and (84)], we obtain



FIG. 5. Same as in Fig. 4 for the quantity  $J(-2)$  which governs all corrections to finite-size scaling.

$$
\frac{\delta_{\beta}}{\beta_c} \sim -3\pi^2 \lambda \epsilon, \quad \frac{\delta_{\nu}}{\nu} \sim 6\pi^2 \lambda \epsilon \quad \text{for } D = 2 + \epsilon \; . \tag{89}
$$

Let us restrict ourselves to nearest-neighbor couplings in order to compare our predictions with actual data. The relative convergence amplitudes  $\delta_{\beta}/\beta_c$  and  $\delta_{\nu}/\nu$  for nearest-neighbor interactions are plotted as functions of D on Figs. 6 and 7, respectively. In three dimensions, they read

$$
\delta_{\beta} = 0.027 8073... ,
$$
  
\n
$$
\delta_{\nu} = -0.150 144... .
$$
 (90)

The phenomenological-renormalization equations (3) and (4) are very easy to handle numerically in our  $O(\infty)$ and (4) are very easy to handle numerically in our  $O(\omega)$ <br>model, because the relation between  $m_L = \xi_L^{-1}$  and  $\beta$  is explicit in the case of nearest-neighbor couplings, where (57) gives, by integration,

$$
\beta = \frac{1}{L^{D-1}}
$$
  
 
$$
\times \sum_{0 \le n_{\mu} \le L-1} \left[ \left( m_{L}^{2} + 4 + 2 \sum_{\mu} (1 - \cos q_{\mu}) \right) \times \left( m_{L}^{2} + 2 \sum_{\mu} (1 - \cos q_{\mu}) \right) \right]^{-1/2}, \quad (91)
$$

where  $q_{\mu} = (2\pi/L)n_{\mu}$  for  $1 \leq \mu \leq D - 1$ .

Figures 8–11 show our results for  $\beta_{L,L-1}$  and  $v_{L,L-1}$ versus the appropriate power of L, up to  $L = 50$ . The straight lines indicate the asymptotic behaviors according to Eqs. (87)—(90).



FIG. 6. Relative convergence amplitude  $\delta_{\beta}/\beta_c$  of the phenomenological-renormalization estimates for the critical temperature  $\beta_c$ , for nearest-neighbor interactions, as a function of dimensionality.



FIG. 7. Same as Fig. 6, for the critical exponent  $\nu$ .

The agreement for  $\beta_c$  (Fig. 8) is surprisingly bad. We have willingly plotted on this figure the data for  $L = 2$  to 6 exclusively, since  $L = 5$  or 6 seems to be the largest size that can be treated exactly by the transfer-matrix approach for Ising-type three-dimensional systems.<sup>30,31</sup> Even the sign of the correction disagrees with the analytical prediction. If one pursues the analysis to totally unrealistic sizes (Fig. 9), one obtains finally an agreement with the



FIG. 8. Phenomenological-renormalization estimates for the critical temperature  $\beta_c$ , in three dimensions. The straight line represents the asymptotic estimate of Eq. (87).



FIG. 9. Enlargement of Fig. 8 showing larger values of L.

asymptotic behavior, after a maximum at  $L = 11$ . This situation is related to the fact that  $J(-2)$  is anomalously small  $[J(-2)$  vanishes when 4% second neighbor couplings are present].

The convergence of the estimates  $v_{L,L-1}$  is much more regular, and agrees with its asymptotic estimate even for small sizes, after a smooth minimum at  $L = 4$ . A more realistic situation, namely 2D percolation, also exhibits this wild discrepancy between finite-size corrections up to  $L \sim 10$  and their asymptotic regime.<sup>14</sup> These "crossover sizes"  $L \sim 10$  or 11 have of course no precise meaning. One has only to be aware of the fact that they may be large, and larger than the numerically tractable sizes.



FIG. 10. Same as Fig. 8, for the critical exponent  $\nu$ , in three dimensions.



FIG. 11. Enlargement of Fig. 10 showing larger values of L.

### C. The marginal case ( $D = D<sub>c</sub> = 4$ )

This section is devoted to the upper critical dimensionality ( $D<sub>c</sub> = 4$ ), where logarithmic corrections affect the bulk properties. We shall show how similar logarithmic behaviors are exhibited by quantities on bars of size I..

For  $D=4$ , the Mellin transform of t has only double poles at  $s = -2, -4, -6, \ldots$ . We have then

$$
t(m) = -\frac{1}{8\pi^2}m^2\ln\frac{m}{\Lambda_0} + O(m^4\ln m)
$$
 (92)

 $(\Lambda_0 = 10.978...$  in the nearest-neighbor model).

Therefore, the scaling variables  $x$  and  $z$  are related through

$$
2z^{-2}\ln(zL\Lambda_0) - 2x^2\ln(x^{-1}L\Lambda_0) = F_0(z) . \tag{93}
$$

The presence of logarithms of  $L$  in (93) violates finite-size scaling. One can nevertheless recast (93) into a modified scaling form by defining<br> $\int \ln I^{-1/3}$ 

$$
X = \left[\frac{\ln L}{4\pi^2}\right]^{1/3} x ,
$$
  
\n
$$
Z = \left[\frac{\ln L}{4\pi^2}\right]^{-1/3} z .
$$
\n(94)

The relation between  $X$  and  $Z$  is now well behaved in the large- $L$  limit:

$$
Z^3 + (ZX)^2 - 1 = 0 \tag{95}
$$

This modified finite-size scaling relation is as universal as the "normal" one [Eqs. (1) and (72)]. At  $\beta = \beta_c$  (X  $=0 \implies Z = 1$ ) we have<sup>13</sup>

$$
\xi_L(\beta_c) = L \left[ \frac{\ln L}{4\pi^2} \right]^{1/3} \left[ 1 + \frac{4\pi^2}{9} \frac{\ln \ln L}{\ln L} + \cdots \right].
$$
 (96)

Consider now the effects of the modified scaling laws on the phenomenological-renormalization group. Following Sec. II, we estimate first the successive derivatives of  $\xi_L(\beta)$  at  $\beta_c$ . The preceding equations lead to

$$
\frac{d\xi_L}{d\beta}(\beta_c) = \frac{2}{3}L^3 \left[1 + \frac{1}{3\ln L} + \cdots \right],\tag{97}
$$

$$
\frac{d^2 \xi_L}{d\beta^2}(\beta_c) = \frac{8}{9}L^5 \left(\frac{4\pi^2}{\ln L}\right)^{1/3} \left[1 + O\left(\frac{1}{\ln L}\right)\right].
$$
 (98)

These formulas allow us to estimate the fixed point  $\beta_{L,L'}$  of Eq. (2) in the limit  $L,L' \rightarrow \infty$  at fixed ratio  $\lambda = L'/L$ :

$$
\beta_{L,L'} - \beta_c \sim -\frac{1}{2} L^{-2} (2\pi \ln L)^{-2/3} \frac{\ln \lambda}{\lambda^2 - 1} \ . \tag{99}
$$

When  $\lambda \rightarrow 1$ , this becomes

$$
\beta_{L,L'} - \beta_c \sim -\frac{1}{4} L^{-2} (2\pi \ln L)^{-2/3} \ . \tag{100}
$$

The critical exponent v associated with  $\beta_{L, L'}$  through Eq. (4) converges towards the mean-field value  $\frac{1}{2}$  as

$$
\nu_{L,L'} - \frac{1}{2} \sim \frac{1}{6 \ln L} \quad \text{for all } \lambda . \tag{101}
$$

The convergence of phenomenological-renormalization data is therefore very slow at the upper critical dimension. It is also totally independent of the couplings  $K_{ij}$ .

As in the 3D model, we have solved numerically Eqs. (2)–(4), using Eq. (91), up to  $L=100$ . Figures 12 and 13 show plots of the data  $(\beta_{L,L-1} - \beta_c)L^2$  versus  $(\ln L)^{-2/3}$ and  $v_{L,L-1}$  versus  $(lnL)^{-1}$ . The straight lines indicate the asymptotic behaviors (100) and (101). These behaviors are reasonably obeyed by the finite-size data, although the scales are logarithmic.



FIG. 12. Same as Fig. 8, for the critical temperature  $\beta_c$ , in four dimensions.



FIG. 13. Same as Fig. 8, for the critical exponent  $\nu$ , in four dimensions.

### D. The anomalous case ( $D > 4$ )

Let us consider finally dimensionalities larger than the upper critical one. The application of the phenomenological renormalization to realistic systems at  $D > D_c$  seems of no practical significance for at least three reasons: The main goal of the method, namely the critical exponents, are known to be those of the mean-field theory, ' the transfer-matrix method is essentially adapted to low dimensions ( $D = 2$  and 3 in some cases); finally, finite-size scaling is known to be modified.<sup>8,13,2</sup>

We aim nevertheless to consider this case, because the large- $N$  limit allows for an explicit analysis of modified finite-size scaling in mean-field-like models, a subject which has been considered in other circumstances; systems which are infinite in  $(D-1)$  directions,<sup>33</sup> or finite in all directions.  $8,9,14$ 

Another interest of this anomalous case is that some models, for which  $D<sub>c</sub>$  is unknown, and which are easily tractable by the transfer-matrix approach, may exhibit analogous behaviors. For  $D > 4$ , the leading behavior of  $t(m)$  is governed by the pole of M at  $s = -2$ :

$$
t(m)=J(-2)m^{2}+O(m^{2+\Omega}), \qquad (102)
$$

and the correction exponent  $\Omega$  is given by the location of the second nearest pole of  $M$ , namely

$$
\Omega = D - 4 \quad \text{for } 4 < D \le 6 \tag{103}
$$
\n
$$
\Omega = 2 \quad \text{for } D \ge 6 \tag{103}
$$

The relation between  $x = L/\xi$  and  $z = \xi_L/L$  reads therefore

$$
2J(-2)[1-(zx)^2] = L^{4-D}z^3 + O((zL)^{-\Omega}).
$$
 (104)

The power of  $L$  in the right-hand side of  $(104)$  is a source of breaking of finite-size scaling.<sup>13</sup> A modified scaling relation can be found between the variables

$$
X = [2J(-2)L^{D-4}]^{1/3}x ,
$$
  
\n
$$
Z = [2J(-2)L^{D-4}]^{-1/3}z ,
$$
\n(105)

 $31$ 

which satisfy the same universal equation as in  $D = 4$ ,

$$
Z^3 + (ZX)^2 - 1 = 0 \tag{106}
$$

up to corrections of order  $L^{-\omega'}$  with

$$
\omega' = \frac{D-1}{3} \Omega = \begin{cases} \frac{(D-1)(D-4)}{3} & \text{for } 4 < D \le 6 ,\\ \frac{2}{3}(D-1) & \text{for } D \ge 6 . \end{cases}
$$
 (107)

Equation (106) means that  $\xi_L$  and  $\xi$  are asymptotically related through

$$
\xi_L = \xi f((L/\xi)L^{(D-4)/3}), \qquad (108)
$$

and that, for instance, we have at the critical point

$$
\xi_L(\beta_c) \sim L \left[ 2J(-2)L^{D-4} \right]^{1/3} . \tag{109}
$$

It has been suggested<sup>8,9,32</sup> to write the finite-size scaling relation in the case of a box of size  $L^D$  as follows:

$$
Q_L = Q_\infty f_Q(N/N_c) , \qquad (110)
$$

where  $N = L^D$  is the volume of the system and  $N_c$  is a correlation volume:

$$
N_c = \xi^D (D < D_c) \quad \text{or} \quad \xi^{D_c} (D > D_c) \tag{111}
$$

In the present case, since one dimension of our bars is infinite, we propose to extend (110) by introducing a correlation transverse volume:

$$
N_c = \begin{cases} \xi^{D-1} & (D < D_c) \text{ or } \xi^{D_c - 1}, (D > D_c). \end{cases}
$$
 (112)

It is now easy to check that (108) and (110) are equivalent with the definition (112) of  $N_c$ , and with  $N = L^{D-1}$ (transverse volume of the bar).

This proves that the relation (110), proposed by Botet et al. to synthesize in one formula both the normal and modified finite-size scaling laws, is valid in the large- $N$ limit. Let us now forget about this, and apply to the model the usual phenomenological-renormalization group. Consider as above the limit  $L, L' \rightarrow \infty$  at fixed ratio  $\lambda = L'/L$ .

Then Eq. (2) reads, in terms of the variables  $X, Z$ ,

$$
Z(X) = \lambda^{(D-4)/3} Z(X\lambda^{(D-1)/3}) \tag{113}
$$

The solution of  $(113)$  is explicitly given by

$$
Z = Z_0(\lambda) = \left(\frac{\lambda^2 - 1}{\lambda^2 - \lambda^{4-D}}\right)^{1/3},
$$
  
\n
$$
X = X_0(\lambda) = (1 - \lambda^{4-D})^{1/2}(\lambda^2 - \lambda^{4-D})^{-1/6}(\lambda^2 - 1)^{-1/3}.
$$
 (114)

The convergences of  $\beta_{L,L'}$  towards  $\beta_c$  is therefore asymptotically governed by

$$
\beta_{L,L'} - \beta_c \sim -\left[\frac{J(-2)}{4}\right]^{1/3} X_0(\lambda)^2 L^{-(2/3)(D-1)}.
$$
\n(115)

The corresponding estimate  $v_{L,L}$  of the critical exponent v in the  $L, L' \rightarrow \infty$  limit is such that

$$
1 + \frac{1}{\nu_{L,L'}} = \frac{2}{3}(D-1)
$$
  
+ 
$$
\frac{\ln[(\partial Z/\partial X)(X_0\lambda^{(D-1)/3}/(dZ/dX)(X_0)]}{\ln \lambda}
$$
 (116)

Namely,  $v_{L,L'}$  converges as  $L, L' \rightarrow \infty$  towards an *apparent* critical exponent  $v(\lambda)$  depending on the ratio  $\lambda = L'/L$ :

$$
v(\lambda) = v \left[ \frac{1}{\lambda} \right]
$$
  
= 
$$
\frac{\ln \lambda}{\ln[(3\lambda^2 - 2\lambda^{4-D} - 1)/(-3\lambda^{2-D} + 2 + \lambda^{4-D})]}
$$
 (117)

As  $\lambda$  varies from 0 to 1,  $v(\lambda)$  decreases from the correct mean-field value  $\frac{1}{2}$  until

$$
v(1) = \frac{D-1}{3(D-2)} \tag{118}
$$

Just as in  $D = 3$  and 4, we have also solved numerically Eqs. (2)—(4). Figures 14 and 15 show plots of the data  $\mathcal{B}_{L,L-1} - \mathcal{B}_c$  versus  $L^{-8/3}$  and  $v_{L,L-1}$  versus  $L^{-8/3}$ 

Let us conclude this section with a remark which may contradict intuition: If we compute estimates  $\overline{v}_{L,L'}$  of v by using the exact  $\beta_c$ , instead of the fixed point of (2)  $\beta_{L,L}$ , then these estimates  $\bar{v}_{L,L}$  converge towards

$$
\overline{v} = \frac{1}{D - 2} \tag{119}
$$

when  $L, L' \rightarrow \infty$  for arbitrary  $\lambda$ . This value  $\overline{v}$  is always worse, i.e., further from the correct value  $\frac{1}{2}$  than  $v(\lambda)$ .

The anomalous finite-size phenomena, occurring in the mean-field domain  $(D > D<sub>c</sub>)$ , in particular the modified



FIG. 14. Same as Fig. 8, for the critical temperature  $\beta_c$ , in five dimensions.



FIG. 15. Same as Fig. 8, for the critical exponent  $\nu$ , in five dimensions.

scaling law (110), and the dependence of the phenomenological-renormalization results upon the way of defining the flow (here, the value of  $\lambda$ ), are very reminiscent of the fact that the corresponding  $(\vec{\phi}^2)^2$  field theory is not renorrnalizable. In other words, even in the critical limit, physical quantities still depend on the lattice spacing a, and hence scaling laws may involve powers of the dimensionless ratio  $\xi/a$ . Other well-known pathologies of mean-field theory, e.g., the breakdown of hyperuniversality relations such as  $2-\alpha = Dv$ , are also consequences of the fact that two length scales remain present in the critical regime for  $D > D_c$ .

### IV. REMARKS AND CONCLUSIONS

We have presented in this paper two kinds of results concerning the convergence of exact finite-size lattice methods such as the phenomenological-renormalization group. The first class of results is a consequence of an estimation of corrections to finite-size scaling laws in the general framework of field theory: the leading correction to Fisher's ansatz is the product of  $L^{-\omega}$  by another scaling function of dimensionless ratios such as  $tL^{1/\nu}$ . The transfer-matrix estimates for critical points and exponents transter-matrix estimates for critical points and exponents<br>have therefore generally the same  $L^{-\omega}$  asymptotic convergence law. In some cases: use of a nonmultiplicatively renormalizable quantity (specific heat), of characteristics which vary under reparametrization (inflection point) or of two very different sizes, the finite-size estimates may obey a different convergence law.

The large- $N$  limit is one of the very few opportunities of having analytical results, and therefore a good quantitative understanding of finite-size effects. As far as we know, convergence amplitudes such as  $\delta_{\beta}$  or  $\delta_{\nu}$  had been computed exactly only in the 2D Ising model.<sup>1</sup> Our approach shows that the convergence amplitudes, as well as the range of values of  $L$  for which the convergence is close to its asymptotic regime, depend on intricate and nonintuitive quantities, such as  $J(-2)$  in the  $O(\infty)$ model. The prediction of the variation of these corrections with the details of the model, and even the prediction of their sign, is more difficult than solving the model in the thermodynamical limit. It is therefore hopeless to find a procedure which would give the optimal interacions which minimize the finite-size effects, e.g., the equivalent for realistic models of the value of  $r$  which makes  $J(-2)$  vanish in 3D.

Moreover, different quantities in the same model may exhibit very different convergence regimes: the example of  $\beta_c$  and v in 3D is quite illustrative of this phenomenon. These nonmonotonous and long transient regimes before the genuine large- $L$  behavior are certainly not a pathology of the  $N = \infty$  limit. One should therefore be extremely prudent when dealing with corrections to scaling, in particular in extracting the bulk correction-to-scaling exponent  $\omega$  from phenomenological-renormalization data, or reciprocally in using the value of  $\omega$  (when it is known) in order to improve the convergence of these data.

The present analysis of corrections to finite-size scaling, although it has been motivated by transfer-matrix methods, could be applied to other finite-size numerical studies. For instance, in some Monte Carlo renormalization-group methods, when two lattices of size  $L$  and  $2L$  have their couplings adjusted to present the same ratio  $L/\xi$ , the finite-size effects should decrease same ratio  $L/\xi$ , the finite-size effects should decrease<br>only as  $L^{-\omega}$ , i.e., rather slowly for some 3D models. More generally, systematic finite-size effects in whatever system with an extent  $L$  comparable to its correlation length are expected to be of order  $L^{-\omega}$ .

Note added in proof. In Sec. II C we studied the susceptibility as an example of multiplicatively renormalizable quantities. Although the quoted results are valid for a generic multiplicative quantity, our example is not judiciously chosen, since  $\chi_L(\beta)$  has no maximum for finite transverse size L. It scales indeed like  $L^{D-1}$  for  $\beta > \beta_c$ with a continuous symmetry group. We thank V. Privman for having brought this point to our attention.

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