

## Finite-size scaling and the crossover to mean-field critical behavior in the two-dimensional Ising model with medium-ranged interactions

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Critical amplitudes in finite-size scaling relations show a singular dependence on the range of the interactions,  $R$ . The respective power laws are predicted from phenomenological crossover scaling considerations. These predictions are tested by Monte Carlo simulations for medium-ranged Ising square lattices. It is speculated that some deviations between the simulation results and corresponding predictions may be due to logarithmic corrections.

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### I. INTRODUCTION

It is widely recognized that critical fluctuations (say, in an anisotropic ferromagnet become more and more reduced as the range  $R$  of the (exchange) interactions increases [1–18]. As  $R \rightarrow \infty$ , simple mean-field behavior is recovered, as the well-known Ginzburg criterion [4,8] shows. On the other hand, close enough to the critical temperature  $T_c$  for finite  $R$ , one always observes the non-classical critical exponents, differing from those of the Landau theory. As is widely known (e.g., [5,6]), this universality of the critical exponents is true for all (arbitrarily large but finite) values of  $R$ , and a different behavior in the limit  $R \rightarrow \infty$  implies a singular variation of critical amplitudes with  $R$ . For simplicity, let us consider the order parameter  $M(t, R)$  of the ferromagnet at zero field:

$$M = t^{1/2} \tilde{M} \{ t^{(4-d)/2} R^d \}, \quad (1)$$

where  $d$  is the dimensionality,  $t$  the distance from the critical point,  $t = 1 - T/T_c$ , and  $\tilde{M}(\xi)$  some scaling function which describes the crossover from Landau-like critical behavior [ $M = \hat{B}_{\text{MF}} t^{1/2}$ , with  $\hat{B}_{\text{MF}} = \tilde{M}(\infty)$  being the critical amplitude  $\hat{B}_{\text{MF}}$  in the mean-field (MF) limit] to the nontrivial (Ising-like) critical behavior,

$$M = \hat{B}(R) t^\beta, \quad (2)$$

where  $\beta$  is the critical exponent (of the Ising universality class in this case, e.g.,  $\beta = \frac{1}{8}$  for  $d = 2$  [7]). The choice of the crossover scaling variable  $\xi$  in Eq. (1) is motivated by the Ginzburg criterion [4,8], which says that mean-field theory is self-consistent as long as

$$\xi \equiv t^{(4-d)/2} R^d \gg 1, \quad (3)$$

while the crossover to the non-mean-field critical behavior should occur for  $t^{(4-d)/2} R^d$  being of order unity (note  $R$  is measured here in units of the lattice spacing

and hence dimensionless). Now, Eq. (1) is consistent with Eq. (2) only if  $\tilde{M}(\xi \ll 1) \propto \xi^Y$ , with  $Y = (2\beta - 1)/(4 - d)$ , and this implies as well that

$$\hat{B}(R) \propto R^{dY} = R^{d(2\beta - 1)/(4 - d)}. \quad (4)$$

It is the aim of the present paper to consider the analogous problem in the context of finite-size scaling [9,19–21], extending previous work that considered a related problem for polymer mixtures [22,23]. Apart from this work on polymers and early work [24] on the specific-heat rounding in the Baxter model for various ratios of coupling constants, such crossover problems in finite-size scaling have not received much attention. As is well known, critical singularities such as those described by Eq. (2) are rounded (and shifted) in finite systems, e.g., for a (hyper)cubic box with all linear dimensions equal to  $L$ , the absolute value of the order parameter behaves as [19–21]

$$M = B(R) L^{-\beta/\nu}, \quad (5)$$

$\nu$  being the critical exponent of the correlation length. In the present paper, we wish to extend the consideration performed in Eqs. (1)–(4) to finite-size scaling, in order to estimate the singular variation of the finite-size-scaling amplitude  $B(R)$  with  $R$  (and amplitudes for other quantities as well). Section II presents a phenomenological theory that combines finite-size scaling and crossover scaling towards mean-field critical behavior. Some care is necessary here, of course, as mean-field theory does not satisfy hyperscaling relations ( $d\nu = 2\beta + \gamma$ ,  $\gamma$  being the susceptibility exponent [1–3]), and this leads to a different structure of finite-size scaling in the mean-field limit [25–27]. Section III then introduces the Ising model on the square lattice with an extended range of couplings and presents Monte Carlo simulation data for that model. Section IV analyzes these data in terms of the theory of Sec. II and discusses its applicability. Some concluding remarks are given in Sec. V.

## II. PHENOMENOLOGICAL THEORY OF FINITE-SIZE EFFECTS IN ISING-LIKE SYSTEMS WITH A MEDIUM RANGE OF INTERACTIONS

We consider an Ising-type system in a (hyper)cubic lattice of linear dimension  $L$  and periodic boundary conditions. The free energy can be written as [27]

$$F = -k_B T \ln Z = -k_B T \ln \int \mathcal{D}\phi \exp \left[ - \int_L d^d x \left\{ \frac{1}{2} c t_{\text{MF}} \phi^2 + \frac{1}{4} u \phi^4 + \frac{1}{2} k_B T [R \nabla \phi(\mathbf{x})]^2 \right\} \right]. \quad (6)$$

Here,  $k_B$  is Boltzmann's constant,  $Z$  the partition function,  $\phi(\mathbf{x})$  the order-parameter field,  $c$  and  $u$  are constants, and  $t_{\text{MF}}$  is the relative temperature distance from the mean-field critical temperature.

In the limit  $R \rightarrow \infty$ , order-parameter fluctuations get suppressed, and thus the functional integral in Eq. (6) gets replaced by an ordinary integral [25–27],

$$\begin{aligned} F_{\text{MF}} &= -k_B T \ln Z_{\text{MF}} \\ &= -k_B T \ln \int_{-\infty}^{+\infty} d\phi \exp \left[ -L^d \left( \frac{1}{2} c t_{\text{MF}} \phi^2 + \frac{1}{4} u \phi^4 \right) \right]. \end{aligned} \quad (7)$$

From Eq. (7) it is obvious that the probability distribution  $P_L(\phi)$  of the order parameter is simply

$$P_L(\phi) \propto \exp \left[ -L^d \left( \frac{1}{2} c t_{\text{MF}} \phi^2 + \frac{1}{4} u \phi^4 \right) \right].$$

From  $P_L(\phi)$  it is straightforward to derive the finite-size-scaling relations for mean-field systems [25–27]:

$$g_L \equiv -3 + \langle s^4 \rangle_L / \langle s^2 \rangle_L^2 = \bar{g}_{\text{MF}}(t_{\text{MF}} L^{d/2}), \quad (8)$$

$$M_L \equiv \langle |s| \rangle_L = L^{-d/4} \tilde{M}_{\text{MF}}(t_{\text{MF}} L^{d/2}), \quad (9)$$

$$\begin{aligned} \chi_L &\equiv L^d [\langle s^2 \rangle_L - \langle |s| \rangle_L^2] / (k_B T) \\ &= L^{d/2} \tilde{\chi}_{\text{MF}}(t_{\text{MF}} L^{d/2}). \end{aligned} \quad (10)$$

Here,  $s$  is the normalized order parameter of the Ising model considered summing over all lattice sites  $i$ ,

$$s = L^{-d} \sum_i S_i, \quad S_i = \pm 1. \quad (11)$$

The quantities written down in Eqs. (8)–(10), namely, re-normalized coupling constant (or normalized fourth-order cumulant, respectively)  $g_L$ , order parameter  $M_L$ , and susceptibility  $\chi_L$  (for  $t < 0$ ), are the quantities commonly recorded in Monte Carlo simulations [20,21,28] and hence considered here. Now for  $R$  large but finite, Eqs. (8)–(10) hold only in the mean-field critical regime, which according to the Ginzburg criterion [4,8] is given by Eq. (3). In the opposite regime, where  $t^{(4-d)/2} R^d \ll 1$  holds, we must have the standard finite-size-scaling relations [19–21]:

$$g_L = \bar{g}_{\text{Ising}}(R^{\mathcal{H}} t L^{1/\nu}), \quad (12)$$

$$M_L = R^x L^{-\beta/\nu} \tilde{M}_{\text{Ising}}(R^{\mathcal{H}} t L^{1/\nu}), \quad (13)$$

$$\chi_L = R^y L^{\gamma/\nu} \tilde{\chi}_{\text{Ising}}(R^{\mathcal{H}} t L^{1/\nu}). \quad (14)$$

In our notation we have anticipated that the scaling functions  $\bar{g}_{\text{MF}}(\zeta_{\text{MF}})$ ,  $\tilde{M}_{\text{MF}}(\zeta_{\text{MF}})$ , and  $\tilde{\chi}_{\text{MF}}(\zeta_{\text{MF}})$  in the mean-

field critical region will differ from their counterparts  $\bar{g}_{\text{Ising}}(\zeta_I)$ ,  $\tilde{M}_{\text{Ising}}(\zeta_I)$ , and  $\tilde{\chi}_{\text{Ising}}(\zeta_I)$  in the nonclassical Ising critical region. Note that for Eqs. (12)–(14) one must use the distance  $t = 1 - T/T_c$  (from the true critical point, of course), which differs from  $t_{\text{MF}}$  due to a shift of the critical temperature [1–3]:

$$T_c^{\text{MF}} - T_c \propto R^{-d}. \quad (15)$$

Equation (15) can be understood from Eq. (6) by considering nonuniform order-parameter fluctuations in the framework of a Gaussian approximation around the mean-field limit (see also [27]). This shift is not of interest to us here. Furthermore, in Eqs. (12)–(14) we have postulated that the amplitudes of all scale factors (for  $M_L$ , for  $\chi_L$ , and for the temperature scale) must exhibit a *singular* dependence on the range of interaction parameter,  $R$ , while apart from these power-law factors  $R^{\mathcal{H}}$ ,  $R^x$ , and  $R^y$  defining new exponents  $\mathcal{H}$ ,  $x$ , and  $y$ , there is no  $R$  dependence: the functions  $\bar{g}_{\text{Ising}}(\zeta_I)$ ,  $\tilde{M}_{\text{Ising}}(\zeta_I)$ , and  $\tilde{\chi}_{\text{Ising}}(\zeta_I)$  are universal. The prediction of these exponents  $\mathcal{H}$ ,  $x$ , and  $y$  is the main interest of this section.

We do this simply by using Eqs. (8)–(10) in the mean-field critical region, but add the variable  $\zeta$  defined in Eq. (3) as a second argument of the respective scaling functions (actually it is more convenient to use  $\zeta' \equiv \zeta^{2/(4-d)} = t R^{2d/(4-d)}$ ):

$$g_L = \bar{g}(t L^{d/2}, t R^{2d/(4-d)}), \quad (16)$$

$$M_L = L^{-d/4} \tilde{M}(t L^{d/2}, t R^{2d/(4-d)}), \quad (17)$$

$$\chi_L = L^{d/2} \tilde{\chi}(t L^{d/2}, t R^{2d/(4-d)}). \quad (18)$$

Note that here in the argument  $t L^{d/2}$  we have also replaced  $t_{\text{MF}}$  by  $t$ , which is legitimate, because in most cases of interest ( $2 < d \leq 4$ ) the shift of  $T_c$  relative to  $T_c^{\text{MF}}$  is much larger than the temperature range around  $T_c$ , where the crossover from Ising behavior to mean-field behavior occurs. Therefore  $t$ , and not  $t_{\text{MF}}$ , must be used in Eqs. (16)–(18). We shall return to this point at the end of this section.

Obviously, we have to have simply [ $\zeta_{\text{MF}} = t L^{d/2}$ ]

$$\bar{g}(\zeta_{\text{MF}}, \zeta' \rightarrow \infty) = \bar{g}_{\text{MF}}(\zeta_{\text{MF}}), \quad (19)$$

$$\tilde{M}(\zeta_{\text{MF}}, \zeta' \rightarrow \infty) = \tilde{M}_{\text{MF}}(\zeta_{\text{MF}}), \quad (20)$$

$$\tilde{\chi}(\zeta_{\text{MF}}, \zeta' \rightarrow \infty) = \tilde{\chi}_{\text{MF}}(\zeta_{\text{MF}}), \quad (21)$$

in order for Eqs. (8)–(10) to result simply in the limit  $R \rightarrow \infty$ . More interesting, of course, is the inverse limit  $\zeta' \rightarrow 0$ , in which Eqs. (19)–(21) must yield the nontrivial critical behavior [Eqs. (12)–(14)]. This implies a singular variation of the scaling functions  $\bar{g}(\zeta_{\text{MF}}, \zeta')$ ,  $\tilde{M}(\zeta_{\text{MF}}, \zeta')$ ,

and  $\tilde{\chi}(\xi_{\text{MF}}, \zeta')$  in this limit. So,

$$\tilde{g}(\xi_{\text{MF}}, \zeta' \rightarrow 0) = \tilde{g}_{\text{Ising}}(\xi_{\text{MF}}^{2/(d\nu)} \zeta'^a), \quad (22)$$

where

$$\xi_{\text{MF}}^{2/(d\nu)} \zeta'^a = t^{2/(d\nu)} L^{1/\nu} t^a R^{2da/(4-d)} = R^{\mathcal{H}} t L^{1/\nu}. \quad (23)$$

Thus the mean-field-scaling variable  $\xi_{\text{MF}}$  is raised to the power  $2/(d\nu)$ , in order to change the power of  $L$  from  $d/2$  to  $1/\nu$  [compare Eqs. (8) and (12)], and then the power ( $a$ ) of  $\zeta'$  has to be chosen such that  $\xi_{\text{MF}}^{2/(d\nu)} \zeta'^a$  simply yields the scaling variable  $\xi_{\text{Ising}}$ . Obviously, Eq. (23) then implies that

$$2/(d\nu) + a = 1, \quad a = 1 - 2/(d\nu) = -\alpha/(d\nu), \quad (24)$$

where in the last step the hyperscaling relation  $d\nu = 2 - \alpha$  was used,  $\alpha$  being the specific-heat exponent. Using the exponent  $a$  from Eq. (24) again in Eq. (23) then fixes the exponent  $\mathcal{H}$ ,

$$\mathcal{H} = 2da/(4-d) = -2(\alpha/\nu)/(4-d). \quad (25)$$

In  $d=3$ , we have [29]  $\alpha \approx 0.11$ ,  $\nu \approx 0.63$ , and hence  $\mathcal{H} \approx -0.35$ . In  $d=2$ , where  $\alpha=0$  implies a logarithmic divergence of the specific heat, we suspect that  $\mathcal{H}=0$  implies a  $\ln R$  correction in Eq. (23).

Another check on this result [Eqs. (23)–(25)] can be obtained from the following reasoning: in the nonclassical critical region, finite-size scaling [19–21] merely expresses the principle that “ $L$  scales with the correlation length  $\xi$ ,” i.e., the variable  $\xi_{\text{Ising}}$  can also be written as

$$\xi_{\text{Ising}} = R^{\mathcal{H}} t L^{1/\nu} = (L/\xi)^{1/\nu},$$

which implies

$$\chi \propto (R^{\mathcal{H}} t)^{-\nu}, \quad t^{(4-d)/2} R^d \lesssim 1. \quad (26)$$

The factor of proportionality in Eq. (26) should be of order unity. On the other hand, in the mean-field critical region [where Eq. (3) holds] we must have

$$\xi_{\text{MF}} = \hat{\xi} R t^{-1/2}, \quad (27)$$

where  $\hat{\xi}$  is another constant of order unity and  $R$  only enters in as a factor. Now we postulate that the crossover from Eq. (27) to Eq. (26) at  $t^{(4-d)/2} R^d = 1$  must be smooth, i.e., for

$$t = t_{\text{cross}} = R^{-2d/(4-d)}$$

both  $\xi$  and  $\xi_{\text{MF}}$  must be of the same order of magnitude:

$$\xi_{\text{MF}} = \hat{\xi} R R^{d/(4-d)} = \hat{\xi} R^{4/(4-d)} \propto R^{-\mathcal{H}\nu} R^{2d\nu/(4-d)}. \quad (28)$$

Equating the powers of  $R$  on both sides of Eq. (28) again yields Eq. (25).

Figure 1 summarizes this situation in terms of a schematic log-log plot of the characteristic lengths versus  $t$ . For  $t_{\text{cross}} \ll t \ll 1$  (the left part of the plot), we have the mean-field regime; for  $t \ll t_{\text{cross}}$ , the Ising regime. In the mean-field regime,  $L$  needs to be compared to  $l$ ; in the Ising regime,  $L$  needs to be compared to  $\xi$ . Of course, in reality the crossover is smooth and may spread over several decades of  $t$  [17]. In order to derive the exponent

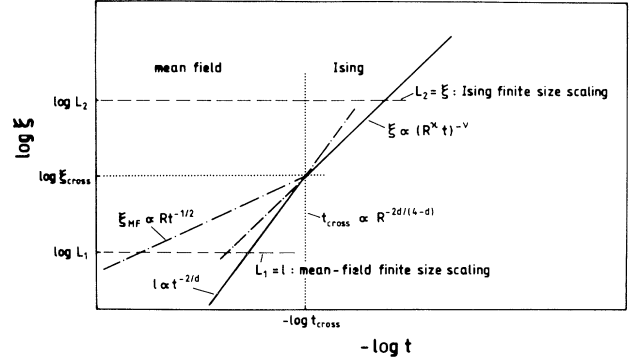


FIG. 1. Schematic log-log plot of the relevant characteristic lengths versus the temperature distance  $t$  from the (true) critical point. In the mean-field regime, where hyperscaling does not hold, there are several characteristic lengths: Apart from the correlation length  $\xi_{\text{MF}}$  of the order-parameter correlation function, a thermodynamic length  $l(t) = [\chi(t)/M^2(t)]^{-2/d}$  matters, since it enters the finite-size scaling with periodic boundary conditions (thus a length  $L_1 < \xi_{\text{cross}}$  scales with  $l$ , while a length  $L_2 > \xi_{\text{cross}}$  scales with  $\xi$ ). At  $t = t_{\text{cross}} \propto R^{-2d/(4-d)}$ , there is a smooth crossover, i.e.,  $\xi_{\text{MF}}(t)$  and  $l(t)$  merge and also match the correlation length  $\xi(t)$  of the Ising critical regime.

$x$  now in Eq. (13), we discuss  $\tilde{M}(\xi_{\text{MF}}, \zeta')$  in Eq. (20) for small  $\zeta'$ :

$$\begin{aligned} M_L &= L^{-d/4} \tilde{M}(\xi_{\text{MF}}, \zeta' \rightarrow 0) \\ &= \xi_{\text{MF}}^{1/2 - 2\beta/(d\nu)} L^{-d/4} \zeta'^b \tilde{M}_{\text{Ising}}(\xi_{\text{MF}}^{2/(d\nu)} \zeta'^a) \\ &= R^x L^{-\beta/\nu} \tilde{M}_{\text{Ising}}(R^{\mathcal{H}} t L^{1/\nu}). \end{aligned} \quad (29)$$

The exponents  $a$  and  $\mathcal{H}$  in Eq. (29) are already fixed, of course, and the power of  $\xi_{\text{MF}} = t L^{d/2}$  in front of the scaling function in Eq. (19) has also been chosen such that the power  $L^{-d/4}$  is turned into a power  $L^{-\beta/\nu}$ . The power  $b$  of  $\zeta'$  in Eq. (29) must now be chosen such that the  $t$  dependence of the prefactors cancels:

$$L^{-\beta/\nu} t^{1/2 - 2\beta/(d\nu)} t^b R^{2db/(4-b)} = L^{-\beta/\nu} R^x; \quad (30)$$

hence,

$$\frac{1}{2} - 2\beta/(d\nu) + b = 0, \quad b = 2\beta/(d\nu) - \frac{1}{2} \quad (31)$$

and ( $d\nu = \gamma + 2\beta$ )

$$x = \frac{2db}{4-d} = \frac{4\beta/\nu - d}{4-d} = \frac{(2\beta - \gamma)/\nu}{4-d}. \quad (32)$$

Using  $\gamma \approx 1.24$ ,  $\beta \approx 0.325$ , and  $\nu \approx 0.63$  for  $d=3$  [28], we estimate  $x \approx -0.95$  in  $d=3$ , while  $\beta = \frac{1}{8}$ ,  $\gamma = \frac{1}{4}$ , and  $\nu = 1$  in  $d=2$  [7] yields

$$x = -\frac{3}{4} \quad (d=2). \quad (33)$$

Again, a check is obtained, noting that for  $L \rightarrow \infty$  in Eq. (13), the powers of  $L$  must cancel out, and therefore,

$$\begin{aligned} M &\propto R^x + \mathcal{H} \beta t^\beta = R^{[(2\beta - \gamma)/\nu - 2\beta\alpha/\nu]/(4-d)} t^\beta \\ &= R^{2d(\beta - 1/2)/(4-d)} t^\beta, \end{aligned} \quad (34)$$

which is the same result as in Eq. (4).

It remains to consider  $\chi_L$  in Eq. (18) for small  $\zeta'$ :

$$L^{d/2} \tilde{\chi}(\zeta_{\text{MF}}, \zeta' \rightarrow 0) = \zeta_{\text{MF}}^{2\gamma/(d\nu-1)} \zeta'^c L^{d/2} \tilde{\chi}_{\text{Ising}}(\zeta_{\text{MF}}^{2/(d\nu)} \zeta'^a) \\ = R^y L^{\gamma/\nu} \tilde{\chi}_{\text{Ising}}(R^y t L^{1/\nu}). \quad (35)$$

Again, the exponents  $c$  and  $y$  follow from requiring that the exponent of  $t$  in the factor in front of the scaling function vanish,

$$L^{\gamma/\nu} t^{2\gamma/(d\nu)-1} t^c R^{2dc/(4-d)} = L^{\gamma/\nu} R^y; \quad (36)$$

hence,

$$2\gamma/(d\nu) - 1 + c = 0, \quad c = 1 - 2\gamma/(d\nu), \quad (37)$$

and

$$y = \frac{2dc}{4-d} = \frac{2d-4\gamma/\nu}{4-d} = \frac{(4\beta-2\gamma)/\nu}{4-d} = 2x. \quad (38)$$

If one considers the limit  $L \rightarrow \infty$  in Eq. (14), powers of  $L$  must cancel, and, hence,

$$\chi \propto R^y - \gamma^y t^{-\gamma} = R^{(4\beta-2\gamma+2\alpha\gamma)/[(4-d)\nu]} t^{-\gamma} \\ = R^{2d(1-\gamma)/(4-d)} t^{-\gamma}. \quad (39)$$

On the other hand, this result can be derived directly from a crossover scaling assumption for the susceptibility analogous to Eqs. (1)–(4):

$$\chi = \hat{A} t^{-1} \tilde{\chi}(R^d t^{(4-d)/2}) \propto t^{-\gamma} R^{2d(1-\gamma)/(4-d)}, \quad (40)$$

as expected.

Here we note that this treatment can also be used to derive crossover scaling forms right at  $T_c$ ,  $t=0$ ; we only have to take Eqs. (16)–(18) and construct from the variables  $\zeta_{\text{MF}}, \zeta'$  (which both contain  $t$ ) two other variables  $\zeta_{\text{MF}}, \zeta_{\text{MF}}/\zeta'$ : in the latter variable,  $t$  has canceled out, and now the limit  $t \rightarrow 0$  can easily be taken. This yields the following scaling forms [using  $(\zeta_{\text{MF}}/\zeta')^{2/d}$  instead of  $\zeta_{\text{MF}}/\zeta'$ , for convenience]:

$$g_L|_{T_c} = \tilde{g}'(LR^{-4/(4-d)}), \quad (41)$$

$$M_L|_{T_c} = L^{-d/4} \tilde{M}'(LR^{-4/(4-d)}), \quad (42)$$

$$\chi_L|_{T_c} = L^{d/2} \tilde{\chi}'(LR^{-4/(4-d)}). \quad (43)$$

All these scaling forms can also be used to obtain the exponents  $x$  and  $y$  by requiring that  $M_L|_{T_c} \propto L^{-\beta/\nu}$  and  $\chi_L|_{T_c} \propto L^{\gamma/\nu}$  as  $L \rightarrow \infty$ . As it should, this reasoning confirms Eqs. (32) and (38). We also note that Eqs. (41)–(43) can be considered as special cases of the general crossover finite-size-scaling description given by Binder and Deutsch [22].

We now return to the problem of disregarding the shift of  $T_c$  relative to the mean-field critical temperature  $T_c^{\text{MF}}$ , or the problem of replacing  $t_{\text{MF}}$  with  $t$  [Eq. (15)] which is equivalent. For  $2 < d < 4$ , the shift  $(T_c^{\text{MF}} - T_c)/T_c$  is much larger than the distance  $T_{\text{cross}}$ , but one should note that this fact does not matter, as one can renormalize the original Ginzburg-Landau-Wilson Hamiltonian and define an “effective” renormalized mean-field transition temperature close to the true  $T_c$ . For  $d < 2$ , the shift for

large  $R$  is much smaller than  $T_{\text{cross}}$  and can be treated as a higher-order correction. Hence, we find that the case  $d=2$  is marginal and suspect that this may again be a source of logarithmic corrections [12]. [Another logarithmic correction has already been proposed on the grounds that  $\alpha/\nu=0$  in the  $d=2$  Ising model; see Eq. (25).] Thus, it is a somewhat nontrivial matter to check what happens in the case of the  $d=2$  Ising model with a variable interaction range  $R$ . This will be done, using Monte Carlo simulations, in Secs. III and IV.

### III. MONTE CARLO RESULTS FOR THE ISING MODEL WITH EXTENDED-RANGE COUPLINGS

We consider an Ising model on a square lattice of  $L \times L$  sites with periodic boundary conditions. A spin variable  $\sigma$  is assigned to each site with the values of  $\pm 1$ . The spins couple to all  $z$  sites within a distance of  $R_m$  (in the units of the lattice spacing) with the same interaction constant  $J > 0$ , while the interaction for distances larger than  $R_m$  is zero. Then the effective range  $R$  of interaction is defined as usual:

$$R^2 = \sum_{j(\neq i)} (\mathbf{r}_i - \mathbf{r}_j)^2 J_{ij} / \sum_{j(\neq i)} J_{ij} \\ = \frac{1}{z} \sum_{j(\neq i)} |\mathbf{r}_i - \mathbf{r}_j|^2, \quad |\mathbf{r}_i - \mathbf{r}_j| \leq R_m. \quad (44)$$

In the last step of Eq. (44) we used the fact that  $J_{ij} = J$  independent of distance inside the maximal interaction distance. We study the cases  $R_m^2 = 1$  (which also yields  $R^2 = 1$ ,  $z = 4$ ; this is the nearest-neighbor Ising lattice, for which the solution is known exactly, of course [7]),

$$R_m^2 = 2(R^2 = \frac{3}{2}, z = 8),$$

$$R_m^2 = 4(R^2 = \frac{7}{3}, z = 12),$$

$$R_m^2 = 8(R^2 = \frac{25}{6}, z = 24),$$

$$R_m^2 = 10(R^2 = 6, z = 36),$$

$$R_m^2 = 18(R^2 = \frac{49}{6}, z = 48),$$

and

$$R_m^2 = 32(R^2 = \frac{27}{2}, z = 80).$$

We have located the transition temperatures for the Ising model with extended-range coupling, by carrying out a Monte Carlo sampling of the fourth-order cumulant of the magnetization distribution  $g_L(T)$  defined in Eq. (8). This quantity is believed to be particularly useful, since within both Ising and mean-field limits one expects [20,24] that the curves  $g_L(T)$  intersect at  $T_c$  in common intersection points  $g^{\text{Ising}}(T_c)$ ,  $g^{\text{MF}}(T_c)$ . It presents a difficulty, of course, that no such unique intersection property holds in the crossover regime between both limits [cf. Eq. (41)], where a crossover occurs between both limiting values, given as [26,30]

$$g^{\text{Ising}}(T_c) \approx -1.835, \quad g^{\text{MF}}(T_c) \approx -0.812. \quad (45)$$

As a consequence,  $T_c$  can be found only by studying rather large lattices where  $g_L(T_c)$  has actually settled down at its asymptotic (Ising) value  $g^{\text{Ising}}(T_c)$ . Figure 2 shows the behavior of  $g_L$  for selected values of  $R$ . Thus, we have found it necessary to include linear dimensions up to  $L = 80$  for  $R_m^2 \leq 18$  and up to  $L = 220$  for  $R_m^2 = 32$ . Since the medium range of the interactions slows down the speed of the algorithm considerably, it is not straightforward to study this problem for still larger choices of either  $R$  or  $L$ , although this would clearly be very desirable.

Once  $T_c(R)$  has been determined (Fig. 3), we can proceed with the analysis of the data for  $g_L|_{T_c}$ ,  $M_L|_{T_c}$ , and  $\chi_L|_{T_c}$  in order to compare with the predictions of Sec. II. On each run, about  $10^6$  Monte Carlo steps per spin have been used for the small systems and about  $10^5$  for the systems with large  $R^2$ ; independent runs were used to estimate the statistical errors. Our data are collected in Tables I and II (data for the nearest-neighbor case can be found in many papers and hence are not listed here; since the interpretation of our data for larger values of  $R$  is not completely straightforward, we feel it may be useful to document them for future use).

Figure 3 shows that only data for  $R^2 > \frac{25}{6}$  roughly follow the asymptotic relation for the shift of  $T_c$ , Eq. (15). This is no surprise, because Eq. (15) is expected to hold as  $R \rightarrow \infty$  and there is no reason why it should hold for  $R < 2$ , in particular since then the depression of  $T_c$  relative to the mean-field value is more than 20%. It is conceivable that there is a logarithmic correction in the shift of  $T_c$ , too. Also, the whole crossover scaling treatment of Sec. II is expected to hold in the limit  $R \rightarrow \infty$ ,  $LR^{-2}$  of order unity only, and the question of which of the data in Tables I and II are already within that limit needs serious discussion. This problem will be discussed in Sec. IV.

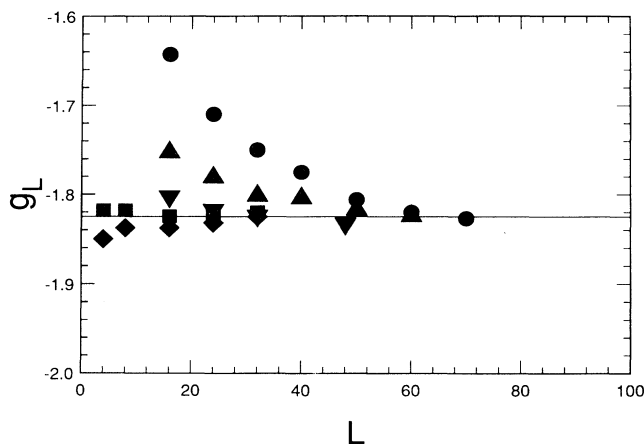


FIG. 2. Plot of the cumulant  $g_L(T_c)$  versus  $L$ . The horizontal straight line indicates the asymptotic Ising value  $g^{\text{Ising}}(T_c) \approx 1.83$  [30], while different symbols give our numerical results for several choices of  $R$  ( $R^2=1$ , diamonds;  $R^2=\frac{3}{2}$ , squares;  $R^2=\frac{7}{3}$ , triangles;  $R^2=\frac{25}{6}$ , inverted triangles;  $R^2=\frac{49}{6}$ , circles).

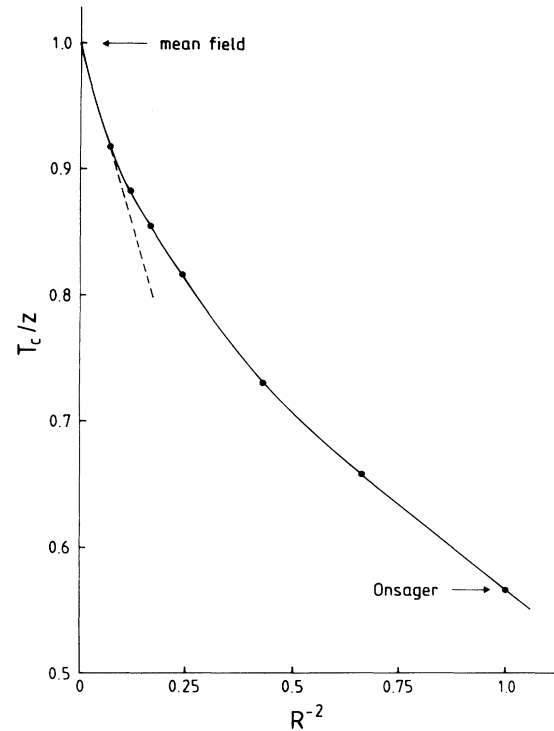


FIG. 3. Plot of  $T_c/z$  versus  $R^{-2}$ . Both exactly known limits (Onsager's exact solution for  $z=4$  and the mean-field result for  $z \rightarrow \infty$ ) are indicated by arrows.

#### IV. ANALYSIS OF THE MONTE CARLO DATA VIA FINITE-SIZE SCALING

Figure 4 gives a log-log plot of all data for  $k_B T_c \chi_L / L$  versus  $L/R^2$ . Obviously, the data for small  $R$  ( $R^2 \leq \frac{25}{6}$ ) do not satisfy the scaling form at all, as was predicted in Eq. (43), but for small  $R$  such a failure of scaling is not unexpected. Figure 4 clearly shows that for small  $R$  we do not encounter at all a mean-field region in which  $k_B T_c \chi_L / L$  would be independent of  $L$ . So in further tests of Eqs. (41)–(43) we only include data for the three largest values of  $R$  (Figs. 5–7): It is seen that for  $\langle |m| \rangle_L$ , there is rough agreement with the proposed scaling form, Eq. (42), while for the other two quantities, systematic deviations from the scaling suggested by Eqs. (41) and (43) are clearly apparent. As was also to be expected, there were somewhat larger errors in the case of the cumulant (Fig. 7), since it is more difficult to sample with high statistical accuracy than low-order moments of the magnetization distribution, and it is also more sensitive to possible small errors in the location of  $T_c$ , since  $g_L(T)$  has a somewhat steeper variation with temperature there than the other quantities.

From Figs. 4–5 we conclude that Eqs. (41)–(43) can be valid only for  $R \gg 1$ , and if this crossover scaling description becomes valid in this limit—which is certainly not proven by our data, although Fig. 5 is suggestive—the approach to this limit is rather slow. As discussed in Sec. II, there are reasons to expect logarithmic

TABLE I. Critical-point properties for the models with  $R_m^2=2, 4,$  and  $8$ .  $T_c$  is in units of the critical temperature of the nearest-neighbor model. We estimate that the statistical error for  $M_L$  is typically at most 1 in the last digit shown, while it is about 2 for  $k_B T_c \chi_L$ , and about 3 for  $g_L$  in the last digit.

$R_m^2=2, T_c \equiv 2.32$				$R_m^2=4, T_c \equiv 3.865$				$R_m^2=8, T_c \equiv 8.63$			
$L$	$M_L$	$k_B T_c \chi_L$	$-g_L$	$L$	$M_L$	$k_B T_c \chi_L$	$-g_L$	$L$	$M_L$	$k_B T_c \chi_L$	$-g_L$
4	0.804	0.826	1.818	4	0.720	1.110	1.699	6	0.609	2.06	1.631
8	0.733	2.67	1.818	6	0.695	1.854	1.748	8	0.586	2.94	1.672
16	0.672	8.61	1.825	8	0.672	2.76	1.771	10	0.568	3.93	1.699
24	0.636	17.3	1.824	10	0.653	3.87	1.782	12	0.555	4.96	1.722
32	0.611	29.6	1.820	12	0.639	5.03	1.794	14	0.545	6.06	1.741
				14	0.627	6.38	1.801	16	0.535	7.29	1.753
				16	0.615	7.98	1.803	24	0.507	13.3	1.781
				24	0.587	15.2	1.817	32	0.491	20.2	1.802
				32	0.566	24.2	1.824	40	0.475	29.6	1.804
				48	0.540	47.3	1.833	50	0.464	41.2	1.817
								60	0.455	54.7	1.824

mic correction factors, which might possibly account for the deviations from scaling apparent in Figs. 5–7, but since our speculative treatment of Sec. II yields no information whatsoever on the precise exponents  $p$  of factors  $(\ln R)^p$  that might occur, and the data clearly do not span a wide enough range of  $R$  that one might unambiguously fit such corrections to the data, we have not attempted to follow this possible line of reasoning further to explain these discrepancies.

It is also of interest to try to extract the amplitudes  $A(R)$  of the susceptibility [ $k_B T_c \chi_L = A(R)L^{\gamma/\nu}$ ] and  $B(R)$  of the magnetization [Eq. (5)] directly from the data, without relying at all on the crossover scaling analysis: This way, the theory of Sec. II is tested in a very direct manner, unbiased by any assumptions of how to analyze the data.

However, while the data for  $\langle |m| \rangle_L$  at  $T_c$  do have a significantly broad regime where we can see Eq. (5) and hence extract  $B(R)$  rather unambiguously, the reliable estimation of  $A(R)$  is more of a problem, as Fig. 8 shows where  $k_B T_c \chi_L / L^{1.75}$  is plotted versus  $L$ : One sees only a rather slow approach to the “plateau” value which is our

estimate of  $A(R)$ . An alternative estimation was also tried, plotting  $k_B T_c \chi_L$  versus  $L^{1.75}$  and fitting a straight line to the data. This approach is preferable, if the dominating correction to scaling is just a regular background term,

$$k_B T_c \chi_L = C_0(R) + A(R)L^{1.75}.$$

In fact, we do expect a background term of order unity. However, a fit to this form shows that  $C_0(R)$  systematically increases with  $R$  and becomes much larger than unity for our largest choices of  $R$ . Moreover, the data for small  $L$  clearly do not fall on the straight line, indicative of other corrections to scaling, presumably with a term  $L^{x_c}$  with a correction to scaling exponent  $x_c$  in between zero [which would yield  $C_0(R)$ ] and  $\gamma/\nu$  (the leading term). In the absence of knowledge of the precise form of such corrections in our model, we have not tried to include them in the analysis. The above fit, which attributes all corrections to a term  $C_0(R)$ , yields estimates that are only slightly—but systematically—different from our estimates in Fig. 8, and such deviations may

TABLE II. Critical-point properties for the models with  $R_m^2=10, 18,$  and  $32$ .  $T_c$  is in units of the critical temperature of the nearest-neighbor model.

$R_m^2=10, T_c \equiv 13.575$				$R_m^2=18, T_c \equiv 18.67$				$R_m^2=32, T_c \equiv 32.386$			
$L$	$M_L$	$k_B T_c \chi_L$	$-g_L$	$L$	$M_L$	$k_B T_c \chi_L$	$-g_L$	$L$	$M_L$	$k_B T_c \chi_L$	$-g_L$
12	0.504	5.05	1.656	8	0.493	3.15	1.584	80	0.301	52.0	1.774
14	0.494	6.14	1.678	10	0.476	4.13	1.614	100	0.302	73.0	1.801
16	0.486	7.23	1.700	12	0.464	5.14	1.643	120	0.300	91.9	1.823
20	0.473	9.50	1.732	14	0.453	6.20	1.643	140	0.292	121	1.824
24	0.463	12.2	1.752	16	0.449	7.22	1.709	180	0.287	187	1.833
32	0.448	18.0	1.782	24	0.423	11.9	1.710	220	0.274	252	1.813
40	0.438	24.3	1.804	32	0.411	17.0	1.750				
50	0.427	34.0	1.815	40	0.400	23.0	1.775				
60	0.420	44.3	1.823	50	0.393	29.5	1.806				
70	0.411	56.9	1.830	60	0.385	38.6	1.820				
				70	0.378	48.6	1.827				

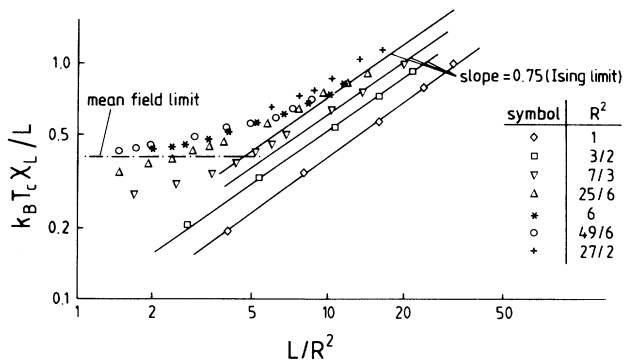


FIG. 4. Log-log plot of the normalized susceptibility at  $T_c$ ,  $k_B T_c \chi_L / L$  versus  $L/R^2$ . Various choices of  $R$  are indicated by different symbols. The straight lines drawn indicate the finite-size scaling in the Ising limit,  $k_B T_c \chi_L = A(R)L^{1.75}$ , which implies  $k_B T_c \chi_L / L = A(R)R^{3/2}(L/R^2)^{0.75}$ . Note that the mean-field limit (where  $k_B T_c \chi_L / L = \text{const}$ ) is barely reached only for our largest values of both  $R$  and  $L$ .

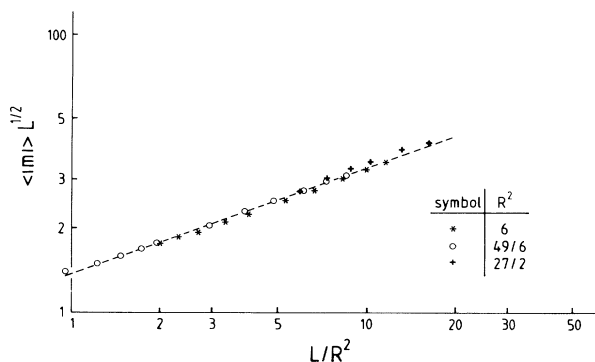


FIG. 5. Log-log plot of the normalized magnetization  $\langle |m| \rangle L^{1/2}$  versus  $L/R^2$ . Only the three largest values of  $R$  are included, and they are indicated by different symbols. The straight line indicates the finite-size scaling in the Ising limit,  $\langle |m| \rangle = B(R)L^{-1/8}$ , which implies  $\langle |m| \rangle L^{1/2} = B(R)R^{3/4}(L/R^2)^{3/8}$ .

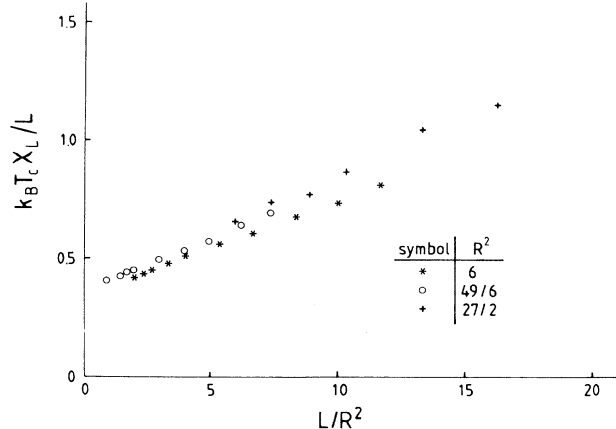


FIG. 6. Plot of  $k_B T_c \chi_L / L$  versus  $L/R^2$  for the three largest values of  $R^2$ .

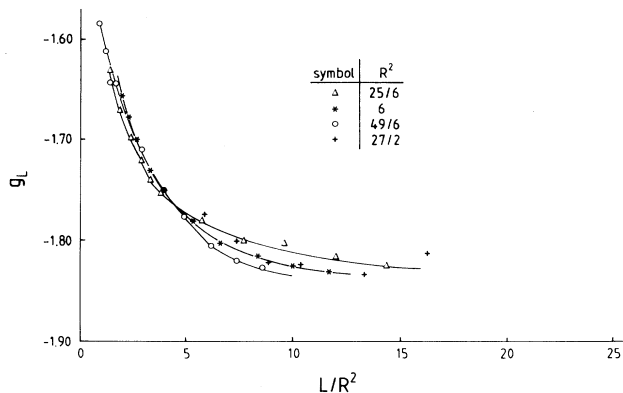


FIG. 7. Plot of  $g_L(T_c)$  versus  $L/R^2$ , including the four largest values of  $R^2$ .

again be taken as an indication of the inaccuracies still present in our analysis.

Finally, Fig. 9 presents a log-log plot of  $A(R)$  and  $B(R)$  versus  $R^2$ . It is clearly seen that for the available range of  $R^2$  we do not (yet?) see the predicted exponents,  $x = -3/4$  for  $B(R)$  [Eq. (33)] and  $y = -3/2$  for  $A(R)$  [Eq. (38)]. But there is slight curvature present on the log-log plot and so one may suspect that the theoretical exponents do apply, but only for much larger values of  $R$ .

### V. DISCUSSION

In this paper, a phenomenological theory was developed to describe the crossover in the critical behavior of Ising-like systems to mean-field behavior as the range  $R$  of the interaction becomes large. We have

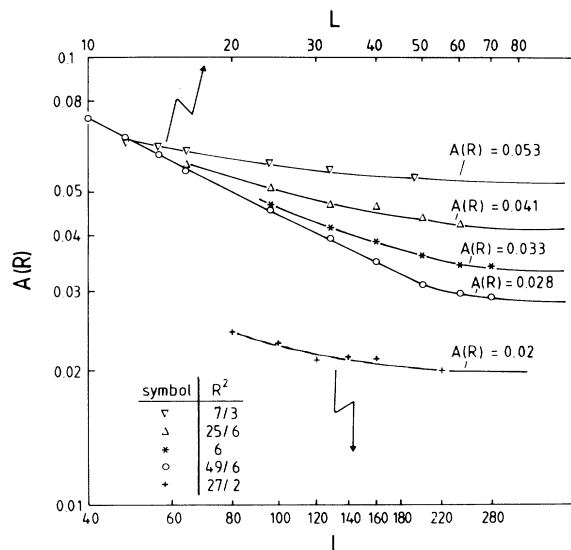


FIG. 8. Log-log plot of  $k_B T_c \chi_L / L^{1.75}$  versus  $L$  for several choices of  $R^2$  as indicated. The resulting estimates for the amplitude  $A(R)$  are also shown. The curves are drawn only to guide the eye.

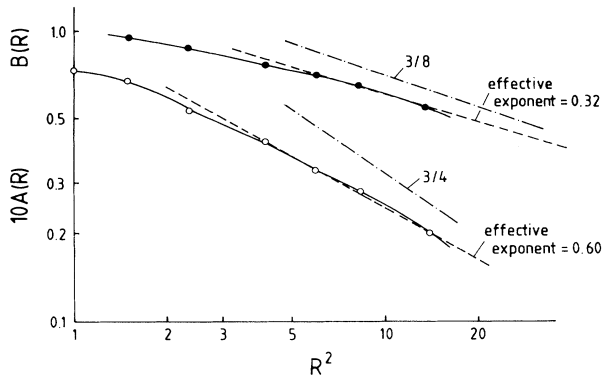


FIG. 9. Log-log plot of the order-parameter amplitude  $B(R)$  and the susceptibility amplitude  $A(R)$  versus  $R^2$ .

incorporated a crossover scaling description based on the Ginzburg criterion in the finite-size-scaling [22] description and derived predictions for the singular variation of finite-size-scaling amplitude factors  $A(R)$  for the susceptibility, and  $B(R)$  for the order parameter at  $T_c$ . This theory should hold for all dimensionalities  $1 < d < 4$ .

An attempt has also been made to test these predictions for the  $d=2$  Ising model, by carrying out simulations in the two-dimensional Ising model with constant interaction of a spin with  $z$  neighbors, where  $z$  varied from  $z=4$  (the nearest-neighbor case) to  $z=80$  (which corresponds to  $R \cong 3.67$ ). Our data show clearly, however, that for  $R \lesssim 2$ , there is not yet any sign of a crossover to mean-field behavior, and even our largest value of  $R$  has presumably not yet reached the regime where the theoretical predictions are valid. It is not, however, straightforward to study significantly larger values of  $R$ , since increasing  $R$  means slowing down the speed of the program, and at the same time one needs to significantly increase  $L$ , since one needs to stay in the regime  $L \gg R^2$  (for a meaningful test of our predictions, one needs to locate  $T_c$  very accurately). As critical slowing down then becomes more and more of a problem, development of a

cluster algorithm for these medium-range Ising models may become necessary. Another theoretical development which could be very useful would be to clarify the presence or absence of logarithmic corrections in  $d=2$ . We do think despite these caveats, however, that the theory of Sec. II should be useful in  $d=3$ , where no logarithmic corrections are suspected and the approach to the mean-field limit with increasing  $R$  is presumably faster than in  $d=2$ .

An interesting variation of the present problem would be the study of a model where the interaction is of medium range but decays to zero smoothly: It is possible that the sharp cutoff of the present model complicates convergence to universality.

Finally, we wish to draw attention to some other related problems: One is the approach towards the mean-field spinodal criticality with  $R \rightarrow \infty$ , when one simulates metastable states in Ising models [31]; the other is the crossover from Ising to mean-field critical behavior in a kinetic Ising model with competing flip and exchange dynamics [32]. In the latter case, however, the inverse problem of the problem considered here occurs, since any small admixture of random exchanges between arbitrary distant spins makes the asymptotic critical behavior mean-field-like, and thus unlike Fig. 3 (where a line of transitions with  $d=2$  Ising exponents ends in a mean-field critical point), one has a line of mean-field transitions at  $T_c(p)$  ending in Ising (non-mean-field) criticality, if the fraction  $p$  of random spin exchanges is zero. But a crossover finite-size-scaling analysis similar in spirit to the one presented here might be useful for these problems, too.

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- [1] M. E. Fisher, *Rev. Mod. Phys.* **46**, 587 (1974).
- [2] L. P. Kadanoff, W. Götze, D. Hamblen, R. Hecht, E. A. S. Lewis, V. V. Parciauskas, M. Rayl, J. Swift, D. Aspnes, and J. Kane, *Rev. Mod. Phys.* **39**, 395 (1967).
- [3] K. Binder, in *Phase Transformations in Materials*, edited by P. Haasen (VCH, Weinheim, Germany, 1991), p. 143.
- [4] V. L. Ginzburg, *Fiz. Tverd. Tela (Leningrad)* **2**, 2031 (1960) [*Sov. Phys. Solid State* **2**, 1824 (1960)].
- [5] E. Riedel and F. J. Wegner, *Z. Phys.* **225**, 195 (1969).
- [6] A. Sariban and K. Binder, *J. Chem. Phys.* **86**, 5859 (1987).
- [7] R. J. Baxter, *Exactly Solved Models in Statistical Mechanics* (Academic Press, New York, 1982).
- [8] J. Als-Nielsen and R. J. Birgeneau, *Am. J. Phys.* **45**, 554 (1977).
- [9] M. E. Fisher, in *Critical Phenomena*, edited by M. S. Green (Academic Press, New York, 1971), p. 1.
- [10] J. Rudnick and D. R. Nelson, *Phys. Rev. B* **13**, 2208 (1976).
- [11] A. D. Bruce and D. J. Wallace, *J. Phys. A* **9**, 1117 (1976).
- [12] J. F. Nicoll and J. Bhattacharjee, *Phys. Rev. B* **32**, 389 (1981).
- [13] C. Bagnuls and C. Bervillier, *J. Phys. (Paris) Lett.* **45**, L95 (1984); *Phys. Rev. B* **32**, 7209 (1985); *Phys. Lett. A* **115**, 84 (1986).
- [14] J. F. Nicoll and P. C. Albright, *Phys. Rev. B* **31**, 4576 (1985).
- [15] Z. Y. Chen, P. C. Albright, and J. V. Sengers, *Phys. Rev. A* **41**, 3161 (1990).
- [16] Z. Y. Chen, A. Abbaci, S. Tang, and J. V. Sengers, *Phys. Rev. A* **42**, 4470 (1990).
- [17] M. Y. Belyakov and S. B. Kiselev, *Physica A* **190**, 75 (1992).
- [18] M. A. Anisimov, M. Y. Belyakov, S. B. Kiselev, and J. V. Sengers, *Physica A* **188**, 487 (1992).
- [19] M. N. Barber, in *Phase Transitions and Critical Phenomena*, edited by C. Domb and J. L. Lebowitz (Academic,



- New York, 1983), Vol. 8, p. 145.
- [20] K. Binder, *Z. Phys. B* **43**, 119 (1981); *Ferroelectrics* **73**, 43 (1987).
- [21] *Finite Size Scaling and Numerical Simulation of Statistical Systems*, edited by V. Privman (World Scientific, Singapore, 1990).
- [22] K. Binder and H.-P. Deutsch, *Europhys. Lett.* **18**, 667 (1992).
- [23] H.-P. Deutsch and K. Binder, *Macromolecules* **25**, 6214 (1992); *J. Phys. (France) II* **3**, 1049 (1993).
- [24] E. Domany, K. K. Mon, G. V. Chester, and M. E. Fisher, *Phys. Rev. B* **12**, 5025 (1975).
- [25] K. Binder, M. Nauenberg, V. Privman, and A. P. Young, *Phys. Rev. B* **31**, 1498 (1985).
- [26] K. Binder, *Z. Phys. B* **61**, 13 (1985).
- [27] E. Brezin and J. Zinn-Justin, *Nucl. Phys. B* **257**, 867 (1985).
- [28] K. Binder and D. W. Heermann, *Monte Carlo Simulation in Statistical Physics: An Introduction* (Springer, Berlin, 1988).
- [29] J. Zinn-Justin and J. C. Le Guillou, *Phys. Rev. B* **21**, 3976 (1980).
- [30] T. W. Burkhardt and B. Derrida, *Phys. Rev. B* **32**, 7273 (1985); A. D. Bruce, *J. Phys. A* **18**, L873 (1985).
- [31] D. W. Heermann, W. Klein, and D. Stauffer, *Phys. Rev. Lett.* **49**, 1262 (1982).
- [32] M. Droz, Z. Racz, and P. Tartaglia, *Physica A* **177**, 401 (1991); *Phys. Rev. A* **41**, 6621 (1990).