# Test of renormalization predictions for universal finite-size scaling functions

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We calculate universal finite-size scaling functions for systems with an $n$-component order parameter and algebraically decaying interactions. Just as previously found for short-range interactions, this leads to a singular $\varepsilon$ expansion, where $\varepsilon$ is the distance to the upper critical dimension. Subsequently, we check the results by numerical simulations of spin models in the same universality class. Our systems offer the essential advantage that $\varepsilon$ can be varied continuously, allowing an accurate examination of the region where $\varepsilon$ is small. The numerical calculations turn out to be in striking disagreement with the predicted singularity.
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In order to analyze numerical results obtained by Monte Carlo or transfer-matrix studies of phase transitions and critical phenomena, *finite-size scaling* [1] is a very widely used technique. This hypothesis, which was properly formulated for the first time by Fisher [2], allows the extrapolation of properties of finite systems, which do not exhibit a phase transition, to the thermodynamic limit. In 1982, Brézin [3] achieved a breakthrough by showing that finite-size scaling laws can actually be derived from renormalization-group (RG) theory, provided that the RG equations are not singular at the fixed point. This implies a breakdown of finite-size scaling for dimensionalities $d \geqslant 4$, and consequently an expansion of the finite-size scaling functions in powers of $\varepsilon = 4-d$ is *singular* at $\varepsilon = 0$. This rather surprising result was confirmed by explicit calculations for the $n$-vector model in the large-$n$ limit. In addition, it follows from Ref. [3] that the finite-size scaling relation for the free energy is a universal function depending only on two nonuniversal metric factors, without an additional nonuniversal prefactor. This result was derived from different arguments by Privman and Fisher [4], and subsequently confirmed analytically for the spherical model [5]. Pioneering work [6,7] then showed that a field-theoretic calculation of finite-size scaling functions is actually possible. Specifically, Brézin and Zinn-Justin [6] developed a systematic $\varepsilon$ expansion for these functions. Unlike the standard expansion in powers of $\varepsilon$ for critical exponents and scaling functions of bulk properties, one finds, for a fully finite geometry, an expansion in powers of $\sqrt{\varepsilon}$. More recently, Esser *et al.* [8] introduced a promising perturbation approach at fixed $d$ which is applicable below the critical temperature as well. However, here we focus on the expansion in $\varepsilon$ and in particular on the singular nature of this expansion.

The systems under consideration have an $n$-component order parameter $\phi$ with $O(n)$ symmetry and periodic boundary conditions. A quantity of central interest is the amplitude ratio $Q = \lim_{L\to\infty} \langle \phi_L^2 \rangle^2 / \langle \phi_L^4 \rangle$, which is directly related to the cumulant introduced by Binder [9]. At the critical temperature $T_c$ it takes a universal, although geometry-dependent, value (cf. Ref. [4]). In Ref. [6], an expansion for $Q(T_c)$ was obtained in powers of $\sqrt{\varepsilon}$, up to $O(\varepsilon)$, which is shown in Fig. 1 for $n=1$, along with numerical results for integer $d$. Given the low order of the expansion and the fact that it can only be checked for integer values of $\varepsilon$, hardly any conclusions can be drawn from a comparison to numerical results, and any confirmation of the singular nature of the $\varepsilon$ expansion will have to wait until the RG calculation has been carried to substantially higher order. Thus, we propose a different route: that is we replace the short-range (SR) forces by long-range attractive interactions decaying as a power law, $J(r) \propto r^{-(d+\sigma)}$, where $0<\sigma<2$. It was shown in Refs. [10,11] that these systems have an upper critical dimension $d_c = 2\sigma$, and that, for $d<d_c$, the critical exponents can be calculated in terms of an expansion in $\varepsilon' = 2\sigma - d$, very similar to the original $\varepsilon$ expansion, which is recovered for $\sigma \to 2$. Since the upper critical dimension is now a continuous parameter, we have the opportunity to verify $\varepsilon'$-expansion results for arbitrarily small $\varepsilon'$. So, even if actual physical realizations of this system may be scarce, it constitutes a very valuable mathematical model. Interest-

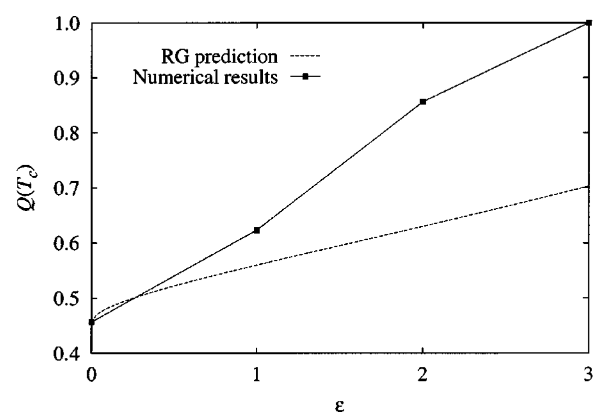


FIG. 1. The amplitude ratio $Q(T_c)$ for systems with short-range interactions. The dashed line shows the $\sqrt{\varepsilon}$ expansion of Ref. [6].

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ingly, finite-size scaling functions for the spherical model with power-law interactions have been calculated by several authors [12] for $d/2<\sigma<d$, but the nature of a possible singularity in the limit $\sigma\to d/2$ appears not to have been examined. The first part of this paper is therefore devoted to a generalization of the treatment of Ref. [6] to systems with algebraically decaying interactions. For notational convenience we redefine $\varepsilon=\varepsilon'=2\sigma-d$. Throughout our analysis we will closely adhere to the approach outlined in Ref. [6]. Additional details can also be found in Ref. [13], Chap. 36.

We consider a system with a hypercubic geometry, with linear dimension $L$ and periodic boundary conditions. It is represented by the following Landau-Ginzburg-Wilson Hamiltonian in momentum space,

$$\mathcal{H}(\phi_{\mathbf{k}})/k_BT=\frac{1}{2}\sum_{\mathbf{k}}\sum_{i}(k^{\sigma}+r_0)\phi_{i,\mathbf{k}}\phi_{i,-\mathbf{k}}+\frac{1}{4!}\frac{1}{L^d}u_0 \times\sum_{\mathbf{k}_1,\mathbf{k}_2,\mathbf{k}_3}\sum_{i,j}\phi_{i,\mathbf{k}_1}\phi_{i,\mathbf{k}_2}\phi_{j,\mathbf{k}_3}\phi_{j,-\mathbf{k}_1-\mathbf{k}_2-\mathbf{k}_3}, \tag{1}$$

where the factor $k^{\sigma}$ $(0<\sigma<2)$ arises from the isotropic long-range interactions. Compared to the SR case, it leads to the general replacement $k^2\to k^{\sigma}$ in all propagators. The indices $i$ and $j$ refer to the components of the field. It has been well established that this system belongs to the same universality class as a discrete spin model with algebraically decaying interactions; in particular the $\varepsilon$-expansion results [10,11] for the critical exponents have been confirmed (see Refs. [14,15], and references therein). Due to the finite geometry all components of the wave vectors are integer multiples of $2\pi/L$. The sums run to infinity, which corresponds to a vanishing lattice spacing $a$; however, the ratio $L/\xi$ is finite, whereas $L/a$ and $\xi/a$ are both sent to infinity [6]. Expectation values are computed from a partition function in which Eq. (1) is replaced by an effective Hamiltonian, consisting of the exactly calculated $\mathbf{k}=\mathbf{0}$ (homogeneous) mode contribution and a perturbatively calculated part, which contains the contribution of all nonzero modes. Only the latter contribution is affected by the changeover to long-range interactions, cf. Ref. [14]. To one-loop order this consists of a shift of the critical temperature and a renormalization of the coupling constant. Higher operators do not contribute at this order. We introduce the dimensionless coupling constant $g_0=\mu^{-\varepsilon}u_0$, and work in the system of units where $\mu=1$. The parameter $r_0$ is split into $r_{0c}+t$, where $t=r_0-r_{0c}\propto T-T_c$, and we require $t\geq 0$. The RG calculations are carried out in the minimal subtraction scheme [16,17], where it is a crucial ingredient of the calculation that, despite the quantization of all momenta, the UV divergences are taken care of by the bulk renormalization constants. As we do not go beyond one loop, we have ignored the field renormalization constant.

The leading contribution to the shift of $T_c$ is

$$\frac{n+2}{6}g_0\frac{1}{L^d}\sum_{\mathbf{k}}{}'\frac{1}{|\mathbf{k}|^{\sigma}+t}, \tag{2}$$

where the prime indicates that the $\mathbf{k}=\mathbf{0}$ mode is omitted from the sum. In the Schwinger parametrization this can be rewritten as

$$L^{-d}\int_0^{\infty}ds\,e^{-st}\left[\sum_{m_1=-\infty}^{\infty}\cdots\sum_{m_d=-\infty}^{\infty}e^{-s(m^2)^{\sigma/2}(2\pi/L)^{\sigma}}-1\right], \tag{3}$$

where $m^2=\Sigma_{i=1}^{d}m_i^2$ and we have omitted the prefactor $[(n+2)/6]g_0$. For $d\geq\sigma$, the UV divergence in Eq. (2) is reflected by the divergence of the integral at small $s$. Thus we isolate this divergence by rewriting Eq. (3) as

$$\frac{L^{\sigma-d}}{(2\pi)^{\sigma}}I_1(d,\sigma,t) +\frac{L^{\sigma-d}}{(2\pi)^{\sigma}}S_{d-1}\frac{1}{\sigma}\Gamma\left(\frac{d}{\sigma}\right)\int_0^{\infty}du\,u^{-d/\sigma}e^{-ut(L/2\pi)^{\sigma}}, \tag{4}$$

with

$$I_1(d,\sigma,t)\equiv\int_0^{\infty}du\,e^{-ut(L/2\pi)^{\sigma}}\left[\sum_{m_1}\cdots\sum_{m_d}e^{-u(m^2)^{\sigma/2}}-1 -S_{d-1}\frac{1}{\sigma}\Gamma\left(\frac{d}{\sigma}\right)u^{-d/\sigma}\right], \tag{5}$$

which is finite. $S_{d-1}=2\pi^{d/2}/\Gamma(d/2)$ is the surface area of a $d$-dimensional unit sphere. The second term in Eq. (4) can be continued analytically for $\mathrm{Re}(d)\geq\sigma$, and has a simple pole for $d=2\sigma$ $(\varepsilon=0)$. Upon expansion around this pole we find for Eq. (4),

$$-\frac{2t}{(4\pi)^{\sigma}\Gamma(\sigma)\varepsilon}+\frac{t}{(4\pi)^{\sigma}\Gamma(\sigma)}\left\{\frac{2}{\sigma}\ln t-[\ln 4\pi+\Psi(\sigma)]\right\} +\frac{1}{(2\pi L)^{\sigma}}I_1(2\sigma,\sigma,t)+O(\varepsilon), \tag{6}$$

where $\Psi(\sigma)$ denotes the digamma function. The addition of the $\phi^2$-insertion counterterm leads to the replacement of $t$ by $tZ_{\phi^2}$. To one-loop order, the renormalization constant has the same form as for SR interactions [18]; the pole is canceled and the shifted reduced temperature is given by

$$\tilde{t}=t+\frac{n+2}{6\sigma}\hat{g}_0t\ln t+\frac{2^{\sigma}}{12}(n+2)\Gamma(\sigma)\hat{g}_0\frac{1}{L^{\sigma}}I_1(2\sigma,\sigma,t) +O(\hat{g}_0^2), \tag{7}$$

with $\hat{g}_0=2[(4\pi)^{\sigma}\Gamma(\sigma)]^{-1}g_0\{1+\frac{1}{2}\varepsilon[\ln 4\pi+\Psi(\sigma)]+O(\varepsilon^2)\}$. The renormalized coupling constant $g$ is calculated in a similar fashion. The leading finite-size contribution is given by $-[(n+8)/6]g_0^2L^{-d}\Sigma_{\mathbf{k}}'(|\mathbf{k}|^{\sigma}+t)^{-2}$, which has a UV divergence for $\mathrm{Re}(d)\geq 2\sigma$. The $1/\varepsilon$ pole is canceled by the counterterm, where the renormalization constant to one-loop order is given by $Z_g=1+[(n+8)/6\varepsilon]\hat{g}$. After some algebra, we find, for the renormalized coupling constant,

$$g=g_0\left[1+\frac{n+8}{6\sigma}\hat{g}_0(1+\ln t)-\frac{n+8}{12}\hat{g}_0\frac{\Gamma(\sigma)}{\pi^\sigma}I_2(2\sigma,\sigma,t)+O(\hat{g}_0^2)\right], \tag{8}$$

with

$$I_2(d,\sigma,t)\equiv\int_0^\infty du\, u e^{-ut(L/2\pi)^\sigma}\left[\sum_{m_1}\cdots\sum_{m_d}e^{-u(m^2)^{\sigma/2}}-1-S_{d-1}\frac{1}{\sigma}\Gamma\left(\frac{d}{\sigma}\right)u^{-d/\sigma}\right]. \tag{9}$$

Equations (7) and (8) suffice to calculate the finite-size scaling functions close to criticality to $O(\varepsilon)$. To this order, the fixed-point value of $\hat{g}_0$ only differs from the SR case in the definition of $\varepsilon$, $\hat{g}_0^*=[6\varepsilon/(n+8)]+O(\varepsilon^2)$. We are now able to calculate $\tilde{t}L^{d/2}g^{-1/2}$ at the fixed point, which, as we shall see shortly, is the parameter appearing in the finite-size scaling functions. This also provides a simple consistency check for our calculations, since all factors $\ln L$ have to disappear upon introduction of the appropriate scaling variable $y=tL^{1/\nu}$. We find $1/\nu=\sigma-[(n+2)/(n+8)]\varepsilon+O(\varepsilon^2)$, which indeed agrees with Ref. [10], and the final expression is

$$\tilde{t}L^{d/2}g^{-1/2}|_{\text{f.p.}}=\frac{1}{\sqrt{g_0^*}}\left[y-\frac{1}{2\sigma}\varepsilon y+\frac{n-4}{2\sigma(n+8)}\varepsilon y\ln y+\frac{1}{4}\varepsilon y\frac{\Gamma(\sigma)}{\pi^\sigma}I_2(2\sigma,\sigma,yL^{-1/\nu})+\frac{2^{\sigma-1}(n+2)}{n+8}\varepsilon\Gamma(\sigma)I_1(2\sigma,\sigma,yL^{-1/\nu})+O(\varepsilon^2)\right]. \tag{10}$$

We are particularly interested in the amplitude ratio $Q$ at criticality, for $n=1$. The even moments of the magnetization distribution are calculated from $\langle(\phi^2)^p\rangle=\int_{-\infty}^{+\infty}d\phi(\phi^2)^p\exp[-S(\phi)]/\int_{-\infty}^{+\infty}d\phi\exp[-S(\phi)]$, with $S(\phi)=L^d(\frac{1}{2}\tilde{t}\phi^2+(1/4!)g\phi^4)$. We carry out the rescaling $\phi\to(L^dg)^{-1/4}\phi$, and expand in terms of the parameter $x\equiv\tilde{t}L^{d/2}g^{-1/2}$. Elementary algebra leads to

$$Q=\frac{4\Gamma^2\left(\frac{3}{4}\right)}{\Gamma^2\left(\frac{1}{4}\right)}\left[1+\left(4\frac{\Gamma\left(\frac{3}{4}\right)}{\Gamma\left(\frac{1}{4}\right)}-\frac{1}{2}\frac{\Gamma\left(\frac{1}{4}\right)}{\Gamma\left(\frac{3}{4}\right)}\right)\sqrt{6}x+\left(13\frac{\Gamma^2\left(\frac{3}{4}\right)}{\Gamma^2\left(\frac{1}{4}\right)}+\frac{1}{16}\frac{\Gamma^2\left(\frac{1}{4}\right)}{\Gamma^2\left(\frac{3}{4}\right)}-2\right)6x^2+O(x^3)\right]. \tag{11}$$

At criticality, $y=0$ and $x$ takes the value

$$x_0=\sqrt{\varepsilon}\left\{\frac{1}{2}\frac{n+2}{\sqrt{3(n+8)}}\sqrt{\frac{\Gamma(\sigma)}{\pi^\sigma}}I_1(2\sigma,\sigma,0)+O(\varepsilon)\right\}. \tag{12}$$

A comparison to Eq. (3.33) in Ref. [6] shows that $x_0$ only differs from the SR case by a redefinition of $\varepsilon$, a geometric factor, and the integral $I_1$, and thus we see that the singular structure is preserved in the generalization to long-range forces. For completeness we remark that one may also calculate $x_0$ by carrying out all manipulations at criticality. This permits a different parametrization and leads to the same expression for $x_0$, in which $I_1(2\sigma,\sigma,0)$ is replaced by $\hat{I}_1(2\sigma,\sigma)/\Gamma(\sigma/2)$, where $\hat{I}_1(d,\sigma)\equiv\int_0^\infty du\, u^{\sigma/2-1}[(\sum_{m=-\infty}^{\infty}e^{-um^2})^d-1-(\pi/u)^{d/2}]$. As a side note, we conjecture $\hat{I}_1(4,2)$, which has been evaluated numerically in Refs. [6,13,19], to be exactly equal to $-8\ln 2$. For lower dimensionalities, the upper critical dimension shifts toward smaller values of $\sigma$, and numerical evaluation yields $I_1(d,d/2,0)=-2.92$, $-3.900$, and $-4.8227$ for $d=1$, 2, and 3, respectively. Substitution into Eqs. (12) and (11) suggests that for each of these values a reasonable convergence may be expected for $\varepsilon<1$.

In order to verify these predictions, we have carried out extensive Monte Carlo simulations of spin models with $n=1$ and algebraically decaying interactions, for $d=1$ and 2. Accurate results could be obtained by means of an efficient cluster algorithm [20]. We investigated system sizes $10\leqslant L\leqslant 150\,000$ for $d=1$ and $4\leqslant L\leqslant 400$ for $d=2$, for several values of the decay parameter $\sigma$. These were chosen such that $0<\varepsilon\lesssim 1$, where it should be noted that for very small $\varepsilon$ the analysis is hampered by strong corrections to scaling. Simulational details can be found in Ref. [14], where the classical regime $0<\sigma\leqslant d/2$ was discussed. The numerical results were analyzed using an expression similar to Eq. (13) in Ref. [14], $Q_L(T)=Q+r_1tL^{y_t}+r_2t^2L^{2y_t}+\cdots+s_1L^{y_i}+\cdots$. Here $y_t$ and $y_i$ are the thermal and leading irrelevant exponents, respectively, $r_i$ and $s_i$ are nonuniversal coefficients, and the ellipses denote higher-order terms. An extensive analysis of the data will be presented elsewhere. The resulting estimates for $Q(T_c)$ are shown in Figs. 2 and 3. For the one-dimensional case (Fig. 2), the region $0.1\leqslant\varepsilon\leqslant 0.9$ has been covered. For $\sigma\to 1$, the data points approach $Q(T_c)=1$, in agreement with the occurrence of a Kosterlitz-Thouless transition at $\sigma=1$ [21]. However, for $0<\varepsilon\lesssim 0.5$, the numerical results are described by a perfectly linear dependence on $\varepsilon$, in strong contrast with the predicted square-root behavior. This discrepancy is reinforced by the two-dimensional results (Fig. 3), which are also well described by a linear relation for $0<\varepsilon\lesssim 1.2$. For larger $\sigma$, the error bars increase, signaling a crossover to short-range criticality.

In summary, we have calculated universal finite-size scaling functions to second order in $\sqrt{\varepsilon}$ for systems with algebraically decaying interactions. These calculations are essentially a generalization of those for systems with short-range interactions [6], and exhibit the same singular dependence on $\varepsilon$. Subsequently, we have compared our results to accurate simulations for one- and two-dimensional systems belonging to the same universality class as the field-theoretical Hamil-

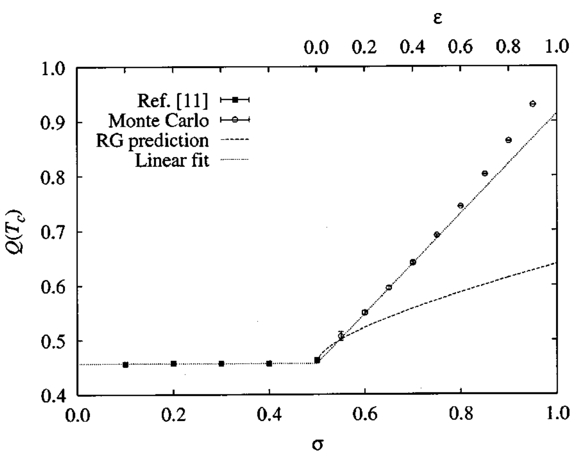


FIG. 2. The critical value of the amplitude ratio $Q$ as a function of the decay parameter $\sigma$ for $d=1$. The corresponding values of $\varepsilon$ are shown at the upper axis. The data in the regime $0<\sigma\leqslant 0.5$ are taken from Ref. [14].

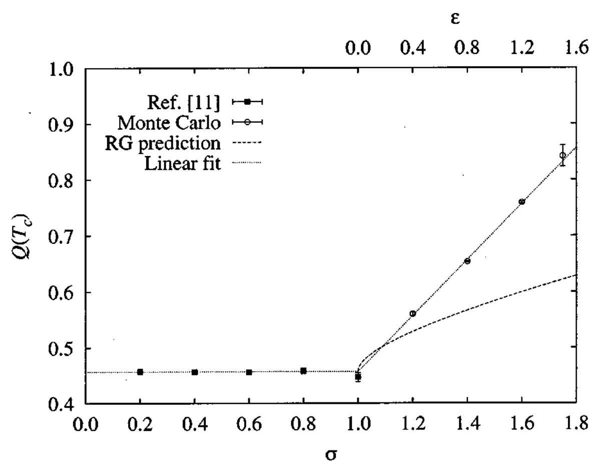


FIG. 3. The analog of Fig. 2 for $d=2$.

tonian. The presence of long-range interactions offers the advantage that $\varepsilon$ is a continuous parameter, so that one can reach the regime where the convergence of the $\varepsilon$ expansion does not have to be doubted. Nevertheless, no agreement is found: the numerical data exhibit a linear rather than a square-root dependence on $\varepsilon$. Currently, we do not have an explanation for this striking discrepancy. Although higher-order terms might yield some improvement, it is difficult to envisage that this would fully resolve the problems. It would be very remarkable if the apparent linear variation over such a wide range in Figs. 2 and 3, which includes the point from which our $\sqrt{\varepsilon}$ expansion starts, were accidental. In Ref. [22], it was suggested that $Q$ contains *nonuniversal* contributions, depending on the cutoff used in the integration of the order parameter probability distribution. However, apart from the validity of this suggestion, it is difficult to envisage how this would lead to the (dis)appearance of a square-root contribution in the $\varepsilon$ expansion. Furthermore, it is an open question as to what extent the breakdown of the field-theoretic description of finite-size scaling for $d\geqslant 4$ [19] influences the nature of the $\varepsilon$ expansion. We feel that an understanding of these problems is of some significance for an understanding of finite-size scaling of critical phenomena in general.

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[1] M.N. Barber, in *Phase Transitions and Critical Phenomena*, edited by C. Domb and J.L. Lebowitz (Academic, London, 1983) Vol. 8; *Finite Size Scaling and Numerical Simulation of Statistical Systems*, edited by V. Privman (World Scientific, Singapore, 1990).
[2] M.E. Fisher, in *Critical Phenomena*, Proceedings of the 51st Enrico Fermi Summer School, Varenna, Italy, edited by M. S. Green (Academic, New York, 1971).
[3] E. Brézin, J. Phys. (Paris) **43**, 15 (1982).
[4] V. Privman and M.E. Fisher, Phys. Rev. B **30**, 322 (1984).
[5] S. Singh and R.K. Pathria, Phys. Rev. B **31**, 4483 (1985).
[6] E. Brézin and J. Zinn-Justin, Nucl. Phys. B **257**, 867 (1985).
[7] J. Rudnick, H. Guo, and D. Jasnow, J. Stat. Phys. **41**, 353 (1985).
[8] A. Esser, V. Dohm, M. Hermes, and J.S. Wang, Z. Phys. B: Condens. Matter **97**, 205 (1995).
[9] K. Binder, Z. Phys. B: Condens. Matter **43**, 119 (1981).
[10] M.E. Fisher, S.-k. Ma, and B.G. Nickel, Phys. Rev. Lett. **29**, 917 (1972).
[11] M. Suzuki, Y. Yamazaki, and G. Igarashi, Phys. Lett. **42A**, 313 (1972).
[12] M.E. Fisher and V. Privman, Commun. Math. Phys. **103**, 527 (1986); J.G. Brankov and N.S. Tonchev, J. Stat. Phys. **52**, 143 (1988); S. Singh and R.K. Pathria, Phys. Rev. B **40**, 9238 (1989).
[13] J. Zinn-Justin, *Quantum Field Theory and Critical Phenomena*, 3rd ed. (Clarendon, Oxford, 1996).
[14] E. Luijten and H.W.J. Blöte, Phys. Rev. Lett. **76**, 1557, 3662(E) (1996); Phys. Rev. B **56**, 8945 (1997).
[15] E. Luijten, *Interaction Range, Universality and the Upper Critical Dimension* (Delft University Press, Delft, 1997).
[16] E. Brézin, J.C. Le Guillou, and J. Zinn-Justin, in *Phase Transitions and Critical Phenomena*, edited by C. Domb and M. S. Green (Academic, London, 1976), Vol. 6.
[17] D.J. Amit, *Field Theory, The Renormalization Group, and Critical Phenomena*, 2nd ed. (World Scientific, Singapore, 1984).
[18] Y. Yamazaki and M. Suzuki, Prog. Theor. Phys. **57**, 1886 (1976).
[19] X. S. Chen and V. Dohm, Int. J. Mod. Phys. C **9**, 1007 (1998).
[20] E. Luijten and H.W.J. Blöte, Int. J. Mod. Phys. C **6**, 359 (1995).
[21] J.M. Kosterlitz, Phys. Rev. Lett. **37**, 1577 (1976).
[22] R. Hilfer, Z. Phys. B: Condens. Matter **96**, 63 (1994); R. Hilfer and N.B. Wilding, J. Phys. A **28**, L281 (1994).