Scaling functions of the three-dimensional $Z(2)$, $O(2)$, and $O(4)$ models and their finite-size dependence in an external field

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We analyze scaling functions in the 3D $Z(2)$, $O(2)$, and $O(4)$ universality classes and their finite-size dependence using Monte Carlo simulations of improved ϕ^4 models. Results for the scaling functions are fitted to the Widom-Griffiths form, using a parametrization also used in analytic calculations. We find good agreement on the level of scaling functions and the location of maxima in the universal part of susceptibilities. We also find that an earlier parametrization of the $O(4)$ scaling function, using 14 parameters, is well reproduced when using the Widom-Griffiths form with only three parameters. We furthermore show that finite-size corrections to the scaling functions are distinctively different in the $Z(2)$ and $O(N)$ universality classes and determine the volume dependence of the peak locations in order parameter and mixed susceptibilities.

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I. INTRODUCTION

Universal critical behavior in the 3D $Z(2)$ and $O(N)$ universality classes plays an important role in the analysis of phase transitions in many statistical models as well as quantum field theories. In the fundamental theory of strong interactions, quantum chromodynamics (QCD), phase transitions that occur at finite temperature and vanishing as well as nonvanishing conserved charge chemical potentials belong to these universality classes. The spontaneous breaking of chiral symmetry in QCD is expected to exhibit universal critical behavior in the 3D $O(4)$ universality class [1], and the 3D $Z(2)$ universality class is expected to describe critical behavior at the so-called critical end point, a yet to be discovered second-order phase transition that is expected to occur in QCD with nonzero quark mass values and nonvanishing baryon chemical potential. A second-order phase transition in the $Z(2)$ universality class also occurs in QCD at nonvanishing, imaginary values of chemical potentials at the so-called Roberge-Weiss end point [2]. Also, the $O(2)$ universality class plays a role in the studies of the phase diagram of QCD, as many calculations are performed in a discretized version of the theory, using so-called staggered fermions, in which only this smaller symmetry is realized.

Numerical studies of the phase structure of statistical models, and, in particular, of complicated theories such as QCD, are being performed on finite lattices. A good understanding of finite-size effects, thus, is generally of importance. In the limit of small external symmetry-breaking fields and large volumes also these finite-size effects are universal, i.e., characteristic for a given universality class. For this purpose, a powerful renormalization group framework has been developed in statistical physics which leads to a detailed finite-size scaling theory for critical behavior [3,4]. This framework has been used to analyze finite-size scaling behavior of systems in the 3D $Z(2)$ and $O(N)$ universality classes. The finite-size dependence of thermodynamic observables in 3D $O(N)$ spin models has been examined using Monte Carlo simulations [5–7], and finite-size scaling functions have been derived using the functional renormalization group approach [8]. For the $O(4)$ universality class, we provided an updated parametrization for the infinite volume scaling functions [9] and presented a parametrization of the finite-size scaling functions $f_G(z, z_L)$ and $f_\chi(z, z_L)$ [10], which describe finite volume corrections to the singular behavior of the order parameter and its susceptibility. In this work, we will extend these studies and provide finite-size scaling functions also for the $Z(2)$ and $O(2)$ universality classes, by performing Monte Carlo simulations with improved Hamiltonians [11–13], which have been constructed to suppress contributions from corrections-to-scaling and, thus, allow for easier access to the desired scaling functions. We furthermore present a parametrization of the infinite volume scaling functions, determined from Monte Carlo simulations, using the Widom-Griffiths (WG) form [14–17] of these scaling functions. In the $Z(2)$ [18] and $O(2)$ [7] universality classes, the relevant parameters entering this analytic form have been determined previously using ϵ expansion and other field theoretic methods applied directly in 3D.

This paper is organized as follows. In the next section, we introduce the $Z(2)$ and $O(N)$ models for which we present new Monte Carlo results and define the basic observables studied by us. In Sec. III, we introduce basic relations for finite-size scaling functions. Section IV is devoted to the determination of the infinite volume scaling functions for the $Z(2)$, $O(2)$, and $O(4)$ models, using a parametrization based on the Widom-Griffiths form. Here, we also determine the nonuniversal parameters for the improved $Z(2)$ and $O(2)$ models that are needed to introduce the scaling variables z and z_L. In Sec. V, we present our results for the finite-size scaling functions. We give our conclusions in Sec. VI. In Appendix A, we discuss the determination of the two nonuniversal scales H_0 and L_0, and in Appendix B, we give explicit expressions for the expansion coefficients d_1^- and d_2^- appearing in the scaling function $f_G(z, z_L = 0)$ at asymptotically large, negative arguments.

II. LATTICE SETUP AND OBSERVABLES

We discuss here universal scaling properties for three-dimensional, N-component ϕ^4 models, i.e., spin models in the 3D $Z(2)$ ($N = 1$, Ising model), $O(2)$ (XY model), and $O(4)$ universality classes described by the Hamiltonian

$$\mathcal{H} = -J\sum_{\langle x,y\rangle}\Phi_x\Phi_y + \sum_x[\Phi_x^2 + \lambda(\Phi_x^2 - 1)^2] - H\sum_x \phi_{x,1}, \tag{1}$$

with $\Phi_x \equiv \phi_{x,1}$ for the 3D $Z(2)$ spin model, (x, y) denoting nearest-neighbor sites on the lattice, and $\Phi_x \equiv (\phi_{x,1}, \ldots, \phi_{x,N})$ for the 3D $O(N)$ spin models. For specific choices of λ, the above Hamiltonian is called "improved" since the quartic coupling λ appearing in the potential term of the spin models has been optimized to reduce the effect of contributions from subleading relevant scaling variables to universal scaling behavior of these models [11]. We use the parameters $\lambda = 1.1$ [12] in the case of $Z(2)$ and $\lambda = 2.1$ for $O(2)$ spin models [13], respectively. In the $O(4)$ case, we use the standard, unimproved Hamiltonian, corresponding to $\lambda = \infty$. The temperature T is defined as the inverse of the coupling J, i.e., $T \equiv 1/J$, and the external field coupling H controls explicit symmetry breaking in the Hamiltonian. We introduce this symmetry-breaking term such that it couples only to the first component of the spin variable Φ_x, defined on the sites x of a three-dimensional lattice of size L^3.

Using the Hamiltonian introduced in Eq. (1), the partition functions of the 3D $Z(2)$ and $O(N)$ models are given by

$$Z(T, H, L) = \int \prod_x \mathrm{d}\Phi_x \mathrm{e}^{-\mathcal{H}}. \tag{2}$$

From this, one obtains the free energy density in units of temperature T: $f(T, H, L) = -L^{-3} \ln Z(T, H, L)$. The derivative of the free energy density with respect to the external field H defines the order parameter M for spontaneous symmetry breaking:

$$M(T, H, L) = -\frac{\partial f}{\partial H}. \tag{3}$$

The (longitudinal) susceptibility χ_h and the mixed susceptibility χ_t are obtained as derivatives of the order parameter with respect to H and J, respectively:

$$\chi_h(T, H, L) = \frac{\partial M}{\partial H}, \tag{4}$$

$$\chi_t(T, H, L) = \frac{\partial M}{\partial J} = -T^2 \frac{\partial M}{\partial T}. \tag{5}$$

In the absence of explicit symmetry breaking ($H = 0$), the $Z(2)$ and $O(N)$ spin models undergo second-order phase transitions at critical temperatures $T_c \equiv 1/J_c$. The critical temperatures of the 3D improved $Z(2)$ [12], $O(2)$ [7], and unimproved $O(4)$ [19] spin models, with couplings λ, as introduced above, are well determined. We give the critical temperatures together with other universal and nonuniversal model parameters in Table I.

In the case of the $O(4)$ spin model, we do not perform new MC calculations, but reparametrize results for scaling functions already obtained in Ref. [9]. We therefore give in Table I the parameters actually used in that calculation. They are consistent with analytic results [18] but differ somewhat from recent MC results [22].

For $H \neq 0$ as well as for finite lattice sizes $L < \infty$, pseudocritical temperatures $T_{pc,o}(H, L)$, with $o = h$ or t, can be defined as locations of maxima in the susceptibilities χ_h and χ_t.

Monte Carlo simulations have been performed by us for the improved $Z(2)$ and $O(2)$ models. For our calculations we use a code which has been developed and used previously in simulations of $Z(2)$ and $O(2)$ models.[1] The statistics collected in calculations with the $Z(2)$ and $O(2)$ models on different size lattices is given in Tables II–IV.

[1]We use a cluster update [23,24] code developed in the group of Jürgen Engels. The algorithm and its implementation are described in more detail in Ref. [21].

TABLE I. Critical exponents in the 3D $Z(2)$, $O(2)$ and $O(4)$ universality classes and nonuniversal parameters for the improved Hamiltonians used in our simulations. $Z(2)$ critical exponents are taken from Zinn-Justin [18], and the $O(2)$ values are taken from Ref. [20]. Exponents used for the $O(4)$ case are taken from Ref. [19]. Other critical exponents are obtained using the hyperscaling relations. The critical temperature ($T_c = 1/J_c$) of the $Z(2)$ model with $\lambda = 1.1$ is taken from Ref. [12], and T_c for the $O(2)$ model with $\lambda = 2.1$ is taken from Ref. [7]. All other nonuniversal parameters have been obtained in this study. For the $Z(2)$ model, we find results for the scales t_0 and H_0 that are in good agreement with previous results obtained in Ref. [21]; t_0 agrees to better than 1%, and the result for H_0 is smaller by about 2%. In the $O(4)$ case, we give critical exponents and nonuniversal parameters used also in a previous analysis of scaling functions [9] (see the text for further references).

	$Z(2)$	$O(2)$	$O(4)$
	Universal parameter		
β	0.3258(14)	0.34864(7)	0.380(2)
δ	4.805(15)	4.7798(5)	4.824(9)
	Nonuniversal parameter		
λ	1.1	2.1	∞
T_c	2.665980(3)	1.964055(23)	1.06849(11)
L_0	1.0262(18)	0.97917(55)	0.7686
H_0	0.79522(17)	1.36632(28)	4.845(66)
t_0	0.303376(45)	0.4540(11)	1.023(16)

TABLE II. Number of configurations generated per parameter set (J, H) on lattices of size L^3 for $J \neq J_c$. Data generated on the largest ($L = 120$) lattices were used for consistency checks but were not used in the final fits.

	$L = 48$	$L = 96$	$L = 120$
$Z(2)$	200 000	100 000	…
$O(2)$	200 000	200 000	24 000

TABLE III. Number of configurations generated per parameter set (J_c, H), i.e., at the infinite volume critical temperature, on lattices of size L^3. These datasets were used for the determination of the scale parameters H_0 and L_0, discussed in Appendix A. The data sets generated on the $L = 96$ lattice were also used in finite-size fits discussed in Sec. V.

	$L = 48$	$L = 96$	$L = 120$
$Z(2)$	200 000	350 000	150 000
$O(2)$	200 000	100 000	84 000

III. SCALING FUNCTIONS

In order to analyze universal critical behavior in the vicinity of the second-order phase transitions occurring in the 3D $Z(2)$ and $O(N)$ spin models, the free energy is split in a singular and regular contribution, respectively:

TABLE IV. Number of configurations generated per parameter set (J, H) on lattices of size L^3 in the region $z < -2$. These data have been primarily used for the determination of the scale parameter t_0 obtained together with the determination of the infinite volume scaling functions discussed in Sec. IV.

	$L = 96$	$L = 120$	$L = 160$	$L = 200$
$Z(2)$	76 000	38 000	18 000	…
$O(2)$	…	480 000	184 000	120 000

$$f(T, H, L) = f_s(T, H, L) + f_{\rm reg}(T, H, L). \quad (6)$$

The scaling behavior of, e.g., the order parameter M and the susceptibilities χ_h and χ_t is derived from the renormalization group analysis of the singular part of the free energy:

$$f_s(t, h, l, \ldots) = b^{-d} f_s(b^{y_t} t, b^{y_h} h, bl, \ldots), \quad (7)$$

where b is a free scale parameter and y_t and y_h are two relevant critical exponents.[2] In Eq. (7), we introduced the reduced temperature (t), external field (h), and finite volume (l) scaling variables:

$$t = \frac{1}{t_0} \frac{T - T_c}{T_c}, \qquad h = \frac{H}{H_0}, \qquad l = \frac{L_0}{L}. \quad (8)$$

They are normalized by nonuniversal scale parameters t_0, H_0, and L_0, respectively. The exponents y_t and y_h define the two independent critical exponents of the universality class under consideration:

$$y_t = 1/\nu, \qquad y_h = \beta\delta/\nu. \quad (9)$$

Here β, δ, and ν are critical exponents which are related to each other through the hyperscaling relation $\delta = d\nu/\beta - 1$. In our current analysis, we use results for the exponents β and δ as basic input. These critical exponents are well determined for the 3D $Z(2)$ and $O(N)$ universality classes. We use here the $Z(2)$ results obtained in Ref. [18] and the $O(2)$ values from Ref. [20]. They are given in Table I. In the $O(4)$ case, we use critical exponents and nonuniversal parameters that have also been used in a previous analysis of scaling functions [9].

Choosing the scale parameter $b = h^{-1/y_h}$, we obtain for the free energy density

$$f(T, H, L) = H_0 h^{1+1/\delta} f_f(z, z_L) + f_{\rm reg}(T, H, L), \quad (10)$$

[2] We ignore here possible contributions from corrections-to-scaling terms and irrelevant scaling fields. The former are suppressed in our analysis due to the use of an optimized Hamiltonian, and the latter are irrelevant for the scaling analysis.

where we have introduced the finite-size scaling function $f_f(z, z_L)$:

$$f_f(z, z_L) = H_0^{-1} f_s(t/h^{1/\beta\delta}, 1, l/h^{\nu/\beta\delta}), \tag{11}$$

with arguments (z, z_L) defined as

$$z = t/h^{1/\beta\delta}, \qquad z_L = l/h^{\nu/\beta\delta}. \tag{12}$$

Using Eqs. (3) and (10), we obtain the order parameter M:

$$M(T, H, L) = h^{1/\delta} f_G(z, z_L) + \mathrm{reg} \tag{13}$$

and its susceptibilities

$$\chi_h(T, H, L) = H_0^{-1} h^{1/\delta - 1} f_\chi(z, z_L) + \mathrm{reg}, \tag{14}$$

$$\chi_t(T, H, L) = -\frac{T^2}{t_0 T_c} h^{(\beta-1)/\beta\delta} f'_G(z, z_L) + \mathrm{reg} \tag{15}$$

with scaling functions $f_G(z, z_L)$, $f'_G(z, z_L)$, and $f_\chi(z, z_L)$ defined, respectively, as

$$f_G(z, z_L) = -\left(1 + \frac{1}{\delta}\right) f_f(z, z_L) + \frac{z}{\beta\delta} \frac{\partial f_f(z, z_L)}{\partial z} + \frac{\nu}{\beta\delta} z_L \frac{\partial f_f(z, z_L)}{\partial z_L}, \tag{16}$$

$$f'_G(z, z_L) = \frac{\partial f_G(z, z_L)}{\partial z}, \tag{17}$$

$$f_\chi(z, z_L) = \frac{1}{\delta}\left(f_G(z, z_L) - \frac{z}{\beta} f'_G(z, z_L)\right) - \frac{\nu}{\beta\delta} z_L \frac{\partial f_G(z, z_L)}{\partial z_L}. \tag{18}$$

The finite-size scaling functions can be determined in the vicinity of the critical point $(t, h, l) = (0, 0, 0)$, where regular contributions to the order parameter and its susceptibilities, given in Eqs. (13)–(15), are negligible[3]:

$$f_G(z, z_L) = h^{-1/\delta} M(T, H, L), \tag{19}$$

$$f'_G(z, z_L) = -\frac{t_0 T_c}{T^2} h^{(1-\beta)/\beta\delta} \chi_t(T, H, L), \tag{20}$$

$$f_\chi(z, z_L) = H_0 h^{1-1/\delta} \chi_h(T, H, L). \tag{21}$$

The nonuniversal scale parameters t_0 and H_0 are fixed by the following conditions on the order parameter at infinite volume:

$$M(t = 0, h, l = 0) = h^{1/\delta},$$
$$M(t < 0, h = 0, l = 0) = (-t)^\beta, \tag{22}$$

or, equivalently, in terms of the scaling function

$$f_G(0, 0) = 1, \qquad \lim_{z \to -\infty} \frac{f_G(z, 0)}{(-z)^\beta} = 1. \tag{23}$$

The scale L_0 is obtained using a normalization condition for the finite-size scaling function $f_G(0, z_L)$. We define $z_L = 1$ as the point at which the order parameter, evaluated at T_c, is 30% smaller than its infinite volume value, i.e.,

$$\frac{f_G(0, 1)}{f_G(0, 0)} = 0.7. \tag{24}$$

This differs from the choice used in Ref. [10] but has the advantage of allowing better comparison of finite-size scaling functions obtained in different universality classes.

In the following two sections, we will discuss results for the infinite and finite volume scaling functions, respectively. In order to judge which lattice sizes and external field parameters are needed to get close to the infinite volume, universal scaling regime, we first analyzed the z_L dependence of the scaling functions at some fixed values of z on different size lattices. The three scaling functions $f_G(z, z_L)$, $f'_G(z, z_L)$, and $f_\chi(z, z_L)$ have been calculated at a few values of z as functions of z_L. Using z and z_L as variables, of course, does require the determination of the nonuniversal scales (t_0, H_0, L_0) which we are going to discuss in the next section and in Appendix A.

Results from the calculations of the scaling functions for some fixed values of z, performed on lattices of size L^3 with $L = 48$ and 96, are shown in Fig. 1. As can be seen, the finite-size effects in all three scaling functions are almost negligible for $z_L < 0.4$. This is consistent with findings obtained in calculations with the standard $O(4)$ model [10] and can also be concluded from Fig. 8, shown in Appendix A, where we compare results for $f_G(z = 0, z_L)$ in different universality classes.

In the following, we thus use our numerical results for $z_L < 0.4$ as approximation for infinite volume limit results.

IV. INFINITE VOLUME SCALING FUNCTIONS

In our discussion of scaling functions in the infinite volume limit $z_L = 0$, we suppress the second argument of the scaling functions; i.e., we introduce $f_G(z) \equiv f_G(z, 0)$ and similarly for $f'_G(z)$ and $f_\chi(z)$. These scaling functions have been determined previously using ϵ expansions [25] and perturbative field theoretic approaches applied directly in three dimensions [7,18,26], as well as in Monte Carlo (MC) simulations [5,6,21]. For the $Z(2)$ universality class,

[3]To arrive at Eqs. (19)–(21), one actually takes the limit $(H \to 0, L \to \infty)$ at fixed z_L.

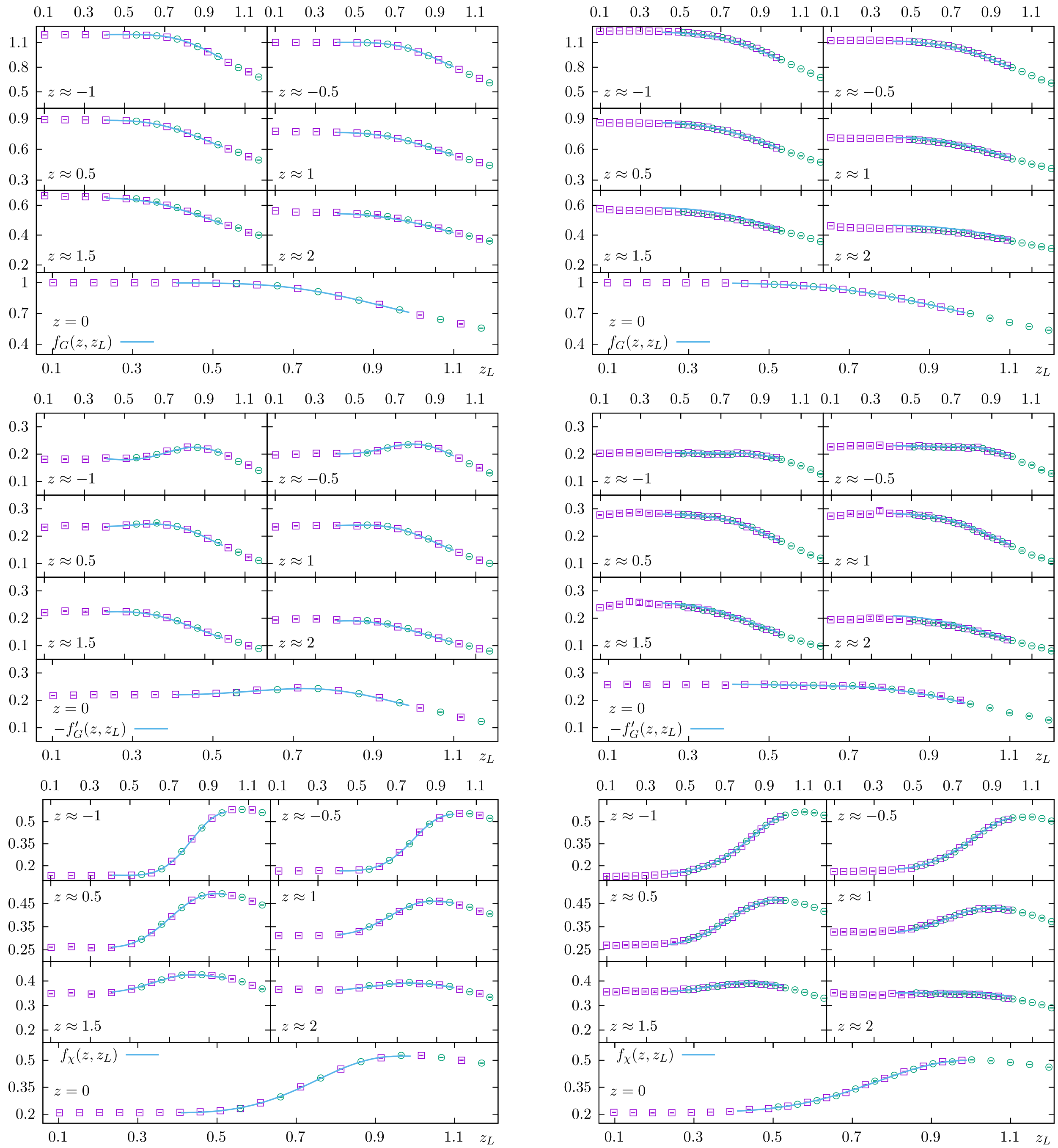

FIG. 1. Finite-size scaling functions $f_G(z, z_L)$ (top), $f'_G(z, z_L)$ (middle), and $f_\chi(z, z_L)$ (bottom) in the 3D $Z(2)$ (left) and $O(2)$ (right) universality classes. Shown are results for several fixed values $z \in [-1.0{:}2.0]$, obtained from calculations on lattices of size L^3, with $L = 48$ (green circles) and 96 (purple squares), in the range $z_L \in [0.1, 1.2]$. The light blue lines show results of joined fits to all three scaling functions performed in the interval $z_L \in [0.4{:}1]$ (see Sec. V). As the values for z and z_L have been fixed *a posteriori*, before nonuniversal scale parameters have been determined in the fits, we have labeled the different panels with approximate z values. Their actual values are (from lowest to highest) $Z(2)$: $z = -0.979, -0.490, 0, 0.490, 0.979, 1.469, 1.958$ and $O(2)$: $z = -1.051, -0.526, 0, 0.526, 1.051, 1.577, 2.010$.

it has been shown that the scaling functions, obtained in MC calculations, are in good agreement with the Widom-Griffiths form [14,15] using a resummed perturbative series for the order parameter obtained in 3D [18]. However, no parametrization based on MC results has been given. The previous determination of the $O(2)$ scaling functions, using the WG *Ansatz* [6], has been performed using an unimproved $O(2)$ Hamiltonian and, thus, had to take care of corrections to scaling, which, in particular, made the determination of scaling functions in the symmetry-broken regime difficult. Scaling functions for the $O(4)$ model, using Monte Carlo results obtained with the standard, unimproved Hamiltonian (corresponding to $\lambda = \infty$), have been presented in Ref. [9]. In none of these cases has a parametrization of $O(N)$ scaling functions been presented, which uses the WG form with only three free parameters.

A. Widom-Griffiths form of scaling functions

We present here a determination of the $Z(2)$ and $O(N)$ ($N = 2$, 4) scaling functions from Monte Carlo simulations. From our new Monte Carlo results and those obtained in Ref. [9], we determine the parameters entering a parametrization of scaling functions using the WG form of the order parameter scaling function [14,15]:

$$M = m_0 R^\beta \theta, \tag{25}$$

$$t = R(1 - \theta^2), \tag{26}$$

$$h = h_0 R^{\beta\delta} h(\theta), \tag{27}$$

where (R,θ) represents an alternate coordinate frame corresponding to the (t, h) plane [16,17]. Aside from the normalization constants m_0 and h_0, this parametrization depends on a function $h(\theta)$, which needs to be determined. For the case of $Z(2)$, it seems that a Taylor series expansion up to $\mathcal{O}(\theta^5)$ is sufficient[4] [18], while in the case of $O(N)$, one needs to take care explicitly of the presence of Goldstone modes in the symmetry-broken phase. This requires that $h(\theta)$ has a double zero at some $\theta_0 > 1$ [7,27]. We, thus, use the *Ansatz* proposed in Refs. [7,18]:

$$h(\theta) = (\theta + h_3\theta^3 + h_5\theta^5)\begin{cases} 1, & \text{for } Z(2). \\ (1 - \theta^2/\theta_0^2)^2, & \text{for } O(N). \end{cases} \tag{28}$$

The normalization constants m_0 and h_0 are determined from the conditions in Eq. (22), which gives us

$$m_0 = \frac{(\theta_0^2 - 1)^\beta}{\theta_0}, \qquad h_0 = \frac{m_0^\delta}{h(1)}, \tag{29}$$

where θ_0 is the first positive zero of $h(\theta)$ in the $Z(2)$ universality class and the double zero of $h(\theta)$ in the $O(N)$ case. Using Eqs. (12) and (19) and the above relations for the normalization constants m_0 and h_0, one can establish the relation between the WG form of the scaling function f_G and the relation between the scaling variables, $z = t/h^{1/\beta\delta}$ and θ:

$$f_G(z) \equiv f_G(\theta(z)) = \theta\left(\frac{h(\theta)}{h(1)}\right)^{-1/\delta}, \tag{30}$$

$$z(\theta) = \frac{1 - \theta^2}{\theta_0^2 - 1}\theta_0^{1/\beta}\left(\frac{h(\theta)}{h(1)}\right)^{-1/\beta\delta}. \tag{31}$$

Obviously, $\theta = 1$ corresponds to $z = 0$ and $\theta = \theta_0$ corresponds to $z = -\infty$, and these, respectively, correspond to the normalization conditions for the scaling function f_G in Eq. (23). Finally, $\theta = 0$ corresponds to $z = \infty$. Using Eqs. (30) and (31), we also obtain $f_G'(z)$ as

$$f_G'(z) \equiv \frac{\mathrm{d}f_G(\theta(z))}{\mathrm{d}z} = \frac{\mathrm{d}f_G}{\mathrm{d}\theta}\Big/\frac{\mathrm{d}z}{\mathrm{d}\theta}. \tag{32}$$

The presence of Goldstone modes in the symmetry-broken ($z < 0$) phase of $O(N)$ symmetric models gives rise to a distinctively different behavior of the $Z(2)$ and $O(N)$ model scaling function f_G in the $z \to -\infty$ limit:

$$\frac{f_G(z)}{(-z)^\beta} = \begin{cases} 1 + d_1^-(-z)^{-\beta\delta} + d_2^-(-z)^{-2\beta\delta} + \mathcal{O}((-z)^{-3\beta\delta}), & \text{for } Z(2), \\ 1 + d_1^-(-z)^{-\beta\delta/2} + d_2^-(-z)^{-\beta\delta} + \mathcal{O}((-z)^{-3\beta\delta/2}), & \text{for } O(N). \end{cases} \tag{33}$$

One can arrive at the above asymptotic form for f_G using Eqs. (30) and (31) with the *Ansatz* for $h(\theta)$ in $Z(2)$ and $O(N)$ universality classes given in Eq. (28). Explicit expressions for d_1^- and d_2^- in terms of the WG parameters h_3, h_5, and θ_0 are given in Appendix B.

B. Representation of $O(4)$ scaling functions using the Widom-Griffiths form

Although earlier parametrizations of the $O(4)$ scaling function $f_G(z)$, determined in Monte Carlo simulations [5], made use of the Widom-Griffiths form, this was done only to establish the behavior of $f_G(z)$ at large $|z|$. The region around $z = 0$ has been parametrized using polynomial *Ansätze*. A recent parametrization of the $O(4)$ scaling function used different fits in the small and large z regions and obtained a parametrization that uses 14 parameters [9].

[4]Note that $h(\theta)$ needs to be an odd function in θ. Using the normalization constant h_0, one can assure that the coefficient of the leading-order term is unity.

TABLE V. Fit parameters h_3, h_5, and θ_0 for $O(4)$ infinite volume scaling functions in the Widom-Griffiths form appearing in the function $h(\theta)$ introduced in Eq. (28). In the lower part of the table, we give results for several universal constants computable from the WG parametrization.

	$O(4)$	
	Monte Carlo	Monte Carlo
	WG fit to Ref. [9]	Engels-Karsch [9]
h_3	0.306(34)	⋯
h_5	−0.00338(25)	⋯
θ_0	1.359(10)	⋯
d_1^-	0.2481(20)	0.2737(29)
d_2^-	0.1083(50)	0.0036(49)
z_t	0.732(10)	0.74(4)
z_p	1.347(9)	1.374(30)

In order to establish the validity of the WG form using an *Ansatz* for the function $h(\theta)$ as suggested in Ref. [7], we reparametrized the fit results presented in Ref. [9]. We used the WG form for the $O(4)$ scaling functions as given in the previous subsection and determined optimal parameters (θ_0, h_3, h_5) in an interval around $z = 0$; i.e., we do not make use of the large z behavior of the scaling function given in Eq. (33). The structure of this asymptotic form is implemented already in the Widom-Griffiths *Ansatz*, and the expansion parameters d_1^- and d_2^- are determined directly from (θ_0, h_3, h_5) (see Appendix B), which can be determined from any set of z values. We determined these parameters in several intervals $[-z_{\max}: z_{\max}]$ with $1 \le z_{\max} \le 6$. The resulting parameters are given in Table V, where the errors quoted there reflect the spread of results for (θ_0, h_3, h_5) obtained when varying $z_{\max}$. In Fig. 2, we compare the scaling functions $f_G(z)$, $f'_G(z)$, and $f_\chi(z)$, obtained with the WG *Ansatz* using parameters given in Table V, to that obtained in Ref. [9]. As can be seen, we find excellent agreement.

Even though the scaling functions themselves are in good agreement and as such give consistent results for the positions z_t and z_p of the maxima of $-f'_G(z)$ and $f_\chi(z)$, we find different asymptotic behavior at large, negative z as shown for the case of $f_G(z)$ in the inset in Fig. 3 (right). In Ref. [9], the subleading asymptotic correction d_2^- has been found to vanish within errors, while we find $d_2^- \sim 0.1$. This difference, however, may not be too surprising, as the earlier results for the asymptotic expansion parameters d_1^- and d_2^- have been obtained from fits in the interval $z \in [-10, -1]$. We will show in the next subsection that in the $O(2)$ case the asymptotic form is not yet valid in this z range.

Given the good agreement between the WG parametrization of the $O(4)$ scaling functions and the earlier results based on a 14-parameter fit to MC data, we find it encouraging to analyze also the new Monte Carlo simulation results, obtained for the 3D $Z(2)$ and $O(2)$ models using a parametrization based on the WG *Ansatz*.

C. Representation of $Z(2)$ and $O(2)$ scaling functions using the Widom-Griffiths form

In order to use Eqs. (30) and (31) in determination of the scaling functions f_G, f'_G, and f_χ from MC results, as given in Eqs. (19)–(21), one still needs to determine the nonuniversal scale parameters (t_0, H_0, L_0). The nonuniversal scales H_0 and L_0 can be determined from the finite-size dependence of $f_G(z, z_L)$ at T_c, i.e., at $z = 0$. We present a determination of these two scales in Appendix A. Once they have been determined from our results on different size lattices, the scale parameter t_0 can be determined from the asymptotic behavior of $f_G(z)$ in the limit $z \to -\infty$. Using Eq. (13), the second normalization condition in Eq. (22), and writing $z = z_0 z_b$ with $z_0 = H_0^{1/\beta\delta}/t_0$, we obtain t_0 from

$$t_0^{-\beta} = \lim_{z_b \to -\infty} (-z_b)^{-\beta} H^{-1/\delta} M(T, H, \infty). \qquad (34)$$

As this equation relates the scale t_0 to observables calculated in the infinite volume limit, its determination can directly be incorporated into fits which we perform in the

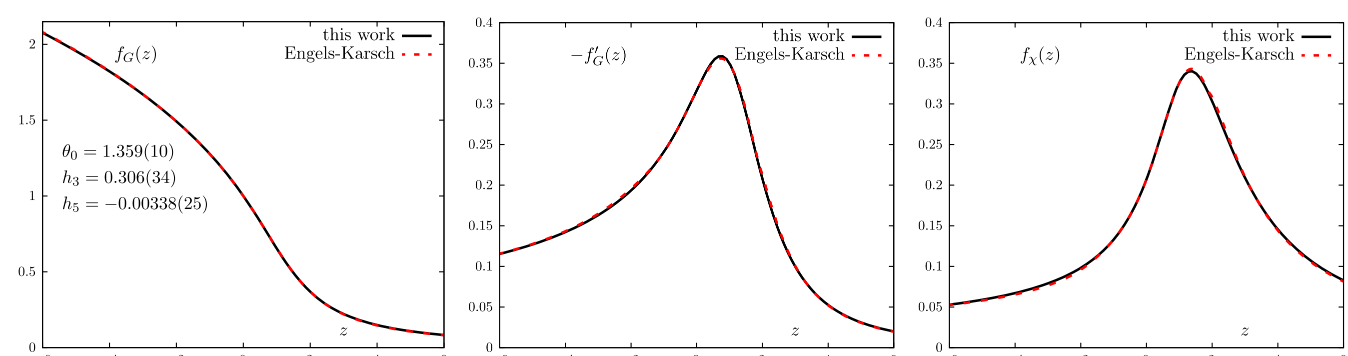

FIG. 2. The $O(4)$ infinite volume scaling functions. The WG parameters have been obtained from a fit to f_G, while f'_G and f_χ have been obtained from there. Dashed red lines show results from previous calculations [9].

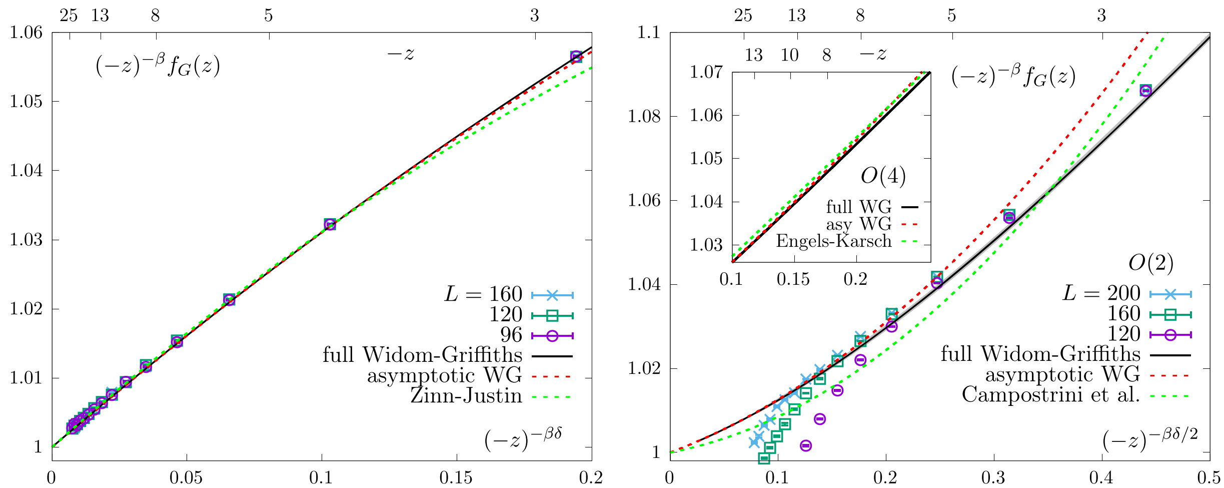

FIG. 3. The scaling function $f_G(z)$ in the $Z(2)$ (left) and $O(2)$ (right) universality classes obtained from the order parameter M using Eq. (19) in the region of large, negative values of z. Monte Carlo data have been obtained in simulations using the 3D $Z(2)$ model with $\lambda = 1.1$ and the $O(2)$ model with $\lambda = 2.1$. All data are from simulations at $T/T_c = 0.99$. The large negative z region of the $O(4) f_G(z)$ scaling function, obtained from our fit to results in Ref. [9], is shown in the inset in the right figure. Solid lines shown in the figures are based on fits using the Widom-Griffiths form of the scaling functions and use also data outside the parameter range shown here (see the text). For $O(2)$, we also show an error band to the WG ansatz obtained from a bootstrap analysis. The green dashed lines show the analytic results obtained in the $Z(2)$ [18] and $O(2)$ [7] universality classes and MC fit results obtained in the $O(4)$ [9] universality class, respectively. The dashed red line shows the asymptotic expansion given in Eq. (33).

infinite volume limit for the determination of the scaling functions. We obtain t_0 and the parameters (h_3, h_5, θ_0) defining $h(\theta)$ using simultaneous fits to the scaling functions $f_G(z)$, $f'_G(z)$, and $f_\chi(z)$ defined in Eqs. (19)–(21). While in the parametrization of $Z(2)$ scaling functions θ_0 is a function of (h_3, h_5), it is an additional free parameter in the $O(N)$ case.

Goldstone modes dominate finite-size effects at large, negative values of z, which are quite different in $O(N)$ universality classes from those in the $Z(2)$ case. In the $O(2)$ universality class, finite-size effects grow rapidly with decreasing values of z. This is evident from Fig. 3, where we show results for $(-z)^{-\beta} f_G(z)$ in the region $z < -2$. The figure shows that we had to perform MC calculations on rather large lattices to extract the scale parameter t_0 from the asymptotic behavior of the order parameter in the symmetry-broken phase. In our simulations of the $O(2)$ model, lattices of size L^3 with $L = 200$ were needed to reach the region $z \leq -10$ without suffering from finite-size effects. In the case of $Z(2)$, lattices with $L = 96$ were already sufficient to perform calculations in a region down to values $z \simeq -20$ without observing a significant finite-size dependence in our results.

For $z > -2$, it was sufficient to perform calculations on lattices with $L = 48$–120. For $z < -2$, however, we also performed calculations with $L = 160$ and 200 for the $O(2)$ model and $L = 160$ in the case of $Z(2)$. The statistics collected in all parameter ranges are given in Tables II–IV.

Our Monte Carlo results obtained for the 3D $Z(2)$ and $O(2)$ models in the large volume limit, $z_L \leq 0.35$, are shown in Fig. 4. We performed joint fits using data in the region $z_L \leq 0.35$ as approximation for the infinite volume limit. All three scaling functions have then been obtained from joint fits to the WG form in the range $z \in [-23:2]$ for $Z(2)$ and $z \in [-12:2]$ for the $O(2)$ model.[5]

We summarize results for the nonuniversal scale parameters (t_0, H_0, L_0), determined by us, in Table I. In Table VI, we give all universal fit parameters entering the definition of $h(\theta)$ and compare with results obtained in 3D analytic calculations [7,18]. In the top section of the two tables, we give the parameters (h_3, h_5), entering fits performed for scaling functions in the $Z(2)$ universality class and (θ_0, h_3, h_5) in the $O(2)$ case. Results for the nonuniversal fit parameter t_0, obtained in the same fits, are given in Table I. The bottom part of the tables gives some universal constants derived from the Widom-Griffiths form of the scaling functions by using, on the one hand, the results from fits to our MC data and, on the other hand, the perturbative results for $h(\theta)$ and θ_0 as input.

Aside from the parameters d_1^- and d_2^- controlling the asymptotic behavior of $f_G(z)$ at large, negative z [Eq. (33)], we also give there the universal constants z_p and z_t, which are the z values at the maxima of $f_\chi(z, 0)$ and $-f'_G(z, 0)$, respectively.

[5]Note that the exact fit range is determined only *a posteriori*, once the scale parameter t_0 has been obtained in our fits.

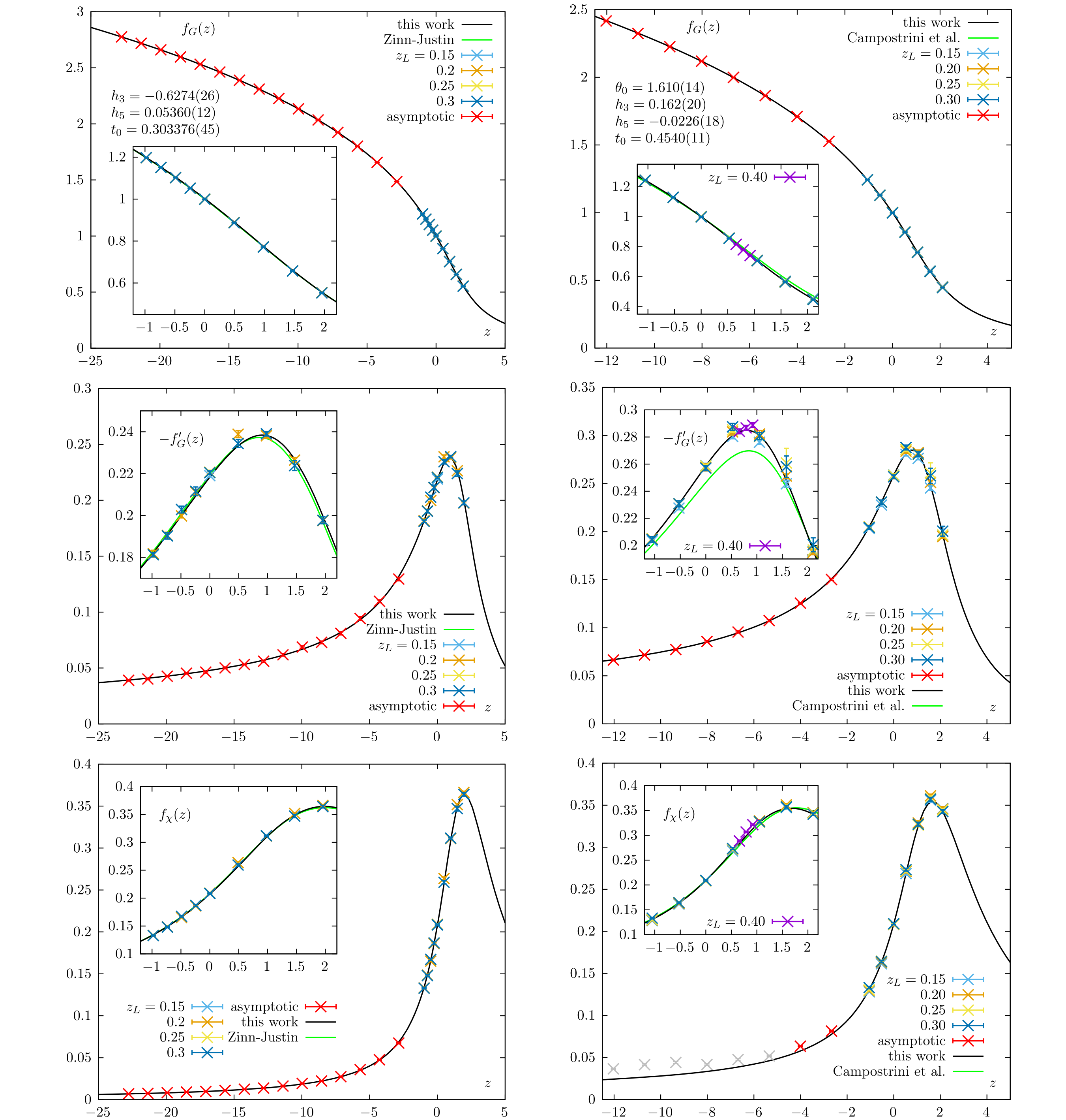

FIG. 4. The $Z(2)$ (left column) and $O(2)$ (right column) infinite volume scaling functions. Shown are Monte Carlo results obtained on lattices of size L^3 with $L = 96$ for $|z| \le 2.1$, $L = 96, 120, 160$ [$Z(2)$, only $L = 160$ is shown], and $L = 200$ [$O(2)$] for $z < -2.5$. All fits are joint fits to data for f_G, f'_G, and f_χ, close to $z = 0$ and in the large, negative z regime. The gray data were not included in the fit. Green lines in the insets show results from analytic calculations [18] [$Z(2)$, left] and [7] [$O(2)$, right].

For the ratio of z_p and z_t, determining pseudocritical temperatures in the $Z(2)$ and $O(N)$ universality classes, we find

$$\frac{z_p}{z_t} = \begin{cases} 2.21(1), & Z(2), \\ 2.09(2), & O(2), \\ 1.84(1), & O(4). \end{cases} \tag{35}$$

TABLE VI. Top: fit parameters h_3 and h_5 for $Z(2)$ infinite volume scaling functions in the Widom-Griffiths form appearing in the function $h(\theta)$ introduced in Eq. (28). Bottom: fit parameters h_3, h_5, and θ_0 for $O(2)$ infinite volume scaling functions in the Widom-Griffiths form appearing in the function $h(\theta)$ introduced in Eq. (28). In the lower part of both tables, we give results for several universal constants computable from the WG parametrization.

$Z(2)$		
	Monte Carlo (this work)	3D perturbative expansion [18]
h_3	−0.6274(26)	−0.76201(36)
h_5	0.05360(12)	0.00804(11)
θ_0	1.3797(24)	1.15369(17)
d_1^-	0.33553(83)	0.348329(13)
d_2^-	−0.2466(71)	−0.368672(53)
z_t	0.8961(10)	0.8578(3)
z_p	1.9770(23)	1.9863(3)

$O(2)$		
	Monte Carlo (this work)	3D improved high-T expansion [7]
h_3	0.162(20)	0.0758028
h_5	−0.0226(18)	0
θ_0	1.610(14)	1.71447
d_1^-	0.0969(38)	0.04870
d_2^-	0.2925(61)	0.36632
z_t	0.7991(96)	0.8438
z_p	1.6675(68)	1.7685

In Fig. 3, we compared the MC results for $f_G(z)$ at large, negative values of z, i.e., for $z < -2$, with the WG form of the scaling function, given in Eq. (30), as well as with the asymptotic form given in Eq. (33). As can be seen, in the $Z(2)$ universality class, the asymptotic expansion using the first two subleading corrections gives a good approximation to the full WG form, in almost the entire region, $z < -2$. In the $O(2)$ and $O(4)$ universality classes, however, the first two subleading corrections agree with the full WG form only for $z < -(8\text{–}10)$ as can be seen in Fig. 3 (right) for the $O(2)$ case and in the inset in Fig. 3 (right) for the $O(4)$ case.

Also shown in Fig. 3 are the results obtained from the 3D analytic calculations [18,27]. While in the $Z(2)$ case differences are insignificant, they clearly are visible in the $O(2)$ case. However, in the asymptotic regime both parametrizations of the WG form differ by less than 1%. We observed the largest differences in the vicinity of the maximum of $-f'_G(z)$, where deviations between the analytic and MC calculation amount to about 5%. This is apparent from the insets shown in Fig. 4.

V. FINITE-SIZE SCALING FUNCTIONS

We now want to determine corrections to the infinite volume scaling functions in the 3D $Z(2)$ and $O(2)$ universality classes arising in a finite volume at small external field H. These corrections are universal when taking the limit $(H \to 0, L \to \infty)$ at fixed z_L as introduced in Eq. (12).

In the limit of small H and in the vicinity of T_c, we obtain the scaling functions $(f_G(z,z_L), f'_G(z,z_L), f_\chi(z,z_L))$ from the order parameter M and the two susceptibilities χ_h and χ_t using Eqs. (19)–(21).

We focus here on the region in the vicinity of T_c and the pseudocritical temperatures $T_{pc,h}$ and $T_{pc,t}$, determined from the maxima of the susceptibilities χ_h and χ_t, respectively. It is this region where correlation lengths are large and where it is of particular importance to get control over finite-size effects in the determination of pseudocritical and critical temperatures in many models belonging to the $Z(2)$ and $O(N)$ universality classes. For this reason, we determine finite-size scaling functions with parameter sets (J,H) corresponding to the interval $z \in [-1:2]$. A similar calculation has been performed previously for finite-size scaling functions in the $O(4)$ universality class [10].

In our analysis of finite-size effects, we use a polynomial *Ansatz* for the scaling functions which has also been used previously for calculations in the 3D $O(4)$ universality class [10]:

$$f_G(z,z_L) = f_G(z,0) + \sum_{n=0}^{n_u} \sum_{m=m_l}^{m_u} a_{nm} z^n z_L^m. \tag{36}$$

For the infinite volume scaling function $f_G(z,0) \equiv f_G(z)$, we use the parametrization determined in the previous section. Here, (n_u, m_l, m_u) denote the lower and upper limits of the sum over the polynomial in powers of z and z_L, respectively. We take the leading-order finite-size correction to be inversely proportional to the volume $\mathcal{O}(1/L^3)$, i.e., $m_l = 3$. The upper limits n_u and m_u are optimized in our fits, using the Bayesian information criterion. We fix $a_{0m_l} = 0$ in both universality classes; additionally, we constrain the fit parameters to $|a_{nm}| < 10$.

From the *Ansatz* used for $f_G(z,z_L)$, one also obtains the parametrization of $f'_G(z,z_L)$, which controls the scaling behavior of χ_t:

$$f'_G(z,z_L) = f'_G(z,0) + \sum_{n=1}^{n_u} \sum_{m=m_l}^{m_u} n a_{nm} z^{n-1} z_L^m, \tag{37}$$

and $f_\chi(z,z_L)$, which controls the scaling behavior of χ_h:

$$f_\chi(z,z_L) = f_\chi(z,0) + \sum_{n=0}^{n_u} \sum_{m=m_l}^{m_u} \left(\frac{1}{\delta} - \frac{n+m\nu}{\beta\delta}\right) a_{nm} z^n z_L^m. \tag{38}$$

Using these polynomial *Ansätze*, we again perform joint fits to the MC data for the three scaling functions (f_G, f'_G, f_χ) in the interval $z \in [-1:2]$ and for $z_L \in [0.4:1.0]$. The data for $z_L < 0.4$ have been excluded from these fits, as they have

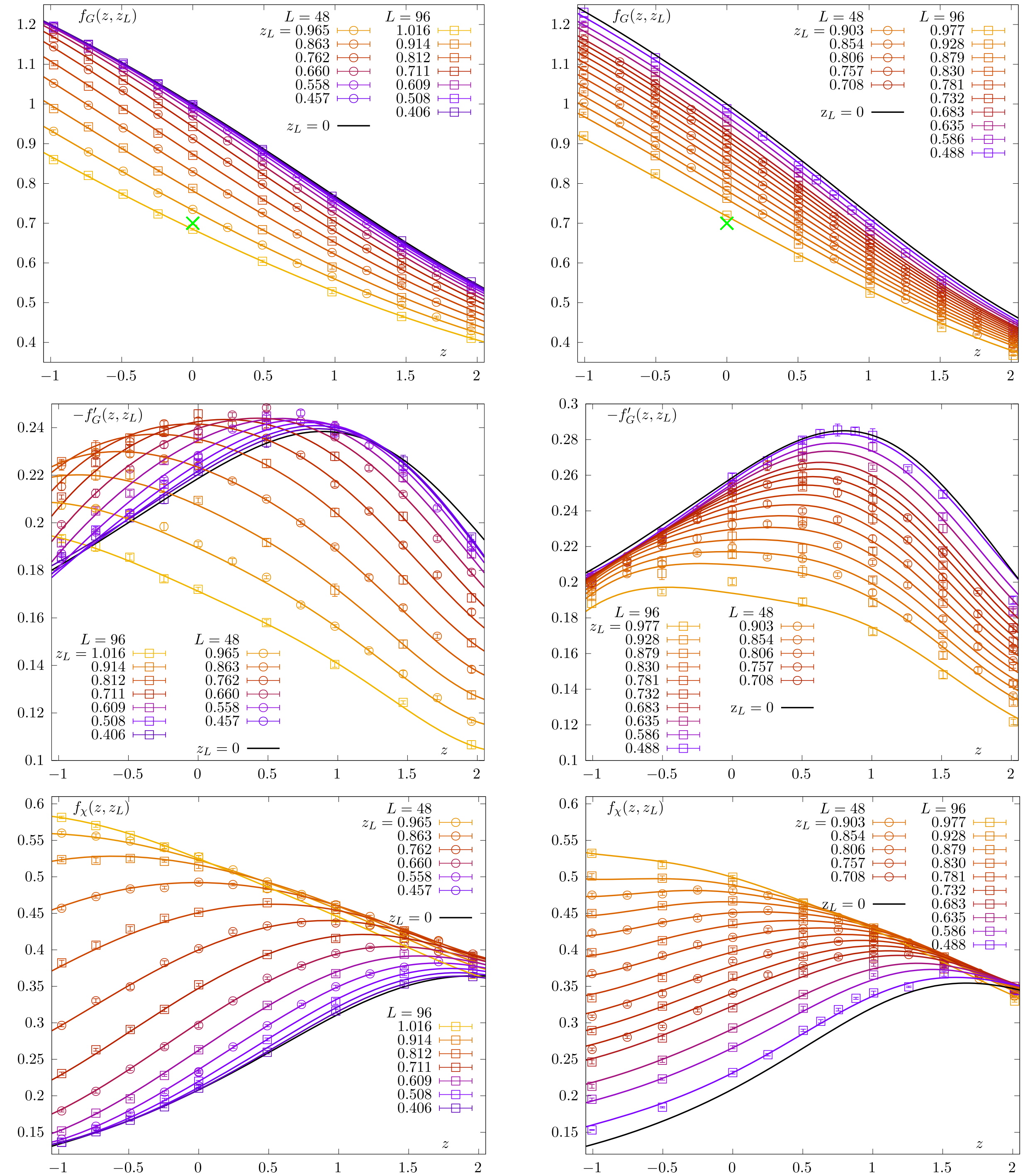

FIG. 5. Fits to data for scaling functions of in the $Z(2)$ (left column) and $O(2)$ (right column) universality class. All fits are joint fits to data for f_G, f'_G, and f_χ, done in the intervals $z \in [-1.0, 2.0]$ and $z_L \in [0.4, 1.0]$ on lattices of size $L = 48$ (circle) and 96 (squares). Also shown are the infinite volume lines for $z_L = 0$. Green crosses in the upper row mark the normalization condition $f_G(0, 1) = 0.7$.

been used already to determine the parameters of the infinite volume scaling functions, as discussed in the previous section.

Results obtained for the finite-size scaling functions in the 3D $Z(2)$ and $O(2)$ universality classes for some fixed values of z have been shown already in Fig. 1. In Fig. 5, we show results for the scaling functions as functions of z for several fixed values of z_L. The fit parameters obtained with the polynomial fit *Ansatz* [Eq. (36)] are given in Table VII for the case of $Z(2)$ and in Table VIII for the case of $O(2)$. These fits provide a good interpolation for our data in the range $z_L \in [0.4 : 1.0]$. However, due to the large number of parameters involved, we cannot give significance to individual parameters entering the polynomial *Ansatz*.

TABLE VII. Parameters of the polynomial fit *Ansatz* for the $Z(2)$ finite-size scaling functions $(f_G, f'_G, f_\chi)(z, z_L)$ with $n_u = 4$, $m_l = 3$, and $m_u = 11$. The fit was restricted to $z \in [-1:2]$ and $z_L \in [0.4, 1.0]$.

a_{nm}	$n = 0$	$n = 1$	$n = 2$	$n = 3$	$n = 4$
$m = 3$	0	−0.948309	0.717317	−0.162262	0.077211
$m = 4$	−1.626176	5.613893	−3.665684	0.705625	−0.389709
$m = 5$	7.182912	−9.594472	4.926683	−1.015233	0.782710
$m = 6$	−7.151294	0.244453	0.803864	0.708351	−0.624599
$m = 7$	−6.583527	7.559574	−3.189855	0.340024	−0.444347
$m = 8$	7.641469	2.794132	−1.881236	−1.199165	0.834052
$m = 9$	7.510637	−4.712291	1.481824	−0.473266	0.548429
$m = 10$	−9.932439	−4.460071	2.132431	2.098657	−1.309965
$m = 11$	2.658208	3.544670	−1.293838	−1.003939	0.524142

TABLE VIII. Parameters of the polynomial fit *Ansatz* for the $O(2)$ finite-size scaling function $(f_G, f'_G, f_\chi)(z, z_L)$ with $n_u = 5$, $m_l = 3$, and $m_u = 8$. The fit was restricted to $z \in [-1:2]$ and $z_L \in [0.4, 1.0]$.

a_{nm}	$n = 0$	$n = 1$	$n = 2$	$n = 3$	$n = 4$	$n = 5$
$m = 3$	0	−0.740936	0.198298	0.020480	−0.219484	0.096802
$m = 4$	−0.735344	4.506235	−0.871942	−0.015341	1.377204	−0.676093
$m = 5$	4.031332	−9.950240	0.340937	−0.456753	−3.161604	1.800423
$m = 6$	−9.769988	9.634183	2.604256	1.621876	3.397707	−2.365422
$m = 7$	8.841449	−3.490053	−3.497933	−1.908686	−1.770614	1.560082
$m = 8$	−2.670471	0.113312	1.259727	0.735997	0.371330	−0.414748

We, therefore, quote our fit result without assigning errors to the fit parameters.

As can be seen, the general z_L dependence of scaling functions $f_G(z, z_L)$ and $f_\chi(z, z_L)$ is similar in the $Z(2)$ and $O(2)$ universality classes. However, it is apparent from the upper row in Fig. 5 that finite-size effects are larger in the $O(2)$ case than for $Z(2)$. In the latter case, results for $f_G(z, z_L)$ are indistinguishable from the infinite volume results already for $z_L < 0.6$, whereas in the $O(2)$ case at $z_L = 0.6$, deviations from the infinite volume values amount to about 3% at $z = -1$ and increase to 4% at $z = 1$ (see also the discussion of Fig. 8 in Appendix A). Furthermore, qualitative differences are evident in the z_L dependence of the scaling function $f'_G(z, z_L)$. In the $Z(2)$ case, the approach to the infinite volume limit is nonmonotonic for $z_L < 0$. A pronounced peak shows up in the symmetry-broken regime ($z \leq 0$) at finite z_l, and the asymptotic infinite volume limit is approached from above. In the case of the $O(2)$ universality class, $f'_G(z, z_L)$ seems to approach the infinite volume limit result from below for all z.

In the case of $f_\chi(z, z_L)$, the approach to the infinite volume limit is nonmonotonic for z values below the pseudocritical scale $z < z_p$. As can be seen in Fig. 1, this is the case in the $Z(2)$ as well as in the $O(2)$ universality class. This nonmonotonic behavior is not that prominently visible in Fig. 5, as it sets in only at rather large values of z_L, i.e., for $z_L > 1$. This regime is not covered in Fig. 5.

While the finite-size effects seen in the scaling functions are generally larger in the $O(N)$ than in the $Z(2)$ universality class, this is not the case for the location of maxima in the scaling functions $-f'_G(z, z_L)$ and $f_\chi(z, z_L)$. These maxima are controlled by universal functions $z_t(z_L)$ and $z_p(z_L)$, respectively. We determined them from the polynomial obtained from the finite-size scaling fits for $Z(2)$ and $O(2)$. In the case of $O(4)$, we have used the finite-size fit given in Ref. [10]. Results are shown in Fig. 6.

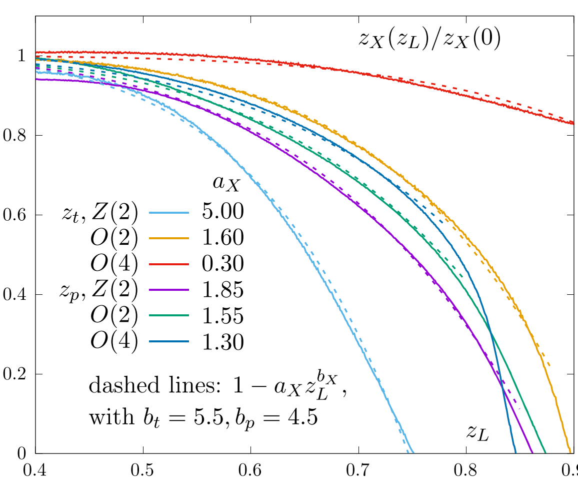

FIG. 6. Finite-size dependence of the location of maxima in the scaling functions $f_\chi(z, z_L)$ and $-f'_G(z, z_L)$. Shown are the universal functions $z_p(z_L)$ and $z_t(z_L)$ for the 3D $Z(2)$ and $O(N)$ universality classes. Dashed lines show simple polynomial approximations [Eq. (39)] with parameters as given in the figure.

It is clearly seen that the finite-size dependence of the maxima in χ_h is stronger than that of χ_t in the $O(N)$ universality classes and vice versa in the $Z(2)$ case. Moreover, the finite-size dependence of z_t and z_p is stronger in the $Z(2)$ universality class than in the $O(N)$ cases. Over a wide range of z_L values, the deviations from the infinite volume limit result are described well with *Ansatz*

$$z_X(z_L) = z_X(0)(1 - a_X z_L^{b_X}), \qquad X = p, t, \tag{39}$$

with $b_p \simeq 4.5$ and $b_t \simeq 5.5$ as shown in Fig. 6.

VI. CONCLUSIONS

We determined the infinite volume scaling functions in the 3D $Z(2)$, $O(2)$, and $O(4)$ universality classes using a two- or three-parameter parametrization based on the analytic Widom-Griffiths scaling form. We find good agreement of the $O(4)$ parametrization with an earlier parametrization that used $\mathcal{O}(10)$ parameters [9]. In the $Z(2)$ case, we find excellent agreement between our parametrization based on Monte Carlo results and the analytic result obtained from a perturbative, field theoretic approach [18]. The largest differences between our Monte Carlo results and analytic calculations [7] we find, in particular, for the scaling function $f'_G(z)$, which controls the scaling behavior of mixed susceptibilities.

We determined the finite-size dependence of the scaling functions and showed that qualitative differences between the $Z(2)$ and $O(N)$ cases show up most prominently in the scaling function $f'_G(z, z_L)$ which controls pseudocritical and critical behavior of the mixed susceptibilities. We could show that the location of the pseudocritical temperature, corresponding to z_t, is less affected by finite-size effects than the pseudocritical temperature determined by the maximum of the order parameter susceptibility (χ_h) at z_p. This difference is particularly striking in the $O(4)$ universality class. The comparison of the finite-size dependence of the scaling functions among different universality classes has been possible with our proposed normalization condition for the nonuniversal scale parameter L_0.

We furthermore find $z_p/z_t \simeq 2$, i.e., at nonzero values of the symmetry-breaking parameter H deviations of the pseudocritical temperature $T_{pc,t}$ from the phase transition temperature T_c are about a factor of 2 smaller than that of $T_{pc,h}$. All data presented in the figures of this paper can be found in Ref. [28].

ACKNOWLEDGMENTS

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APPENDIX A: DETERMINATION OF H_0 AND L_0

In order to extract scaling functions from numerical simulations of the 3D $Z(2)$ and $O(2)$ model using the Hamiltonian given in Eq. (1), we need to determine the nonuniversal scales (t_0, H_0, L_0). In this appendix, we discuss the determination of (H_0, L_0) using the finite-size dependence of the order parameter at T_c.

The critical temperature T_c has been determined with great precision for the improved $Z(2)$ [12] and $O(2)$ [7] models, respectively. For the $Z(2)$ model, also the scale H_0 has been determined previously [21] on similar size lattices as used in this study but using infinite volume scaling *Ansätze* and lower statistics.

For the determination of H_0, we make use of the normalization conditions for the order parameter or, equivalently, the scaling function $f_G(z, 0)$ as introduced in Eq. (23). The scale L_0 is obtained using the normalization condition for the finite-size scaling function $f_G(0, z_L)$ introduced in Eq. (24).

For our determination of the scale parameters, we introduce the (bare) scaling variables z_b and $z_{L,b}$ through $z = z_0 z_b$ and $z_L = z_{0,L} z_{L,b}$, with

$$z_b = \frac{T - T_c}{T_c} H^{-1/\beta\delta}, \tag{A1}$$

$$z_{L,b} = \frac{1}{L H^{\nu/\beta\delta}}, \tag{A2}$$

and

$$z_0 = H_0^{1/\beta\delta}/t_0, \qquad z_{0,L} = L_0 H_0^{\nu/\beta\delta}. \tag{A3}$$

To determine H_0, using Eq. (23), we performed dedicated calculations at T_c on lattices of size $L = 48$, 96, and 120 and for several values of z_L. The statistics collected for each parameter set (J_c, L) is given in Table III. We calculate the order parameter $M(T, H, L)$ in the limit $(H \to 0, L \to \infty)$ for several values of fixed $z_{L,b}$ and then take the limit $z_{L,b} \to 0$ at $T \equiv T_c$:

$$H_0^{-1/\delta} = \lim_{z_{L,b}\to 0} \lim_{H\to 0} (H^{-1/\delta} M(T_c, H, 1/z_{L,b} H^{\nu/\beta\delta})). \tag{A4}$$

Results from this calculation are shown in Fig. 7. The intercept at $z_{L,b} = 0$ yields $H_0^{-1/\delta}$. Also shown in the figure

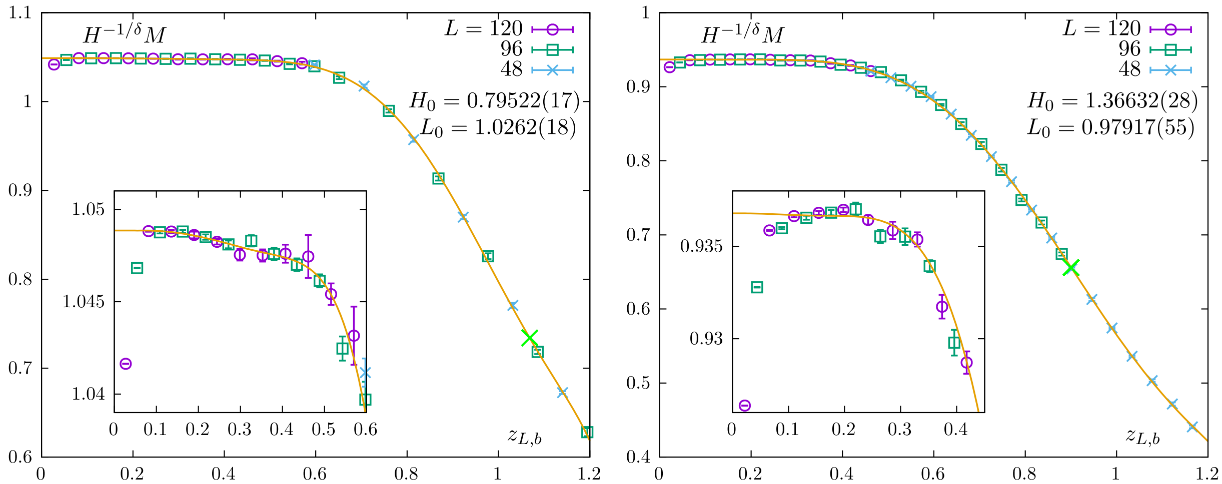

FIG. 7. The rescaled order parameter $H^{-1/\delta}M$ versus the bare finite-size scaling variable $z_{L,b}$ at T_c. The left-hand figure shows results for the 3D $Z(2)$ model with $\lambda = 1.1$, and the right-hand figure is for the $O(2)$ model with $\lambda = 2.1$. The inset shows the region of small $z_{L,b}$ that is used for the determination of the nonuniversal scale parameter H_0. The green cross marks the value of $z_{L,b}$ that determines the scale parameter L_0 using the normalization condition given in Eq. (24).

are results from polynomial fits

$$\tilde{f}_G(z_{L,b}) = H_0^{-1/\delta} + \sum_{m=m_l}^{m_u} b_m z_{L,b}^m \tag{A5}$$

to the right-hand side of Eq. (A4) in different intervals $z_{L,b} \in [0.1 : z_{L,b,\max}]$, with $z_{L,b,\max} \in \{1.1, 1.2, 1.3\}$. H_0 and b_m are then determined by bootstrapping fits with different $z_{L,b,\max}$. The lower and upper limits m_l and m_u are chosen differently from their finite-size counterparts: We use $m_l = 4$ and $m_u = 9$ for $Z(2)$, while $m_l = 3$ and $m_u = 7$ are used for $O(2)$. This determines H_0. Using Eq. (24), we then obtain L_0 from the value $z_{L,b}$, which gives $H_0^{1/\delta}\tilde{f}_G(z_{L,b}) = 0.7$. Using the fit results for $\tilde{f}_G(z_{L,b})$, we then obtain the normalization constants (H_0, L_0) for the $Z(2)$ and $O(2)$ model, which are given in Table I.

The result obtained for H_0 for the $Z(2)$ model from our finite-size scaling fit is about 2% smaller than the value $H_0 = 0.8150(56)$ obtained in Ref. [21] from a fit of the order parameter M at T_c, using the infinite volume scaling *Ansatz* for M.

Using the scale parameters H_0 and L_0, we obtain the scaling function $f_G(z, z_L)$ at $z = 0$ as a function of z_L. A comparison of results obtained in different universality classes is shown in Fig. 8. This suggests that the finite-size dependence of the order parameter is larger in the $O(N)$ universality classes than in the $Z(2)$ universality class.

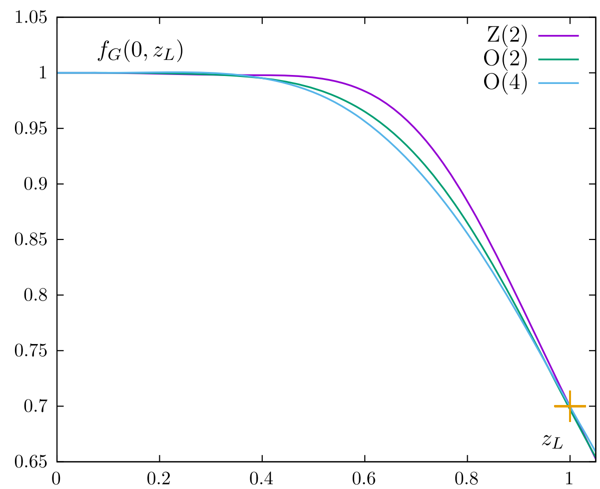

FIG. 8. Comparison of the scaling function $f_G(0, z_L)$ in different 3D universality classes as a function of z_L. The data for the scaling function in the $O(4)$ universality class are taken from Ref. [10]. For this purpose, the scaling variable z_L has been rescaled using $L_0 = 0.7686$ to be consistent with the normalization condition [Eq. (24)] used for the $Z(2)$ and $O(2)$ universality classes.

APPENDIX B: PARAMETRIZATION OF $Z(2)$ AND $O(N)$ SCALING FUNCTIONS

We give here results for the two subleading expansion coefficients d_1^- and d_2^-, appearing in the large, negative z expansion of the infinite volume scaling functions $f_G(z)$ in the 3D $Z(2)$ and $O(N)$ universality classes [cf. Eq. (33)]. We present explicit expressions in terms of the parameters appearing in the definition of the function $h(\theta)$ given in Eq. (28) of scaling functions written in the Widom-Griffiths form [14–17].

The coefficients in the asymptotic expansion for the $Z(2)$ scaling function are

$$d_1^- = -\theta_0^{\delta-1} \frac{(1 + (2\beta - 1)\theta_0^2)}{(\theta_0^2 - 1)} \frac{h(1)}{h'(\theta_0)}, \tag{B1}$$

$$d_2^- = -\frac{\theta_0^{2\delta-1}h(1)^2}{2(\theta_0^2-1)^2 h'(\theta_0)^3}(2\beta\theta_0 h'(\theta_0)(2\delta((2\beta-1)\theta_0^2+1) -(2\beta-1)\theta_0^2-3) - h^{(2)}(\theta_0)(\theta_0^2-1) \times((2\beta-1)\theta_0^2+1)), \tag{B2}$$

and the corresponding expansion coefficients in the $O(N)$ case are

$$d_1^- = \theta_0^{\delta/2-1}\frac{(1+(2\beta-1)\theta_0^2)}{(\theta_0^2-1)}\sqrt{\frac{2h(1)}{h^{(2)}(\theta_0)}}, \tag{B3}$$

$$d_2^- = -\frac{\theta_0^{\delta-1}h(1)}{3(\theta_0^2-1)^2 h^{(2)}(\theta_0)^2}(6\beta\theta_0 h^{(2)}(\theta_0)(\delta((2\beta-1)\theta_0^2+1) -(2\beta-1)\theta_0^2-3) - h^{(3)}(\theta_0)(\theta_0^2-1) \times((2\beta-1)\theta_0^2+1)). \tag{B4}$$

It should be noted that θ_0 is an independent parameter in the parametric representation of $O(N)$ universality class, while it is a function of parameters h_3 and h_5 in the $Z(2)$ case.

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