Scaling functions of the free energy density and its derivatives for the 3d $O(4)$ model

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We derive direct representations of the scaling functions of the 3d $O(4)$ model which are relevant for comparisons to other models, in particular, QCD. This is done in terms of expansions in the scaling variable $z = \bar{t}/h^{1/\Delta}$. The expansions around $z = 0$ and the corresponding asymptotic ones for $z \rightarrow \pm\infty$ overlap such that no interpolation is needed. The expansion coefficients are determined numerically from the data of a previous high statistics simulation of the $O(4)$ model on a three-dimensional lattice of linear extension $L = 120$. From the scaling function of the magnetization we calculate the leading asymptotic coefficients of the scaling function of the free energy density. As a result we obtain the universal amplitude ratio $A^+/A^- = 1.84(4)$ for the specific heat. Comparing the scaling function of the energy density to the data we find the nonsingular part of the energy density $\epsilon_{\mathrm{ns}}(T)$ with high precision and at the same time excellent scaling properties.

I. INTRODUCTION

The aim of the paper is to provide representations of the scaling functions of the three-dimensional $O(4)$ model which can be used in tests of other models on their membership of the corresponding universality class. This is especially of importance for quantum chromodynamics (QCD) with two degenerate light-quark flavors at finite temperature, because it is believed [1–6] to belong to the $O(4)$ universality class at its chiral transition in the continuum limit. There exist already many parametrizations [7–12] of the magnetic equation of state. They differ essentially in the following aspects:

(a) The form of the magnetic equation of state which is initially parametrized. The most used form is the Widom-Griffiths (WG) form [13,14], where both the scaling function and the scaling variable depend on the magnetization M. A second form has the advantage that the scaling variable is independent of M. It is therefore more appropriate for the comparison to M-data with errors. The two forms are completely equivalent in describing the critical behavior of the model and they can be derived from each other. In principle, it is then only necessary to parametrize one form.

(b) The type of parametrization which is used. The parametrization has to describe the correct general scaling laws as deduced from renormalization group (RG) theory, it must satisfy Griffiths's analyticity conditions [14] and take into account the Goldstone singularities in the low temperature phase.

(c) The input from which the parameters are determined. There are two main sources of information: from field-theory methods, for example ϵ-expansions, small-field expansions or high temperature series etc., and secondly, from Monte Carlo (MC) data.

Our paper is inspired by the pioneering work of Toussaint [7]. In his paper the scaling function (of the second kind) for the order parameter was calculated based only on MC data and moreover these data were simulated at finite external field H. The main purpose of the paper was, like ours, to provide the scaling function for the QCD analysis. The parametrization was carried out in a third, unusual form, which has not been used since then, yet the Goldstone effects had still not been taken into account. Like the WG form, this third form has the drawback that the calculation of the second form of the scaling function and, in particular, its derivatives with respect to its scaling variable is an indirect one and it is therefore unhandy. Moreover, scaling functions of the second kind determine via the location of their extrema the important pseudocritical lines. In Refs. [8,10] the WG form was used and parametrized with a combination of a low and a high temperature ansatz in accord with the requirements of (b). The two parts were subsequently connected by an interpolation. The parameters were deduced exclusively from MC data with finite external fields. In Refs. [9,11,12] the WG form was used. All three papers discuss and use variants of the classical parametric representation of the equation of state introduced by Schofield and Josephson [15–17] in 1969, which is valid in the whole critical region. References [9,11] differ in details of the parametrization and in the input: whereas [9] relies essentially on field-theory input and uses the data for testing, Ref. [11] determines its parameters directly from fits to the data. In Ref. [12] the functional RG method is used to calculate the scaling functions. The classical representation had been invented for the WG form, at a time where only few MC data on small lattices were available. Today it is still used for all kind of calculations of universal quantities from field theory. However, as we shall demonstrate,

it is not necessary to work with this representation. Instead we parametrize directly the scaling functions of the second kind, which is the preferred choice of the QCD community in their tests on the universality class of the $O(4)$ model. In addition, this allows us not only to make use of the magnetization data in the determination of the parameters, but also of the data for the susceptibilities.

In order to broaden the tests on the universality class we calculate as well the scaling functions connected to the energy density and the specific heat. Here however, the initially unknown regular or nonsingular part of the energy density and/or specific heat is contained in the data and has to be subtracted correctly. We show how this can be done in principle, when the critical exponent α is negative. The inadequate estimate of the regular parts in a former test for 2-flavor QCD [18] prevented a successful outcome of the test from the beginning and led to unjustified conclusions. Yet, there is a derivative of the energy density, the thermal susceptibility or covariance between the energy density and the magnetization, which does not require a subtraction of the nonsingular term. We shall use also this quantity for our parametrization.

The specific model which we study here is the standard $O(4)$-invariant nonlinear σ-model, which is defined by

$$\beta \mathcal{H} = -J \sum_{\langle \vec{x}, \vec{y} \rangle} \vec{\phi}_{\vec{x}} \cdot \vec{\phi}_{\vec{y}} - \vec{H} \cdot \sum_{\vec{x}} \vec{\phi}_{\vec{x}}, \qquad (1)$$

where $\vec{x}$ and $\vec{y}$ are nearest-neighbor sites on a three-dimensional hypercubic lattice, and $\vec{\phi}_{\vec{x}}$ is a four-component unit vector at site $\vec{x}$. The coupling J and the external magnetic field $\vec{H}$ are reduced quantities, that is they contain already a factor $\beta = 1/T$. In fact, we consider in the following the coupling directly as the inverse temperature, $J \equiv 1/T$.

It is useful to decompose the spin vector $\vec{\phi}_{\vec{x}}$ into longitudinal (parallel to the magnetic field $\vec{H}$) and transverse components

$$\vec{\phi}_{\vec{x}} = \phi_{\vec{x}}^{\parallel} \vec{e}_H + \vec{\phi}_{\vec{x}}^{\perp}, \quad \text{with} \quad \vec{e}_H = \vec{H}/H, \qquad (2)$$

where H is the magnitude of the magnetic field. We define the energy of a spin configuration as

$$E = -\sum_{\langle \vec{x}, \vec{y} \rangle} \vec{\phi}_{\vec{x}} \cdot \vec{\phi}_{\vec{y}}. \qquad (3)$$

The lattice average $\phi^{\parallel}$ of the longitudinal spin components is

$$\phi^{\parallel} = \frac{1}{V} \sum_{\vec{x}} \phi_{\vec{x}}^{\parallel}, \qquad (4)$$

where $V = L^3$ and L is the number of lattice points per direction. The partition function is then

$$Z(T, H) = \int \prod_{\vec{x}} d^4 \phi_{\vec{x}} \delta(\vec{\phi}_{\vec{x}}^2 - 1) \exp(-\beta E + HV \phi^{\parallel}). \quad (5)$$

We introduce the (reduced) free energy density as usual by

$$f(T, H) = -\frac{1}{V} \ln Z, \qquad (6)$$

from which one obtains the order parameter of the system, the magnetization M, as

$$M = -\frac{\partial f}{\partial H} = \langle \phi^{\parallel} \rangle. \qquad (7)$$

The longitudinal susceptibility is the second derivative of $-f$ with respect to the field

$$\chi_L = \frac{\partial M}{\partial H} = V(\langle \phi^{\parallel 2} \rangle - M^2). \qquad (8)$$

The energy density is

$$\epsilon = \frac{\partial f}{\partial \beta} = \frac{\langle E \rangle}{V}, \qquad (9)$$

and the specific heat

$$C = \frac{\partial \epsilon}{\partial T} = \frac{\beta^2}{V}(\langle E^2 \rangle - \langle E \rangle^2). \qquad (10)$$

Finally we define the thermal susceptibility χ_t as the mixed second derivative of f

$$\chi_t = \frac{\partial M}{\partial \beta} = \langle E \rangle \langle \phi^{\parallel} \rangle - \langle E \phi^{\parallel} \rangle. \qquad (11)$$

The rest of the paper is organized as follows. First we discuss the critical behavior of the observables and the universal scaling functions, which we want to calculate. In Sec. III we describe the expansions with which we parametrize the scaling functions. Some details of the used simulations and the parametrizations resulting from the data are presented in Sec. IV. Here we also investigate the role of the nonsingular terms for the scaling of the data. We close with a summary and the conclusions.

II. CRITICAL BEHAVIOR AND SCALING FUNCTIONS

In the thermodynamic limit ($V \to \infty$) the above defined observables show power law behavior close to T_c. It is described by critical amplitudes and exponents of the reduced temperature $t = (T - T_c)/T_c$ for $H = 0$ and the magnetic field H for $t = 0$, respectively. According to RG theory the nonanalytic or singular part f_s of the free energy density is responsible for critical behavior. Besides f_s, the free energy density contains a regular or nonsingular part f_{ns}. Correspondingly, the derivatives of f_{ns} contribute regular terms to the scaling laws, which apart from the cases of the energy density and the specific heat (for $\alpha < 0$) are subleading. In the two-dimensional Ising model such an analytic contribution to the magnetic susceptibility was established [19,20]. In Ref. [7], Toussaint makes a corresponding ansatz $f_{ns} = c_{H2}H^2 + c_{J1}t + c_{J2}t^2 + c_{J3}t^3$, which leads to an additional constant in χ_L, a term $\sim H$ in M and an H-independent $\epsilon_{ns}(T)$. Since in our former scaling fits to M at T_c, e.g. in Refs. [10,21], we never discovered such a regular term we follow Privman *et al.* [22] and assume the nonsingular part f_{ns} to have no field dependence, that is

$$f(T, H) = f_s(T, H) + f_{ns}(T), \tag{12}$$

and

$$\epsilon = \epsilon_s + \epsilon_{ns}(T), \qquad C = C_s + C_{ns}(T). \tag{13}$$

The regular parts do not disappear at $T = T_c$. We may expand $\epsilon_{ns}(T)$ in T at T_c

$$\epsilon_{ns}(T) = \epsilon_{ns}(T_c) + (T - T_c) \cdot C_{ns}(T_c)$$
$$+ \frac{1}{2}(T - T_c)^2 \cdot C'_{ns}(T_c) + \dots. \tag{14}$$

The scaling laws at $H = 0$ are then for the magnetization (from now on β denotes a critical exponent)

$$M = B(-t)^\beta \quad \text{for } t < 0, \tag{15}$$

the longitudinal susceptibility

$$\chi_L = C^+ t^{-\gamma} \quad \text{for } t > 0, \tag{16}$$

and the energy density and the specific heat both for $t < 0$ and $t > 0$

$$\epsilon = \epsilon_{ns}(T) + \frac{A^\pm}{\alpha(1 - \alpha)} T_c t |t|^{-\alpha}, \tag{17}$$

$$C = C_{ns}(T) + \frac{A^\pm}{\alpha} |t|^{-\alpha}. \tag{18}$$

For the thermal susceptibility we have for $t < 0$

$$\chi_t = \beta B T_c (-t)^{\beta - 1}. \tag{19}$$

On the critical line $T = T_c$ or $t = 0$ we have for $H > 0$ the scaling laws

$$M = B^c H^{1/\delta} \quad \text{or} \quad H = D_c M^\delta, \tag{20}$$

$$\chi_L = C^c H^{1/\delta - 1} \quad \text{with} \quad C^c = B^c/\delta. \tag{21}$$

The remaining observables scale as follows:

$$\epsilon = \epsilon_{ns}(T_c) + E_c H^{(1-\alpha)/\Delta}, \tag{22}$$

$$C_s - \frac{2\epsilon_s}{T_c} = \frac{A_c}{\alpha_c} H^{-\alpha_c}, \tag{23}$$

$$\chi_t = X_c H^{(\beta - 1)/\Delta}, \tag{24}$$

where $\alpha_c = \alpha/\Delta$ and $\Delta = \beta\delta$ is the so-called "gap exponent."

Generalizations of these scaling laws to both nonzero t and H-values may be derived from the RG scaling equation for f_s

$$f_s(u_1, u_2, u_3, \dots) = b^{-d} f_s(b^{y_1} u_1, b^{y_2} u_2, b^{y_3} u_3, \dots). \tag{25}$$

Here, the u_j with $j = 1, 2, \dots$ are the scaling fields, b is a positive scale factor and the y_j are the RG eigenvalues. The class of our model has two relevant scaling fields $u_1 = u_t$, $u_2 = u_h$ with $y_t, y_h > 0$ and infinitely many irrelevant ones

with negative y_j. The relevant scaling fields depend analytically on t and H and

$$u_t = c_t t + O(t^2, H^2), \qquad u_h = c_h H + O(tH). \tag{26}$$

The c_t, c_h are two model-dependent (positive) metric scale factors. Choosing $b = u_h^{-1/y_h}$ for $H > 0$ one obtains from Eq. (25) the second form of scaling functions from

$$f_s(u_t, u_h, u_{j>2}) = u_h^{d/y_h} f_s(u_t u_h^{-y_t/y_h}, 1, u_j u_h^{-y_j/y_h}). \tag{27}$$

Close to the critical point, for t, H small, $u_t = c_t t$, $u_h = c_h H$ and the dependence on the irrelevant scaling fields becomes negligible, f_s is a universal scaling function of u_t and u_h and

$$f_s = (c_h H)^{d/y_h} \Psi_2(c_t c_h^{-y_t/y_h} t H^{-y_t/y_h}), \tag{28}$$

where Ψ_2 is again a universal function. By comparison with the scaling laws one obtains

$$y_t = 1/\nu, \qquad y_h = 1/\nu_c = \Delta/\nu, \quad \text{or} \quad \Delta = y_h/y_t, \tag{29}$$

and the hyperscaling relations

$$2 - \alpha = d\nu, \qquad \gamma = \beta(\delta - 1), \qquad d\nu = \beta(1 + \delta). \tag{30}$$

Instead of working with two metric scale factors one usually introduces new temperature and field variables $\bar{t} = tT_c/T_0$ and $h = H/H_0$ which are chosen such that the scaling laws for the magnetization simplify to

$$M(t = 0) = h^{1/\delta} \quad \text{and} \quad H_0 = D_c, \tag{31}$$

$$M(h = 0) = (-\bar{t})^\beta \quad \text{and} \quad T_0 = B^{-1/\beta} T_c. \tag{32}$$

The magnetic equation of state as derived from Eqs. (7) and (28) becomes then

$$M = h^{1/\delta} f_G(z), \tag{33}$$

where f_G is a universal scaling function with the argument

$$z = \bar{t}/h^{1/\Delta}. \tag{34}$$

It fulfills the normalization conditions

$$f_G(0) = 1, \quad \text{and} \quad f_G(z) \underset{z \to -\infty}{\to} (-z)^\beta. \tag{35}$$

Because of Eq. (7), the corresponding scaling equation of the free energy density must then be

$$f_s = H_0 h^{1 + 1/\delta} f_f(z), \tag{36}$$

where $f_f(z)$ is again a universal scaling function, and

$$f_G(z) = -\left(1 + \frac{1}{\delta}\right) f_f(z) + \frac{z}{\Delta} f'_f(z). \tag{37}$$

Since the susceptibility χ_L is the derivative of M with respect to H we obtain from Eq. (33)

$$\chi_L = \frac{\partial M}{\partial H} = \frac{h^{1/\delta-1}}{H_0} f_\chi(z), \tag{38}$$

with

$$f_\chi(z) = \frac{1}{\delta}\left(f_G(z) - \frac{z}{\beta}f'_G(z)\right). \tag{39}$$

For $H \to 0$ at fixed $t > 0$, that is for $z \to \infty$, the leading asymptotic term of f_χ is determined by Eq. (16)

$$f_\chi(z) \underset{z\to\infty}{=} C^+ D_c B^{\delta-1} z^{-\gamma} = R_\chi z^{-\gamma}, \tag{40}$$

where R_χ is a universal amplitude product. For $z \to \infty$ the leading terms of f_G and f_χ are identical, because for $T > T_c$ and small magnetic field $M \propto H$. The rest of our observables are related to $f_f(z)$ and $f_G(z)$ as follows:

$$\epsilon_s = -\frac{T^2}{T_0} H_0 h^{(1-\alpha)/\Delta} f'_f(z), \tag{41}$$

$$C_s - \frac{2}{T}\epsilon_s = -\left(\frac{T}{T_0}\right)^2 H_0 h^{-\alpha/\Delta} f''_f(z), \tag{42}$$

$$\chi_t = -\frac{T^2}{T_0} h^{(\beta-1)/\Delta} f'_G(z). \tag{43}$$

III. EXPANSIONS OF THE SCALING FUNCTIONS

In principle we have to parametrize only one scaling function, either $f_f(z)$ or $f_G(z)$, because they are related by the differential equation (37). We choose as usual $f_G(z)$, because it is directly calculable from the magnetization data. Our representation of the scaling function is composed of three expansions: one around $z = 0$ and two for $z \to \pm\infty$. In the following we derive relations between the expansion coefficients of $f_f(z)$ and $f_G(z)$. We start with the expansions for small z

$$f_f(z) = \sum_{n=0}^\infty a_n z^n, \qquad f_G(z) = \sum_{n=0}^\infty b_n z^n. \tag{44}$$

From Eq. (37) we obtain

$$b_n = \left[-\left(1+\frac{1}{\delta}\right) + \frac{n}{\Delta}\right] a_n, \quad \text{or} \quad a_n = \frac{\Delta b_n}{\alpha + n - 2}. \tag{45}$$

The last equation connects the derivatives of the two scaling functions at $z = 0$

$$f_f^{(n)}(0) = \frac{\Delta}{\alpha + n - 2} \cdot f_G^{(n)}(0), \tag{46}$$

and because of the first of the normalization conditions, Eq. (35)

$$f_G(0) = b_0 \equiv 1, \quad \text{and} \quad f_f(0) = a_0 = \frac{\Delta}{\alpha - 2}. \tag{47}$$

Next we consider the asymptotic expansion in the high temperature region, that is for $z \to \infty$, or for $t > 0$ and

$h \to 0$. Since M is an odd function of H for $t > 0$ (Griffiths's condition), we must have

$$f_G(z) = z^{-\gamma} \cdot \sum_{n=0}^\infty d_n^+ z^{-2n\Delta}. \tag{48}$$

The prefactor is the leading term of f_G and $d_0^+ = R_\chi$ (see Eq. (40) and the remark after it). The corresponding ansatz for $f_f(z)$ is

$$f_f(z) = z^{2-\alpha} \cdot \sum_{n=0}^\infty c_n^+ z^{-2n\Delta}. \tag{49}$$

Using again Eq. (37) we are led to the relation

$$c_{n+1}^+ = \frac{-d_n^+}{2(n+1)}, \quad \text{with} \quad c_1^+ = -\frac{R_\chi}{2}, \tag{50}$$

however, the coefficient c_0^+ is not specified by the last equation.

In the low temperature region, for $t < 0$ and $h \to 0$, that is for $z \to -\infty$, massless Goldstone modes appear. They lead to a divergence of the transverse susceptibility $\chi_T \sim H^{-1}$. In addition also the longitudinal susceptibility χ_L is diverging on the coexistence curve. Here, the predicted divergence in three dimensions is [23–25]

$$\chi_L(T < T_c, H) \sim H^{-1/2}. \tag{51}$$

This is equivalent to a dependence of the magnetization on $H^{1/2}$ near the coexistence curve [8]. Therefore we make the following ansatz for $f_G(z)$ in this region:

$$f_G(z) = (-z)^\beta \cdot \sum_{n=0}^\infty d_n^-(-z)^{-n\Delta/2}, \tag{52}$$

where due to the second normalization condition in Eq. (35), $d_0^- = 1$. The corresponding ansatz for $f_f(z)$ is

$$f_f(z) = (-z)^{2-\alpha} \cdot \sum_{n=0}^\infty c_n^-(-z)^{-n\Delta/2}. \tag{53}$$

Inserting the two expansions into the differential Eq. (37) we find

$$c_{n+2}^- = -\frac{2d_n^-}{n+2}. \tag{54}$$

As in the high temperature phase the coefficient of the leading term, c_0^-, is not fixed, moreover $c_1^- \equiv 0$, and $c_2^- = -1$. In order to completely solve Eq. (37) for $f_f(z)$ we still have to find the coefficients $c_0^\pm$. Since $\alpha < 0$ for the $O(4)$ model we may proceed in the following way. First we consider the small z-expansions for $z > 0$

$$\sum_{n=3}^\infty a_n z^n = \Delta \sum_{n=3}^\infty \frac{b_n z^n}{\alpha + n - 2}$$
$$= \Delta z^{2-\alpha} \int_0^z dy\, y^{\alpha-3} \sum_{n=3}^\infty b_n y^n \tag{55}$$

$$= \Delta z^{2-\alpha} \int_0^z dy y^{\alpha-3} [f_G(y) - 1 - b_1 y - b_2 y^2] \quad (56)$$

$$= f_f(z) - a_0 - a_1 z - a_2 z^2. \quad (57)$$

That enables us to calculate c_0^+

$$c_0^+ = \lim_{z \to \infty} f_f(z) z^{\alpha-2}$$

$$= \Delta \int_0^\infty dy y^{\alpha-3} [f_G(y) - 1 - b_1 y - b_2 y^2], \quad (58)$$

or, by partial integration

$$c_0^+ = \frac{\Delta}{2-\alpha} \int_0^\infty dy y^{\alpha-2} [f_G'(y) - f_G'(0) - y f_G''(0)]. \quad (59)$$

In the same manner we can calculate c_0^- from an integral over negative z by starting from

$$f_f(z) = a_0 + a_1 z + a_2 z^2 + \Delta(-z)^{2-\alpha} \int_z^0 dy(-y)^{\alpha-3}$$

$$\times [f_G(y) - 1 - b_1 y - b_2 y^2], \quad (60)$$

and taking the limit $z \to -\infty$

$$c_0^- = \lim_{z \to -\infty} f_f(z)(-z)^{\alpha-2}$$

$$= \Delta \int_{-\infty}^0 dy(-y)^{\alpha-3} [f_G(y) - 1 - b_1 y - b_2 y^2], \quad (61)$$

or

$$c_0^- = \frac{-\Delta}{2-\alpha} \int_{-\infty}^0 dy(-y)^{\alpha-2} [f_G'(y) - f_G'(0) - y f_G''(0)]. \quad (62)$$

The function $f_f(z)$ is universal as a whole and so are each of its expansion coefficients, that is c_0^+ and c_0^- are universal. In fact, it can be shown, that these coefficients are the universal products of critical amplitudes

$$c_0^\pm = f_s^\pm (B^c)^\delta B^{-(1+\delta)}, \quad (63)$$

where

$$f_s^\pm = \frac{A^\pm}{-\alpha(1-\alpha)(2-\alpha)}, \quad (64)$$

are the critical amplitudes of the free energy density for $H = 0$ and $t \neq 0$

$$f = f_{ns}(T) + f_s^\pm |t|^{2-\alpha}. \quad (65)$$

Because of Eqs. (63) and (64) we can now calculate the universal ratio

$$\frac{A^+}{A^-} = \frac{c_0^+}{c_0^-} \quad (66)$$

from the two integrals in Eqs. (59) and (62). A similar formula is known for the magnetic equation of state in the Widom-Griffiths form [26]. It was, for example, used to determine the ratio A^+/A^- in the case of the $O(2)$ model [27].

IV. THE PARAMETRIZATIONS

The data we use in the following to parametrize the scaling functions were all obtained from simulations described in detail in Ref. [21]. We repeat here only the main features of these simulations. They were performed on three-dimensional lattices with periodic boundary conditions and linear extension $L = 120$. The coupling constant region which was explored is $0.90 \leq J \leq 1.2$, the magnetic field was varied from $H = 0.0001$ to $H = 0.007$. In general 100 000 measurements were done at each fixed H and J. We have reevaluated the raw data to obtain the magnetization, the longitudinal and the thermal susceptibilities, the energy density and the specific heat. Because of the large spatial volume of the lattice, most of the finite size effects have disappeared from the data. This is, in particular, true for the energy density and the magnetization, to a smaller extent also for the susceptibilities and the specific heat. We shall discuss the remaining effects when the scaling of the respective observables is analyzed. A further source of difficulties is, at larger $|t|$ and H-values, the possible appearance of corrections to scaling because of the influence of irrelevant scaling fields. These violations of scaling should be visible in the scaling plots for the data. However, as we shall show below, we find perfect scaling properties without any sign of these corrections to scaling for our values of t and H for the energy density and the magnetization. This not the case for the corresponding nonlinear $O(2)$ model, see e.g. Fig. 5 of Ref. [28], where strong scaling violations were found for $T < T_c$. An explanation for this striking difference can be inferred from two papers, by Hasenbusch and Török [29] for $N = 2$ and by Hasenbusch [30] for $N = 4$. In these papers the leading corrections to scaling could be eliminated by using instead of the nonlinear $O(N)$ invariant models the corresponding $O(N)$ symmetric ϕ^4 models and the tuning of the additional parameter λ. It turned out that the optimal parameter value is 2.1 for $N = 2$ and 12.5(4.0) for $N = 4$. The nonlinear case corresponds to $\lambda = \infty$. One expects therefore to find significantly weaker corrections for $N = 4$ as compared to $N = 2$. The remarkable lack of scaling corrections had already been noted in Ref. [8], where for the first time the critical exponents for the $3d$ $O(4)$ model were determined from magnetization data at finite external fields. Later, in Ref. [10], the result for the exponent δ could be improved with better data and fits where correction-to-scaling terms had been taken into account. Yet, these terms were contributing at best marginally and could as well be neglected.

In order to define our variables t, $\bar{t}$, h and z we use the same critical amplitudes, temperature and exponent values as in Refs. [10,21]. These are

$$J_c = T_c^{-1} = 0.93590, \quad T_0 = 1.093, \quad H_0 = 4.845, \quad (67)$$

$$\beta = 0.380, \quad \delta = 4.824, \quad \Delta = 1.83312, \quad (68)$$

and from the hyperscaling relations

$$\alpha = -0.2131, \qquad \nu = 0.7377, \qquad \gamma = 1.4531. \quad (69)$$

We have compared the exponents from Eqs. (68) and (69) to the field-theory results of Guida and Zinn-Justin [31], displayed in their Table 3. Apart from the value for $\delta = 4.824(9)$ (from [10]) which corresponds to the value $\eta = 0.0302(16)$ via the hyperscaling relation $\eta = (5 - \delta)/(1 + \delta)$ our numbers are always close to the respective central values of Guida and Zinn-Justin and they are always inside their error bars.

We proceed in the following way. First we calculate $f_G(z)$ from the magnetization data and fit the large z parts to the asymptotic expansions. The small z region is more intricate, because the derivative $-f_G'(z)$ has a peak for $z > 0$, which determines the pseudocritical line. In order to model the corresponding variation properly we fit directly the derivative for small z. It can be obtained either from the data for χ_t, Eq. (43), or from χ_L and M, using Eqs. (33), (38), and (39). After completion of the parametrization of $f_G(z)$ we compute the leading asymptotic coefficients $c_0^\pm$ of $f_f(z)$. The scaling function of the free energy density is then also entirely known. In the next step we determine the nonsingular contributions to the energy density and the specific heat, first at T_c and then at all our T-values. We show that the results for $\epsilon_{\rm ns}$ shape a smooth function of T, where T_c is not a distinguished point. With this function $\epsilon_{\rm ns}(T)$ it is then possible to compare the scaling functions to the data for the energy density and specific heat.

In Fig. 1 we show the data obtained from the magnetization for the scaling function $f_G(z)$ and our parametrizations. Obviously the data scale very well, apart from the data for $H = 0.0001$ and $z < 0$, which show some finite size effect (in the figure at $z = -1.534$ and -5.219). We have fitted f_G in the asymptotic regions with the first three terms of the respective expansions from Eqs. (48) and (52). For the positive z-range [1.5, 15] we found the coefficients

$$d_0^+ = 1.10599 \pm 0.00555,$$

$$d_1^+ = -1.31829 \pm 0.1087, \qquad d_2^+ = 1.5884 \pm 0.4646. \quad (70)$$

In the negative z-range $[-10, -1]$ we discarded the data with $H = 0.0001$ and obtained

$$d_0^- \equiv 1, \qquad d_1^- = 0.273651 \pm 0.002933,$$
$$d_2^- = 0.0036058 \pm 0.004875. \quad (71)$$

Since $d_0^+ = R_\chi$ we have a new value for this quantity, which is compatible with the old values $R_\chi = 1.084(18)$ from Ref. [10] and $R_\chi = 1.12(11)$ from Ref. [9] but somewhat more accurate. Astonishingly, the asymptotic expansions describe the function $f_G(z)$ very well down to rather small $|z|$-values, and as can be seen in Fig. 1 they overlap
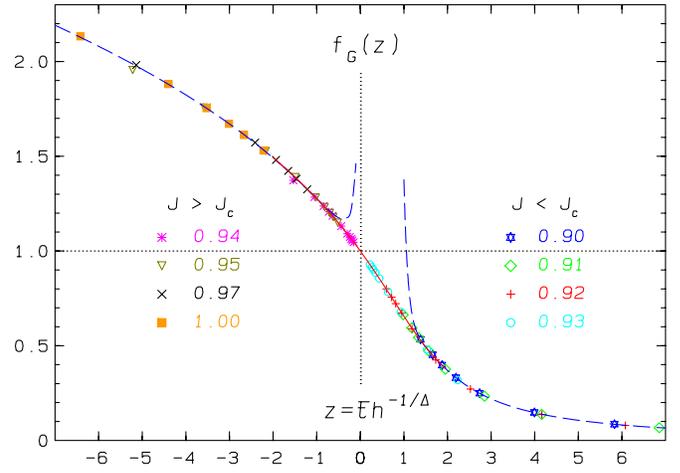

FIG. 1 (color online). The scaling function $f_G = Mh^{-1/\delta}$ as a function of $z = \bar{t}h^{-1/\Delta}$. The dashed lines show the asymptotic expansions, the solid line the Taylor expansion at $z = 0$. The numbers refer to the different $J = 1/T$-values of the data.

with our approximation to the Taylor expansion at $z = 0$. As mentioned already, we use the derivative $-f_G'(z)$ to determine the coefficients of the Taylor expansion. In Fig. 2 we show the data which we obtained from χ_t (filled circles) and χ_L and M (crosses) for the derivative. Obviously, the data involving χ_L suffer from large finite size effects in the whole low temperature region ($z < 0$) for already moderately small H-values. This behavior is known and a consequence of Eq. (51), the divergence of χ_L near the coexistence line. In contrast to that, the data from χ_t show a consistent scaling behavior for $z < 0$ (apart from the $H = 0.0001$ point for $J = 0.94$ at $z = -1.534$). For $z > 0$ but close to the critical point we find still larger finite size effects for the χ_L-data as compared to the ones
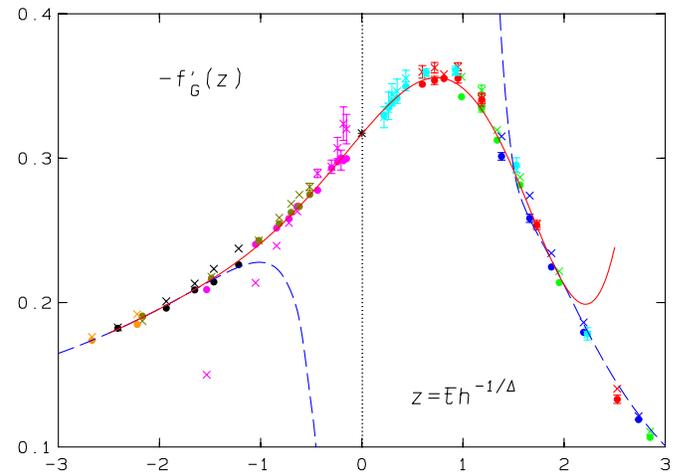

FIG. 2 (color online). The derivative $-f_G'(z)$ as a function of $z = \bar{t}h^{-1/\Delta}$. The filled circles denote the data calculated from χ_t, the crosses the data obtained from χ_L and M. The dashed lines show the asymptotic expansions, the solid line the Taylor expansion around $z = 0$.

for the χ_t-data, because of the stronger divergence of χ_L on the critical line. At larger positive z-values beyond the peak region we observe however, that the χ_t-data are systematically smaller than the χ_L-data. The reason for this lies in the cluster update [32] which was used to produce the data. That update diminishes very efficiently the autocorrelation time for the order parameter, but is less efficient for the energy density. For increasing temperature and/or decreasing H the cluster size drops and if the number of cluster updates is not correspondingly increased the autocorrelation times for the energy density data increase faster than those for the magnetization data. An increasing decorrelation of ϵ and M takes then place with increasing z, that is the χ_t-data become too small. In view of all these considerations we use in our Taylor fits only χ_t-data for $z < 1.3$ and in the z-interval [1.3, 2] both types of data.

From our data at T_c we have calculated an additional data point at $z = 0$, denoted by a star in Fig. 2. To this end we have used Eq. (43) at T_c

$$- f'_G(0) = \frac{T_0}{T_c^2} h^{-(\beta-1)/\Delta} \chi_t(T_c). \qquad (72)$$

The corresponding data are shown in Fig. 3. At small H we have again finite size effects, at large H corrections to scaling set in. A fit to the remaining data points leads to the result $-f'_G(0) = 0.3173(5)$. We have approximated the Taylor series with polynomials. Instead of using a single very high order polynomial, we started with two fits to sixth-order polynomials, that is for $f'_G(z)$ with the ansatz

$$f'_G(z) = b_1 + 2b_2 z + 3b_3 z^2 + 4b_4 z^3 + 5b_5 z^4 + 6b_6 z^5, \qquad (73)$$

in the overlapping z-intervals $[-2.5, 0.75]$ and $[-0.75, 2]$. The lowest coefficients of the two polynomials should, at the end of the process, coincide to generate a smooth parametrization close to $z = 0$. In the second step we took therefore the arithmetic averages of the results of the two fits for b_1 and b_2, fixed them and repeated the two fits to determine the remaining coefficients. In step three b_3 was
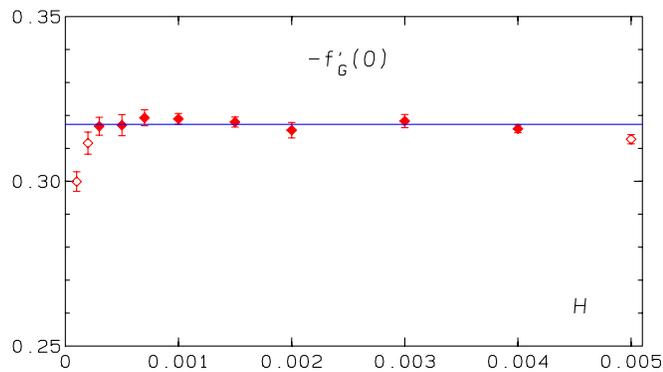

FIG. 3 (color online). The quantity $-f'_G(0)$ as a function of the magnetic field H. The filled data points were used for the fit, the solid line shows the fit result.

fixed by averaging the corresponding means of the first and the second step. The last fits were performed with fixed b_1, b_2 and b_3 in the intervals $[-2.5, 0.75]$ and $[-0.5, 2]$, including some points from the fits to the asymptotic regions. Our final result is

$$b_0 \equiv 1, \qquad b_1 = -0.3166125 \pm 0.000534, \qquad (74)$$

$$b_2 = -0.04112553 \pm 0.001290, \qquad (75)$$
$$b_3 = 0.00384019 \pm 0.000667.$$

The remaining coefficients are different for $z < 0$ and $z > 0$. We find for $z > 0$

$$b_4^+ = 0.006705475 \pm 0.001704, \qquad (76)$$
$$b_5^+ = 0.0047342 \pm 0.001429,$$

$$b_6^+ = -0.001931267 \pm 0.000312, \qquad (77)$$

and for $z < 0$

$$b_4^- = 0.007100450 \pm 0.000160, \qquad (78)$$
$$b_5^- = 0.0023729 \pm 0.000095,$$

$$b_6^- = 0.000272312 \pm 0.000021. \qquad (79)$$

We note that b_4^- and b_4^+ still coincide inside their error bars. In Fig. 2 we have plotted the respective approximations to $-f'_G(z)$ in the z-ranges $[-2.5, 0]$ and $[0, 2.5]$. Obviously, there is a large range for $z < 0$ and a shorter range for $z > 0$ where the approximations overlap and coincide with the respective asymptotic expansions. In the rest of the paper we use therefore the Taylor expansions in the z-range $[-2, 1.95]$ and outside the asymptotic expressions.

It is now straightforward to calculate the coefficients of the leading asymptotic terms of $f_f(z)$ from Eqs. (59) and (62). We find

$$c_0^+ = 0.422059886 \pm 0.010595, \qquad (80)$$
$$c_0^- = 0.229176194 \pm 0.010669.$$

The errors of $c_0^\pm$ have been determined using the complete correlation matrix of the contributing parameters. The main contributions to $c_0^\pm$ are coming from the two terms proportional to b_1 and b_2. The second, larger term is the same for both coefficients, the first only changes the sign, that is for c_0^+ we have the sum, for c_0^- the difference of these terms and as a consequence the $c_0^\pm$ are strongly correlated. That allows us to estimate the correlation between c_0^+ and c_0^- to $C_{+-} = -\sigma_1^2 + \sigma_2^2$, where the $\sigma_{1,2}$ are the errors of the two terms. From Eqs. (66) and (80) we obtain then the universal ratio

$$\frac{A^+}{A^-} = 1.842 \pm 0.043. \qquad (81)$$

Our value for the ratio is in agreement with the final estimates found in Refs. [9], 1.91(10), and [11], 1.8(2).

We note however, that our error estimate does not include a possible variation of the critical exponents used.

With the results from Eq. (80) we have completely specified the parametrizations of $f_G(z)$ and of $f_f(z)$. In order to test the scaling function of the free energy density and/or its temperature derivatives we still need the regular contributions. Quite generally, the exponent α must be always less than 1 for continuous transitions, because the energy density at T_c is finite and there is no latent heat (which would be possible for $\alpha = 1$). From Eqs. (17) and (22) we know therefore that

$$\epsilon_s(T_c, H = 0) = 0, \quad \text{or} \quad \epsilon(T_c, H = 0) = \epsilon_{ns}(T_c). \quad (82)$$

We may then determine $\epsilon_{ns}(T_c)$ from our data for the energy density at T_c. In Fig. 4 we see that the data at $T = T_c$ fulfill the expected scaling law, Eq. (22) and (41) accordingly

$$\epsilon_s(T_c) = -\frac{T_c^2}{T_0} H_0 h^{(1-\alpha)/\Delta} f'_f(0). \quad (83)$$

Moreover, there is no sign of a finite size dependence at small external fields. We have fitted the data directly with Eq. (22) and find

$$\epsilon_{ns}(T_c) = -0.991888(13), \quad E_c = -0.8500(06),$$
$$f'_f(0) = 0.47723(32). \quad (84)$$

Evidently we have a very precise result for the nonsingular part of the energy density at T_c. The derivative $f'_f(0)$ can also be calculated from $b_1 = f'_G(0)$ and Eq. (46). That leads to $f'_f(0) = 0.47843(81)$ and is consistent with the previous result.

For positive α the specific heat is diverging and it is therefore unclear how to determine the regular term $C_{ns}(T_c)$. If however α is negative, then $C_s - 2\epsilon_s/T$ disappears at T_c for $h = 0$, because of Eq. (23), the finite regular term remains and we can calculate $C_{ns}(T_c)$. Usually, the specific heat has nevertheless a sharp peak at T_c and $H = 0$,

which just means that the critical amplitudes are negative. That sign is taken care of by the factors $1/\alpha$ and $1/\alpha_c$, respectively, in our amplitude definitions, so that $A^\pm$ and A_c are positive. In Fig. 5 we show our data for $C - 2\epsilon/T$ at T_c and the corresponding fit to Eqs. (23) and (42). We find

$$\left(C_{ns} - \frac{2\epsilon_{ns}}{T}\right)(T_c) = 6.2669(195), \quad \text{and}$$
$$C_{ns}(T_c) = 4.4103(195), \quad (85)$$
$$A_c = 0.32041(468), \quad \text{or} \quad f''_f(0) = 0.7151(104), \quad (86)$$

which is compatible to the value $f''_f(0) = 0.7075(221)$ calculated from b_2.

In Fig. 6 we show the scaling function $f'_f(z)$ which is obtained from our parametrization. We plot the asymptotic expansions and the Taylor expansion separately and find that they are overlapping in the same regions as for $f_G(z)$, that is our calculation of the $c_0^\pm$ is consistent. The data which we also show have been calculated assuming that

$$\epsilon_{ns}(T) = \epsilon_{ns}(T_c) + (T - T_c) \cdot C_{ns}(T_c), \quad (87)$$

where the numbers are from our fits at $T = T_c$. We note here, that without the term proportional to $C_{ns}(T_c)$ the data would scale nowhere apart from the point $z = 0$. In Fig. 6 we observe scaling for small $|z|$ and coincidence with the predicted scaling function, but not at larger values. The reason for that is the assumption, Eq. (87), for the function $\epsilon_{ns}(T)$, which leads to inaccurate ϵ_{ns}-values for larger $|T - T_c|$. We can test this and the scaling behavior at fixed T and varying H at the same time. If we have scaling then Eq. (41) must hold and

$$\epsilon_{ns}(T) = \epsilon(T, H) + T^2 \frac{H_0}{T_0} h^{(1-\alpha)/\Delta} f'_f(z), \quad (88)$$

where the $\epsilon(T, H)$ are the energy density data at fixed T and $f'_f(z)$ is the predicted scaling function. The test is successful, if we obtain the same value $\epsilon_{ns}(T)$ for all H inside the
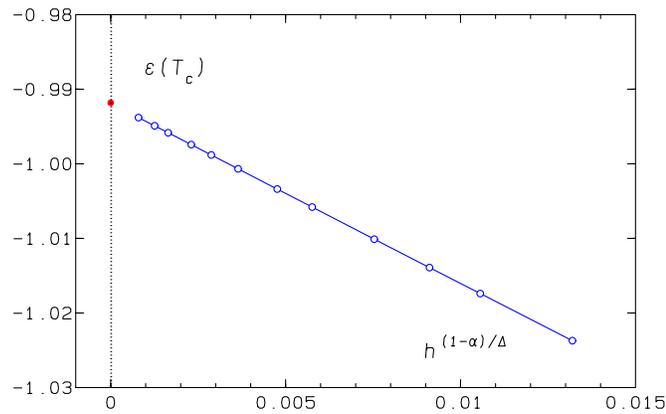

FIG. 4 (color online).   The energy density at T_c (open circles) as a function of $h^{(1-\alpha)/\Delta}$. The filled circle shows the extrapolation to $h = 0$, that is $\epsilon_{ns}(T_c)$, the points are connected by straight lines.
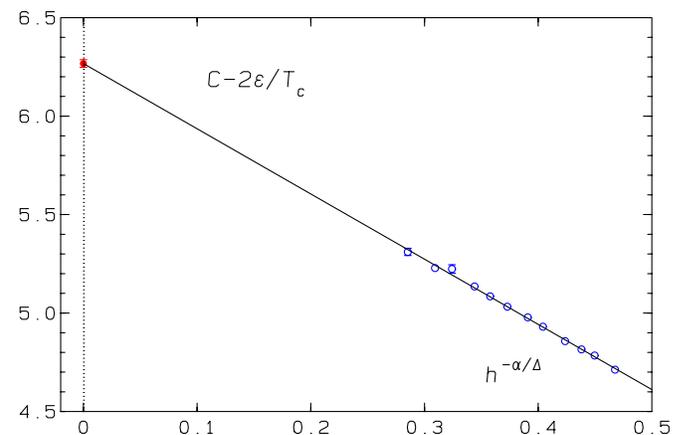

FIG. 5 (color online).   The quantity $C - 2\epsilon/T$ at T_c (open circles) as a function of $h^{-\alpha/\Delta}$. The filled circle shows the extrapolation to $h = 0$, the straight line the fit, Eq. (42).
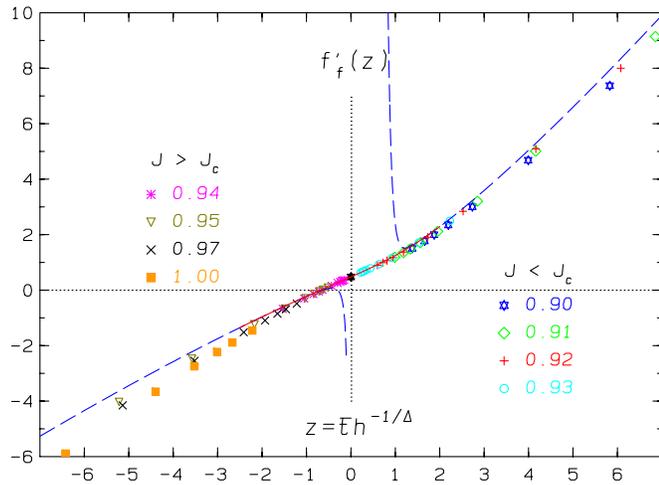
FIG. 6 (color online). The scaling function $f'_f(z)$ as a function of $z = \bar{t}h^{-1/\Delta}$. The dashed lines show the asymptotic expansions, the solid line the polynomial approximations for small z. The star at $z = 0$ is the result from Eq. (84).

FIG. 8 (color online). The scaling function $f'_f(z)$ as a function of $z = \bar{t}h^{-1/\Delta}$. The line shows our parametrization, the data have been calculated using Eqs. (89) and (90).

error bars. This is indeed the case. The errors of the averages are tiny. They vary for $T \leq T_c$ between 6×10^{-6} and 1.4×10^{-5}, and in the hot phase they increase to 3.5×10^{-5}. In Fig. 7 we compare the found values for $\epsilon_{ns}(T)$ with the approximation from Eq. (87), where we have used our previously calculated numbers from Eqs. (84) and (85). Though the differences in Fig. 7 do not seem to be large, they are the reason for the deviation of the data from the scaling function $f'_f(z)$ in Fig. 6. We have fitted our results for $\epsilon_{ns}(T)$ with the Taylor expansion, Eq. (14), up to the third derivative of ϵ_{ns} and find

$$\epsilon_{ns}(T_c) = -0.991792(28), \qquad C_{ns}(T_c) = 4.3910(14), \tag{89}$$

$$C'_{ns}(T_c) = 8.448(108), \qquad C''_{ns}(T_c) = 42.79 \pm 5.13. \tag{90}$$

The new result for $C_{ns}(T_c)$ is in agreement with the one we obtained from our admittedly far extrapolation of $C - 2\epsilon/T$ in h at T_c. We have used the results from the Taylor expansion fit to approximate the functions $\epsilon_{ns}(T)$ and $C_{ns}(T)$ in the calculation of the scaling functions f'_f and f''_f from our data. As can be seen from Fig. 8 we find now perfect scaling for the energy density, even for relatively large $|T - T_c|$-values. In Fig. 9 we compare our parametrization for f''_f with the data. Since the specific heat is proportional to the fluctuation of the energy density, the data are not as precise as for f'_f, especially for high temperatures. Nevertheless we observe satisfactory scaling and a further confirmation for our parametrization.

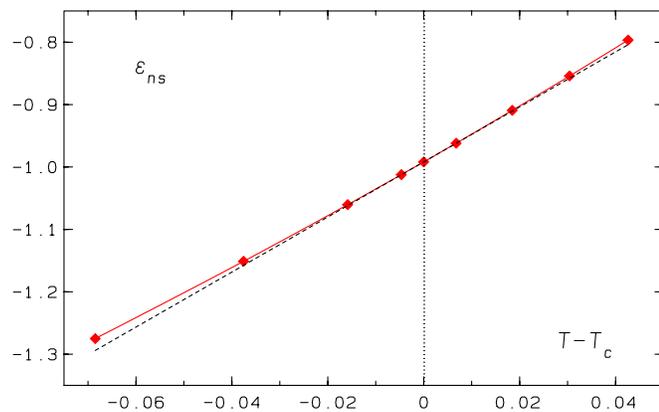Finally we show in Fig. 10 the third derivative of the scaling function $f_f(z)$ with respect to z. It controls the

FIG. 7 (color online). The nonsingular part of the energy density $\epsilon_{ns}(T)$ as a function of $T - T_c$ (filled diamonds). The dashed line shows the approximation from Eq. (87).

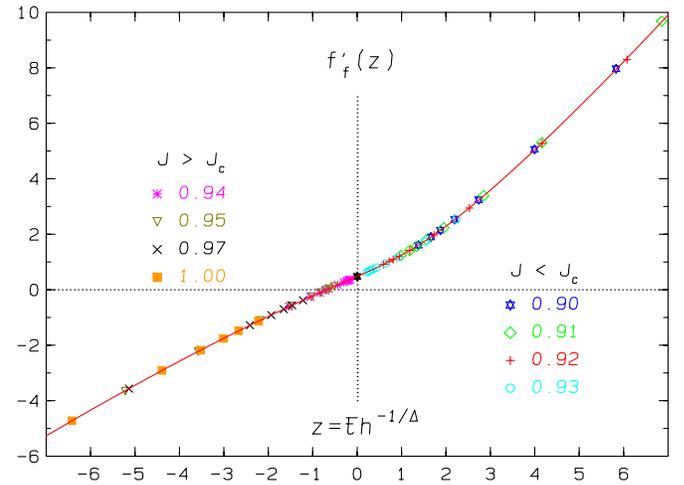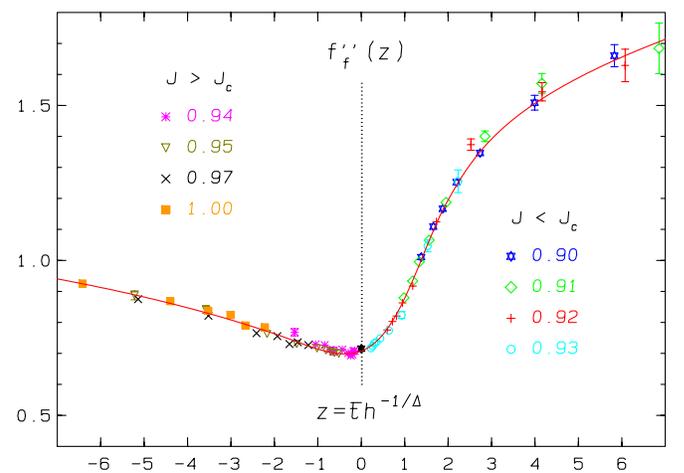FIG. 9 (color online). The scaling function $f''_f(z)$ as a function of $z = \bar{t}h^{-1/\Delta}$. The line shows our parametrization, the data have been calculated using Eqs. (89) and (90), the star at $z = 0$ is the result from Eq. (86).
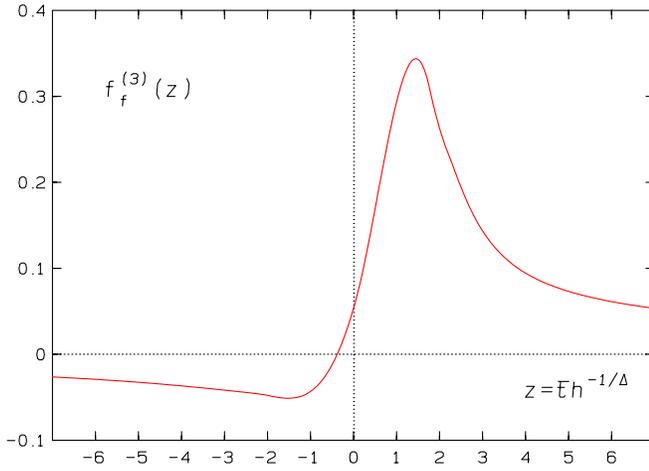
FIG. 10 (color online). The scaling function $f_f^{(3)}(z)$ as a function of $z = \bar{t}h^{-1/\Delta}$. The line shows our parametrization.

singular behavior of the third derivative of the free energy density with respect to temperature,

$$\frac{\partial^3 f}{\partial T^3} \sim \frac{\partial^3 f_s}{\partial T^3} = \frac{H_0}{T_0^3} h^{-(1+\alpha)/\Delta} f_f^{(3)}(z), \qquad (91)$$

and is the first thermal derivative of the free energy density that diverges at T_c in the limit $H \rightarrow 0$. It thus allows a discussion of critical behavior resulting from the structure of the singular part of the free energy density without the need of determining nonsingular contributions to the free energy density. This property of the three-dimensional $O(4)$ model has been exploited in the discussion of critical behavior in the vicinity of the chiral phase transition of 2-flavor QCD [33,34].

V. SUMMARY AND CONCLUSIONS

In this paper we have investigated the scaling functions of the three-dimensional $O(4)$ model, which can be derived from the singular part of the free energy density. In contrast to other papers [8–12] where the scaling functions are parametrized in the Widom-Griffiths form, we have chosen a form which is preferred in tests of other models such as QCD. Here the scaling variable z is independent of the magnetization. These scaling functions can of course be derived from those of the other type, however the explicit functional dependence on z is of value. The major advantages of our parametrization are

(1) derivatives with respect to the variable z can be taken directly and not implicitly; the positions of extrema are easily calculable.

(2) the parameters are determined from direct fits to the data; one can immediately judge how well the data are represented.

In order to carry out the parametrization we have used the best presently available data set for finite magnetic fields

[21]. Furthermore, we have tackled the problem of the scaling of the energy density and the specific heat in the $3d$ $O(4)$ model, to our knowledge for the first time at all, and we were able to clarify the role of the nonsingular part of the energy density for scaling. This is very important for all corresponding checks of QCD with two light flavors (see, for example, Ref. [18]). Our approach in some more detail was the following:

We have parametrized the scaling function $f_G(z)$ of the magnetization with asymptotic expansions for $z \rightarrow \pm\infty$ and Taylor expansions around $z = 0$. The knowledge of the expansion coefficients of $f_G(z)$ enabled us to derive the corresponding coefficients for the scaling function $f_f(z)$ of the singular part of the free energy density. In particular, we could calculate the leading asymptotic coefficients $c_0^\pm$ of $f_f(z)$ and thereby determine the universal amplitude ratio for the specific heat to $A^+/A^- = 1.842(43)$. In the following we have tested our data for the energy density and the specific heat with the respective scaling functions. To this end we have determined the nonsingular parts of the two observables at T_c. Whereas this is always possible for the energy density, we could do that for the specific heat only, because in the three-dimensional $O(4)$ model the exponent α is negative. With these results we found scaling for the energy density in the neighborhood of T_c or small $|z|$ but not outside. As it turned out, we can achieve scaling for all our T or J-values, if we use the correct values of $\epsilon_{ns}(T)$. The latter can be calculated from our function $f_f'(z)$ if the data show scaling in h. We found indeed perfect scaling in h and very accurate $\epsilon_{ns}(T)$-values. They form a smooth function of T in accord with the results from T_c. As expected, T_c is not a distinguished point of this function. For other models the regular parts of the energy density are of course different and may be not so easy calculable, if, for example, correction-to-scaling terms spoil h-scaling. A test of the energy density and/or specific heat on scaling may then be problematic.

As a last result of our parametrization we quote the peak positions of scaling functions which are relevant for the definition of pseudocritical lines. In all cases the peaks are very flat and symmetric around the peak positions z_p. We found the value $z_p^{0,2} = 1.374(30)$ for f_χ, in $-f_G'$ the value $z_p^{1,1} = 0.74(4)$ and for $-f_f''$ the value $z_p^{2,0} = -0.38(8)$. The corresponding observables are χ_L, χ_t, and $C - 2\epsilon/T$, the upper index of z_p denotes the number of derivatives of the free energy density with respect to T and H. Evidently, the pseudocritical lines can be rather different. If, for example, the peak position of χ_t is used to define the pseudocritical temperature, it will be closer to T_c as in the case of χ_L.

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