

Universal properties of 3d $O(4)$ symmetric models: The scaling function of the free energy density and its derivatives

Frithjof Karsch^{*†}

Physics Department, Brookhaven National Laboratory, Upton, NY 11973, USA
Fakultät für Physik, Universität Bielefeld, D-33615 Bielefeld, Germany
E-mail: karsch@bnl.gov

Jürgen Engels

Fakultät für Physik, Universität Bielefeld, D-33615 Bielefeld, Germany
E-mail: engels@physik.uni-bielefeld.de

We present 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 $z = \bar{t}/h^{1/\beta\delta}$. The expansions around $z = 0$ and the corresponding asymptotic ones for $z \rightarrow \pm\infty$ overlap such that no interpolation is needed. We explicitly present the expansion coefficients which have been determined numerically from data of a previous high statistics simulation of the $O(4)$ model on a three-dimensional lattice of linear extension $L = 120$. This allows to derive smooth representations of the first three derivatives of the scaling function of the free energy density, which determine universal properties of up to sixth order cumulants of net charge fluctuations in QCD.

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*Speaker.

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1. Introduction

We 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. Contrary to the often analyzed scaling function of the order parameter, the so-called magnetic equation of state, our main interest here is to determine directly the scaling function of the free energy density and its derivatives. This is especially of importance for applications to quantum chromodynamics (QCD) with two degenerate light-quark flavors at finite temperature. Two-flavor QCD is believed [1]-[6] to belong to the 3d $O(4)$ universality class at its chiral transition in the continuum limit. In the vicinity of the chiral phase transition temperature the reduced temperature variable in QCD also depends quadratically on the quark chemical potential. Derivatives of the singular part of the free energy density of QCD with respect to chemical potential, which define cumulants of fluctuations of net quark number, thus are controlled by scaling functions that are given by derivatives of the scaling function of the free energy density in a three-dimensional $O(4)$ model.

Obtaining explicit parametrizations of higher order derivatives of the scaling functions of the free energy density became of interest recently as these higher order derivatives control the scaling behavior of fluctuations of conserved charges, e.g. the net baryon number [7]. These quantities are currently measured at RHIC [8] and will also be measured in heavy ion experiments at the LHC.

2. The three dimensional $O(4)$ model

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

$$\beta \mathcal{H} = -J \sum_{\langle \vec{x}, \vec{y} \rangle} \vec{\phi}_{\vec{x}} \cdot \vec{\phi}_{\vec{y}} - \vec{H} \cdot \sum_{\vec{x}} \vec{\phi}_{\vec{x}}, \quad (2.1)$$

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, $J \equiv 1/T$. The partition function is then

$$Z(T, H) = \int \prod_{\vec{x}} d^4 \phi_{\vec{x}} \delta(\phi_{\vec{x}}^2 - 1) \exp(-\beta \mathcal{H}). \quad (2.2)$$

We introduce the order parameter M as the derivative of the free energy density, $f(T, H) = -\frac{1}{V} \ln Z$, with respect to the magnitude of the external magnetic field $\vec{H} = H \vec{e}_H$,

$$M = -\frac{\partial f}{\partial H} = \langle \phi^{\parallel} \rangle, \quad (2.3)$$

where ϕ^{\parallel} is the field component parallel to the magnetic field \vec{H} .

In the vicinity of the critical point the free energy density may be splitted into a singular (non-analytic) (f_s) and a non-singular (f_{ns}) part,

$$f(T, H) = f_s(T, H) + f_{ns}(T). \quad (2.4)$$

The singular part is a homogeneous function of the variable $h = H/H_0$ and the reduced temperature $\bar{t} = (T - T_c)/T_0$, where H_0 and T_0 set the scale in the critical region. The singular part may be expressed in terms of a universal scaling function f_f , which itself only depends on the scaling variable $z = \bar{t}/h^{1/\Delta}$, i.e.,

$$f_s = H_0 h^{1+1/\Delta} f_f(z). \quad (2.5)$$

Here we have introduced the gap exponent, $\Delta = \beta\delta$, which is given in terms of the more commonly used critical exponents β and δ . The latter define the scaling properties of the order parameter as function of temperature at $h = 0$ and as function of the external field at $t = 0$, respectively. Eq. 2.5 establishes the relation between the universal scaling function of the order parameter (f_G) and the scaling function of the free energy density (f_f). Using Eq. 2.3 we find

$$M = h^{1/\delta} f_G(z) \quad (2.6)$$

$$f_G(z) = - \left(1 + \frac{1}{\delta} \right) f_f(z) + \frac{z}{\Delta} f_f'(z). \quad (2.7)$$

In the following we will exploit the differential equation, Eq. 2.7, to determine the scaling function $f_f(z)$ from $f_G(z)$.

3. Scaling functions of the free energy density and the order parameter

As the universal scaling functions of the free energy density, $f_f(z)$, and the order parameter, $f_G(z)$, are related through the differential equation, Eq. 2.7, the knowledge of $f_G(z)$ is sufficient to determine $f_f(z)$. We summarize in the following the relevant relations that determine $f_f(z)$, once a suitable parametrization of $f_G(z)$ is known. Further details are given in Ref. [9].

We consider a parametrization of $f_G(z)$ by introducing three series expansions that are valid for small z and in the asymptotic regions $z \rightarrow \pm\infty$, respectively,

$$f_G(z) = \begin{cases} \sum_{n=0}^{\infty} b_n z^n & , z \text{ small} \\ z^{-\gamma} \cdot \sum_{n=0}^{\infty} d_n^+ z^{-2n\Delta} & , z \rightarrow +\infty \\ (-z)^\beta \cdot \sum_{n=0}^{\infty} d_n^- (-z)^{-n\Delta/2} & , z \rightarrow -\infty \end{cases} \quad (3.1)$$

The corresponding parametrization for the scaling function of the free energy density is then given by,

$$f_f(z) = \begin{cases} \sum_{n=0}^{\infty} a_n z^n & , z \text{ small} \\ z^{2-\alpha} \cdot \sum_{n=0}^{\infty} c_n^+ z^{-2n\Delta} & , z \rightarrow +\infty \\ (-z)^{2-\alpha} \cdot \sum_{n=0}^{\infty} c_n^- (-z)^{-n\Delta/2} & , z \rightarrow -\infty \end{cases} \quad (3.2)$$

The relation between the expansion coefficients in the series representations for f_G and f_f are easily obtained by using the differential equation, Eq. 2.7, and comparing coefficients for $n \geq 0$,

$$a_n = \frac{\Delta b_n}{\alpha + n - 2}, \quad c_{n+1}^+ = \frac{-d_n^+}{2(n+1)}, \quad c_{n+2}^- = -\frac{2d_n^-}{n+2}, \quad (3.3)$$

b_0	b_1	b_2	b_3
1	-0.3166125 ± 0.000534	-0.04112553 ± 0.001290	0.00384019 ± 0.000667
	b_4^+	b_5^+	b_6^+
	0.006705475 ± 0.001704	0.0047342 ± 0.001429	$-0.001931267 \pm 0.000312$
	b_4^-	b_5^-	b_6^-
	0.007100450 ± 0.000160	0.0023729 ± 0.000095	0.000272312 ± 0.000021

Table 1: Coefficients of the small z -expansion of the scaling function $f_G(z)$ of the order parameter. For $n \geq 4$ we give different expansion coefficients for negative and positive z -values.

and $c_1^- = 0$. This leaves the coefficients c_0^\pm still undetermined. They can be obtained as

$$c_0^+ = \frac{\Delta}{2-\alpha} \int_0^\infty dy y^{\alpha-2} [f'_G(y) - f'_G(0) - yf''_G(0)] , \quad (3.4)$$

$$c_0^- = \frac{-\Delta}{2-\alpha} \int_{-\infty}^0 dy (-y)^{\alpha-2} [f'_G(y) - f'_G(0) - yf''_G(0)] . \quad (3.5)$$

Here α is the specific heat critical exponent, which is negative in the three dimensional $O(4)$ universality class.

The coefficients a_n for all n and c_n , for $n > 0$, are obtained from a parametrization of the scaling function of the order parameter. The relevant expansion coefficients b_n , b_n^\pm and d_n^\pm have been obtained from numerical data for the order parameter itself as well as its susceptibility [9]. In this step one explicitly makes use of a set of values for critical exponents in the three dimensional $O(4)$ universality class. We used: $\beta = 0.380$ and $\delta = 4.824$. All other critical exponents can be derived using hyperscaling relations. E.g., the specific heat exponent is given by, $\alpha = -0.213$. We list the resulting expansion coefficients in Table 1 and 2. Note that we give different expansion coefficients b_n^+ and b_n^- for $n \geq 4$ to better reproduce the asymmetric form of the scaling function $f_G(z)$ also for small values of z with only a small number of expansion coefficients. The corresponding scaling function of the order parameter and its first derivative is shown in Fig. 1.

Having at hand a parametrization of $f_G(z)$ we finally can determine the remaining coefficients c_0^\pm , which complete the parametrization of $f_f(z)$. These expansion coefficients are listed in Table 3.

d_0^+	d_1^+	d_2^+
1.10599 ± 0.00555	-1.31829 ± 0.1087	1.5884 ± 0.4646
d_0^-	d_1^-	d_2^-
1	0.273651 ± 0.002933	0.0036058 ± 0.004875

Table 2: Coefficients for the asymptotic series expansions of $f_G(z)$ in the region of large positive and negative z -values, respectively.

4. Discussion and Conclusions

The availability of high accuracy numerical data on the order parameter and its susceptibility in a three dimensional, $O(4)$ symmetric spin model allowed us to extract the underlying scaling

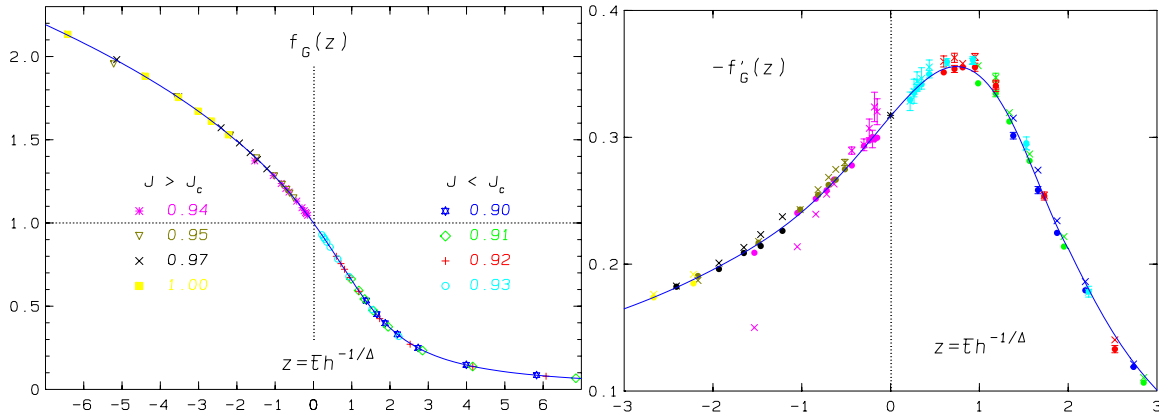


Figure 1: The scaling function of the order parameter (left) and its derivative (right).

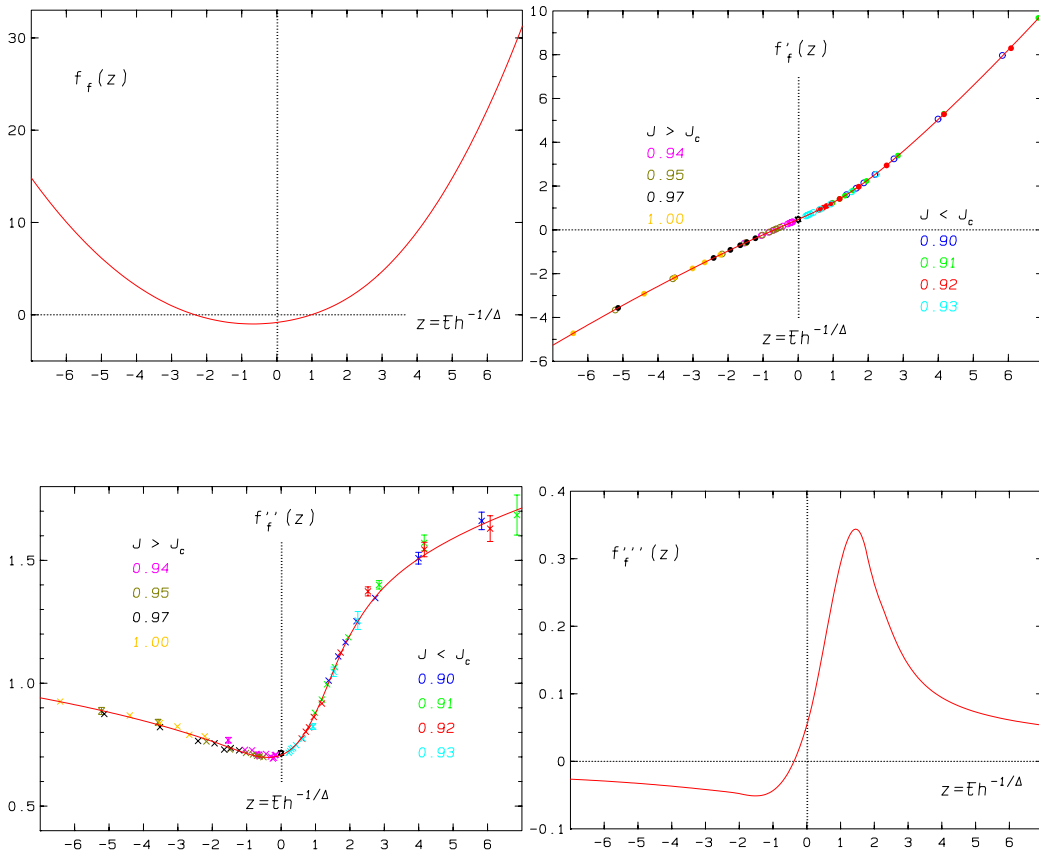


Figure 2: The scaling function of the free energy density and its first three derivatives.

c_0^+	c_0^-
0.422059886 ± 0.010595	0.229176194 ± 0.010669

Table 3: The leading expansion coefficients for the singular part of the free energy density.

function of the free energy density and its first three derivatives. As the specific heat exponent α is negative in the 3d $O(4)$ universality class, it is only the third derivative with respect to temperature, which diverges at the critical point. The corresponding scaling function $f_f'''(z)$ has two extrema; a rather shallow minimum in the symmetry broken phase and a pronounced maximum in the symmetric phase. The latter is located at $z_p^{3,0} \simeq 1.45$. This happens to be close to the location of the peak in the susceptibility of the order parameter, $z_p^{0,2} = 1.374(3)$.

The higher order derivatives of the scaling function of the free energy density play a central role in the discussion of fluctuations of conserved charges in QCD, e.g. the singular behavior of the $2n$ -th order cumulant of net baryon number fluctuations is related to the n -th derivative of $f_f(z)$. The change of sign of $f_f'''(z)$ and its pronounced maximum characterize the QCD transition. In fact, the change of sign of $f_f'''(z)$ suggests that 6th order cumulants of net baryon number are negative in the vicinity of the QCD transition line. This may be detectable in a heavy ion collision, if the production of hadrons (freeze-out) occurs at temperatures and baryon chemical potentials that are close to the QCD crossover transition line.

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