A numerical study of Goldstone-mode effects and scaling functions of the three-dimensional $O(2)$ model

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We investigate numerically the three-dimensional $O(2)$ model on $8^3 - 160^3$ lattices as a function of the magnetic field $H$. In the low-temperature phase we verify the $H$-dependence of the magnetization $M$ induced by the Goldstone modes and determine $M$ in the thermodynamic limit on the coexistence line both by extrapolation and by chiral perturbation theory. We compute two critical amplitudes from the scaling behaviours on the coexistence line and on the critical line. In both cases we find negative corrections to scaling. With additional high temperature data we calculate the scaling function and show that it has a smaller slope than that of the $O(4)$ model. For future tests of QCD lattice data we study as well finite-size-scaling functions.

1. INTRODUCTION

$O(N)$ models are of general relevance to condensed matter physics and to quantum field theory, because many physical systems exhibit a second-order phase transition with the same universal properties. Due to the existence of massless Goldstone modes in $O(N)$ models with $N > 1$ and dimension $d = 3$ and $4$ singularities are expected on the whole coexistence line $T < T_c, H = 0$, in addition to the known critical behaviour at $T_c$. Recently these predictions have been confirmed by simulations of the 3d $O(4)$ model \cite{2}. A further motivation for studying 3d $O(N)$ models is their relation to quantum chromodynamics (QCD). The QCD chiral phase transition for two light-quark flavors is supposed to be of second order in the continuum limit and to be in the same universality class as the 3d $O(4)$ model \cite{3}. In the staggered formulation of QCD on the lattice a part of chiral symmetry is remaining and that is $O(2)$. For the comparison to QCD lattice data it is therefore important to know the $O(2)$ and $O(4)$ universal scaling functions.

The $O(2)$-invariant nonlinear $\sigma$-model (or $XY$ model) on a $d$-dimensional hypercubic lattice is defined by

$$\beta H = -J \sum_{i,j} S_i \cdot S_j - H \cdot \sum_i S_i .$$

(1)

$S_i$ is an 2-component unit vector at site $i$ with a longitudinal (parallel to the magnetic field $H$) and a transverse component

$$S_i = S_i^\parallel \hat{H} + S_i^\perp .$$

(2)

The order parameter of the system, the magnetization $M$, is given by

$$M = < \frac{1}{V} \sum_i S_i^\parallel > = < S^\parallel > .$$

(3)

There is a longitudinal and a transverse susceptibility

$$\chi_L = \frac{\partial M}{\partial H} = V(< S^\parallel^2 > - M^2) ,$$

(4)

$$\chi_T = V < S^\perp^2 > = \frac{M}{H} .$$

(5)

In the broken phase ($T < T_c$) the magnetization attains a finite value $M(T,0)$ at $H = 0$. Consequently the transverse susceptibility diverges as $H^{-1}$ when $H \to 0$ for all $T < T_c$. It is non-trivial that also the longitudinal susceptibility is diverging on the coexistence line for $2 < d \leq 4$. The predicted \cite{4} divergence for $d = 3$ is

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

(6)
which is equivalent to an $H^{1/2}$-behaviour of the magnetization near the coexistence curve

$$M(T < T_c, H) = M(T, 0) + cH^{1/2}. \quad (7)$$

In finite volumes and $H \to 0$ the Goldstone modes induce strong finite-size effects at all $T < T_c$.

2. NUMERICAL RESULTS

Our simulations were done on three-dimensional lattices with periodic boundary conditions and linear extensions $L = 8 - 160$ using the cluster algorithm. In order to eliminate finite-size effects we simulated for increasingly larger values of $L$ at fixed values of $J = 1/T$ (i.e. fixed temperature $T$) and $H$. For $1/T_c$ we took the value $J_c = 0.454165(4)$ from Ref. [5].

In Fig. 1 we show the data for the magnetization as a function of $H^{1/2}$ for six fixed values of $J$ in the low-temperature phase. The picture is rather similar to the one obtained in $O(4)$ [2]: strong finite-size effects appear for small $H$ and persist as one moves away from $T_c$, the results from the largest lattices are at first sight linear in $H^{1/2}$, as predicted by Eq. 7. Very close to $H = 0$ the fixed temperature curves become slightly flatter, leading to a higher value for $M(T, 0)$ than expected from the data at larger $H$ values. This behaviour is more pronounced close to $T_c$ than at lower temperatures.

In order to extrapolate the data to $H \to 0$ and $V \to \infty$ we apply two different strategies. The first is to extend the linear form in $H^{1/2}$, Eq. 7, to a quadratic one

$$M(T < T_c, H) = M(T, 0) + c_1 H^{1/2} + c_2 H, \quad (8)$$

and to fit the data from the largest lattices, which we assume to represent data on an infinite volume lattice, to this form. The second way to find $M(T, 0)$ is just opposite to the first. Here we exploit the $L$ or volume dependence at fixed $J$ and fixed small $H$ to determine via chiral perturbation theory (CPT) [6] the magnetization $\Sigma$ of the continuum theory for $V \to \infty$, $H = 0$, which is related to $M(T, 0)$ by

$$M(T, 0) = \frac{\Sigma}{\sqrt{J}}. \quad (9)$$

We observe in Fig. 1 a remarkable coincidence of the fits according to Eq. 8 (dashed lines) with the CPT results at $H = 0$ (filled circles). In the neighbourhood of $T_c$ the results for $M(T, 0)$ should show the usual critical behaviour. Since we expect here sizeable corrections to scaling [7] we make the following ansatz to determine the critical amplitude $B$ ($\bar{t} = T_c - T$)

$$M(T \lesssim T_c, 0) = B\bar{t}^{\beta} [1 + b_1 \bar{t}^{\omega\nu} + b_2 \bar{t}]. \quad (10)$$

Here and in the following we use the critical exponents from Ref. [6].

Figure 1. The magnetization vs. $H^{1/2}$ in the low-temperature region for fixed $J$ and various $L$. 
3. THE SCALING FUNCTION

In the thermodynamic limit, the dependence of the magnetization on temperature and magnetic field can be expressed \[ M = h^{1/\delta} f_G(t/h^{1/\delta}) \],

where \( f_G \) is a universal scaling function and \( t \) and \( h \) are normalized reduced temperature \( t = (T - T_c)/T_0 \) and magnetic field \( h = H/H_0 \). Here \( H_0 = d_c^{-\delta} = 1.11(1) \), \( T_0 = B^{-1/\beta} = 1.18(2) \), which implies \( f_G(0) = 1 \) and \( f_G(t < 0, h \to 0) \to (-t)^{\beta} h^{-1/\delta} \). Obviously, \( f_G \) does not account for possible corrections to scaling and is the leading term in the Taylor expansion in \( h^{\omega c} \) of a more general form

\[ M h^{-1/\delta} = \Psi(t h^{-1/\delta}, h^{\omega c}) \].

We therefore perform quadratic fits to our data in \( h^{\omega c} \) at fixed values of \( t h^{-1/\delta} \) in the low-temperature region, where the corrections are strong. In the high-temperature region the data scale directly. In Fig. 3 we have plotted \( M h^{-1/\delta} \) from data with \( H \leq 0.0075 \) and \( 0.43 < J < 0.55 \) and the final result for the scaling function \( f_G \).

An alternative scaling form is that of Widom and Griffiths. It is discussed in Ref. [8], where more
Figure 4. (a) $ML^{\beta/\nu}$ from reweighted data from lattices with different $L$ (solid lines) and the scaling function $Q_0$ (dashed line) at $z = 0$. (b) Comparison of $\ln Q_0$ to its asymptotic value (line).

details of our calculations can be found.

In Ref. [9] staggered lattice QCD data for $N_f = 4$ were compared to the $O(4)$ scaling function. The test failed because the data were indicating a steeper scaling function. Since the $O(2)$ scaling function is even flatter than the one for $O(4)$, as can be seen from the inset of Fig. 3, the situation will be worse there. A way out may be the comparison to finite-size-scaling functions, since lattice QCD is presumably far from the thermodynamic limit.

3.1. Finite-size-scaling functions

The general form of the finite-size-scaling function for the magnetization is given by

$$M = L^{-\beta/\nu} Q_0(z L^{1/\nu^*}) + \ldots ,$$

where $Q_0$ is a universal function. Examples of lines of fixed $z$ are the critical line where $z = 0$ and the pseudocritical line, the line of maximum positions of the susceptibility $\chi_L$ in the $(t, h)$-plane for $V \to \infty$. The scaling function contains also all information about $\chi_L$, because

$$\chi_L = \frac{\partial M}{\partial H} = \frac{h^{1/\nu - 1}}{H^0} \left( f_G(z) - \frac{z}{\beta} f'_G(z) \right) .$$

Evidently, the maximum of $\chi_L$ at fixed $h$ and varying $t$ is at the maximum point $z_p$ of the function in the brackets of Eq. (18). $z_p$ is again a universal quantity and we find $z_p = 1.556 \pm 0.10$ from (18). As a check we have also determined the peak positions on lattices with $L = 24 - 96$ which extrapolate to $z_p = 1.65 \pm 0.10$ for $L \to \infty$. In Fig. 4a we show $ML^{\beta/\nu}$ from the reweighted data on the critical line for various $L$ values and also the scaling function $Q_0(z = 0)$. For $L \to \infty$ the scaling function $Q_0$ is related to $f_G$ by

$$Q_0 \to f_G(z)(h L^{1/\nu^*})^{1/\delta} .$$

From Fig. 4b we see that $Q_0(z = 0)$ seems to be asymptotic in the whole variable range considered. At present we investigate the case $z = z_p$.

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