

On the universal critical behavior in 3-flavor QCD

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We analyze the universal critical behavior at the chiral critical point in QCD with three degenerate quark masses. We confirm that this critical point lies in the universality class of the three dimensional Ising model. The symmetry of the Ising model, which is $Z(2)$, is not directly realized in the QCD Hamiltonian. After making an ansatz for the magnetization- and energy-like operators as linear admixtures of the chiral condensate and the gluonic action, we determine several non-universal mixing and normalization constants. These parameters determine an unambiguous mapping of the critical behavior in QCD to that of the 3d-Ising model. We verify its validity by showing that the thus obtained orderparameter scales in accordance with the magnetic equation of state of the 3d-Ising model.

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1. Introduction

A detailed understanding of the phase structure of strongly interacting matter at non-zero temperature and density is one of the major tasks for non-perturbative lattice QCD simulations. It has been conjectured based on renormalization group arguments [1] and verified in numerical calculations [2, 3] that the QCD phase transition with three degenerate quarks flavors is of first order for small masses. This also holds for two light quarks and one heavier strange quark, if the strange quark mass is kept below a critical value. The line that separates the first order region from the crossover region is a critical line on which the nature of QCD phase transition is of second order [4]. It is an open and interesting question how close the critical line passes the physical point, where we know that the QCD transition is a crossover [5]. In fact, recent lattice calculations suggest that the first order region dramatically shrinks with the approach of the continuum limit [6, 7].

In this work we restrict ourselves to three degenerate quark masses. Within this theory the critical point – the endpoint of the line of first order transitions – has been determined before, with standard staggered fermions on $N_\tau = 4$ lattices [2, 3] and on $N_\tau = 6$ lattices [7]. Our analysis is also based on simulations with standard staggered fermions (and the standard Wilson gauge action) on $N_\tau = 4$ lattices. We repeat the determination of the critical endpoint with larger spatial lattice sizes. Moreover we focus on the determination of the correct scaling operators and variables that allow for the mapping of the QCD critical behavior onto the corresponding universality class, which is here the 3-dimensional Ising model. The construction of the operators and fields is done along the line of [2, 8].

For our simulation we use an exact RHMC algorithm [9], which we have implemented to run entirely on GPUs. In other words, all calculations that involve spinors or gauge fields are done on the GPU, whereas the CPU is only used to control the I/O and program flow. The HMC trajectory is done in a mixed-precision manner: the force and evolution calculations are done in single precision, which is corrected by a Metropolis step in double precision. The expectation values which we obtain for the chiral condensate and the plaquette are shown in Fig. 1. In order to analyze the finite size scaling behavior we have performed simulations on spatial volumes of 16^3 , 24^3 in some cases also 32^3 . For each coupling $\beta = 6/g^2$ we have generated between 5000 and 10000 configurations that are separated by 20 RHMC updates. For the bare quark masses, we picked values in the range of $0.024 < am < 0.034$. From Fig. 1 one can already see that the transition becomes stronger for smaller quark masses.

2. Z(2) critical behavior

The dynamics and universal critical behavior of the 3d-Ising model is – as in all generic O(N) models – characterized by two relevant scaling variables. Close to the critical point we thus can assume that the Hamiltonian takes the effective form

$$H_{\text{eff}}(t, h) = tE + hM, \quad (2.1)$$

where t and h are the relevant scaling variables and E, M the corresponding scaling operators. In analogy to a classical spin system we will refer to the fields as reduced temperature and external field, and denote the operators as energy and magnetization.

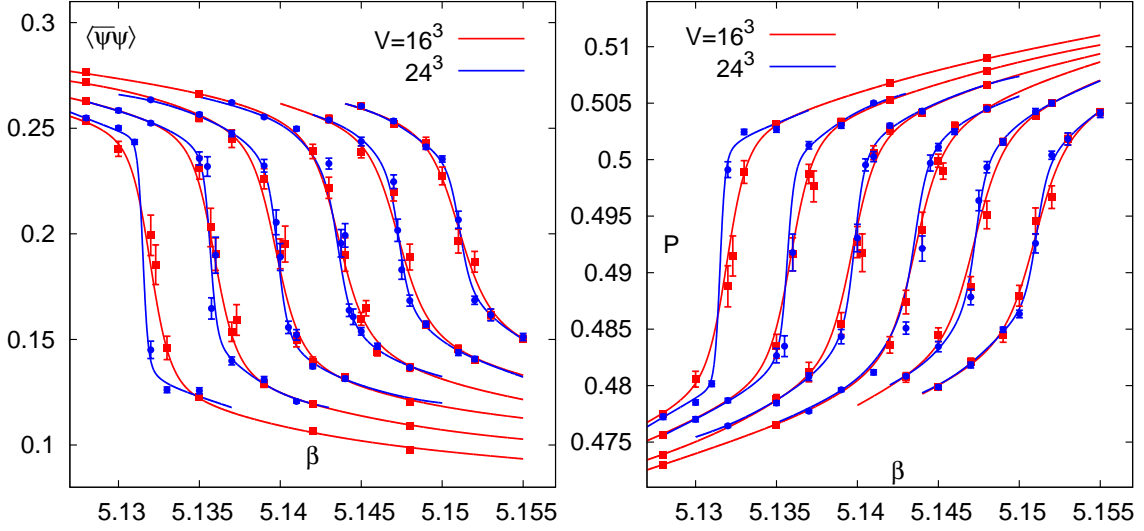


Figure 1: The chiral condensate (left) and the plaquette expectation values for different bare quark masses as a function of the coupling $\beta = 6/g^2$. The values of the bare quark masses are $am = 0.024, 0.026, 0.028, 0.030, 0.032, 0.034$ (from left to right).

Under a renormalization group transformation the singular part of the free energy scales as

$$f_s(t, h) = b^{-3} f_s(b^{y_t} t, b^{y_h} h). \quad (2.2)$$

The dimensionless scale factor b is arbitrary. From here immediately all known scaling and hyperscaling relations follow. Especially the standard finite size scaling behavior (choosing $b = LT = N_\sigma/N_\tau$) of the susceptibilities is given by

$$V^{-1} \langle (\delta E)^2 \rangle \sim L^{\alpha/\nu}, \quad V^{-1} \langle (\delta M)^2 \rangle \sim L^{\gamma/\nu} \quad \text{with} \quad \delta X = X - \langle X \rangle. \quad (2.3)$$

Here L denotes the spatial extent of the system and α, γ, ν are the critical indices that characterize the universality class. In order to map the QCD critical behavior to the $Z(2)$ critical behavior we construct the scaling operators from the operators appearing in the QCD Lagrangian by employing the following linear ansatz [2]

$$E = S_G + r\bar{\psi}\psi, \quad M = \bar{\psi}\psi + sS_G. \quad (2.4)$$

Here S_G denotes the Wilson gauge action and $\bar{\psi}\psi$ the chiral condensate. Similarly, we linearize the scaling fields in the vicinity of the critical point (β_c, m_c) by assuming

$$t = t_0((\beta - \beta_c) + A(m - m_c)), \quad h = h_0((m - m_c) + B(\beta - \beta_c)). \quad (2.5)$$

The mixing parameters of the scaling operators and fields: r, s, A, B as well as the normalization constants t_0, h_0 have to be determined from the QCD simulations. Although there is no apparent reason, we assume in the following the directions t and h as orthogonal, which relates A and B by $A = \tan(\phi) = -B$, where ϕ is the rotation angle between the β and the t direction.

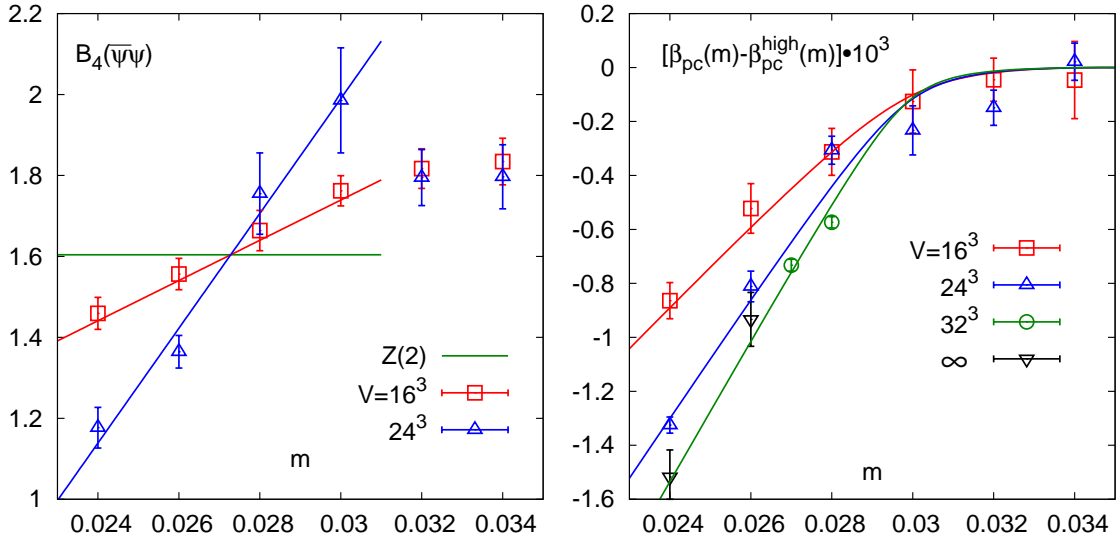


Figure 2: The fourth order Binder cumulant of the chiral condensate (left) and the pseudo-critical coupling from the peak position of the disconnected chiral susceptibility (right).

3. Locating the critical point

The first step to establish the correct scaling operators and fields in the 3-flavor QCD case is the location of the critical point. It has been shown [2] that a good method to do so is by analyzing Binder cumulants. The Binder cumulant of the order parameter is defined by

$$B_4(M) = \langle (\delta M)^4 \rangle / \langle (\delta M)^2 \rangle^2. \quad (3.1)$$

From the scaling behavior of the free energy (2.2) it follows immediately that the Binder cumulant is volume independent at the critical point. Moreover, its value at the critical point is universal. Furthermore, we can conclude from (2.2) that close to the critical point it is not mandatory to analyze the Binder cumulant of the correct order parameter. As long as the operator of consideration has non-vanishing overlap with M , the strongest singularity corresponding to $L^{1/\nu}$ will dominate and the correct universal value of B_4 is obtained. This means that in our analysis of Binder cumulants we can choose the mixing parameter s arbitrarily¹. In Fig. 2 (left) we plot the Binder cumulant of the chiral condensate ($s = 0$) along the pseudo-critical line. *I.e.* for each mass we evaluate B_4 at the pseudo-critical coupling $\beta_{pc}(m)$ which we have determined from the peak position of the chiral susceptibility. The two volumes $V = 16^3$ and 24^3 clearly suggest an intersection point close to the universal value of the 3d-Ising model, which is $B_4^{\text{Ising}} = 1.604$. We can thus confirm that the critical point lies in the $Z(2)$ universality class. Furthermore, we obtain for the intersection point of the 16^3 -lattice with the universal Ising value a mass value of $am_c = 0.0268(6)$, which is in good agreement with the previously obtained value from RHMC simulations $am_c = 0.0263(3)$ [4]. Combining the results of the 24^3 , and 16^3 -lattices into a common fit that restricts the intersection point of the two volumes to Ising universal value, we obtain a critical mass of $am_c = 0.0273(4)$.

¹As long as we have not $s = 1/r$, where the leading order singularity exactly cancels.

This fit is shown as straight lines in Fig. 2 (left). For both of the above described fits we restrict the fitting range to $am \in [0.024, 0.030]$. Larger quark masses do not seem to fall into the scaling region, as the data does not follow the approximate linear behavior for $am \geq 0.032$.

In Fig. 2 (right) we show the pseudo critical couplings for different volumes as function of mass. For better visibility we have subtracted the linear function $\beta_{pc}^{\text{high}}(am) = 1.8281 \cdot am + 5.0889$ and multiplied the differences by 10^3 . We see that for large masses ($am > am_c$) the pseudo critical couplings seem to be volume independent within errors, whereas at sub-critical masses we observe a distinct scaling with the volume. Assuming that the two masses $am = 0.024$ and 0.026 lie in the first order region we perform to extrapolations of the pseudo critical couplings to the thermodynamic limit, using $\beta_{pc}(N_\sigma) = \beta_c(\infty) + cN_\sigma^{-3}$. Here c is a constant that we fit. We find that the infinite volume can, to a good approximation, already be described by the 32^3 -lattices. For $am < am_c$ we obtain a parameterization of the critical couplings in the thermodynamic limit as a function of the quark mass, as $\beta_c(am) = 2.12(3) \times (am - 0.0268)5.1372(1)$. This is by definition a parameterization of the (negative) t-axis. We can thus obtain a value of the mixing parameter B through the relation

$$B^{-1} = - \left. \frac{\partial \beta_c(am)}{\partial (am)} \right|_{am=am_c}, \quad (3.2)$$

which arises due to the fact that in the Ising model the line of first order phase transitions defines the temperature direction. We estimate $B = -0.47(1)$. Assuming that the scaling directions are orthogonal, this also determines the parameter A .

4. The mixing parameters r and s

So far we have determined the critical point as well as the proper scaling directions. Before we can consider the magnetic equation of state we still have to clarify the correct order parameter M through the determination of the mixing parameter s . We fix s by demanding that the linear combination $M = \bar{\psi}\psi + sS_G$ fulfills basic properties of an order parameter, namely that M vanishes at the critical point and stays zero for $t > 0, h = 0$. While the former condition is easy to fulfill and yields a mixing parameter $s = 0.048(2)$, the latter condition is equivalent with the fact that energy and magnetization operators are statistically independent:

$$\langle (\delta M)(\delta E) \rangle = 0. \quad (4.1)$$

Using this relation together with the definition of the scaling operators (2.4) and directions (2.5), we obtain the following conditions for the mixing parameters:

$$r = -B \quad \text{and} \quad s = \frac{\langle (\delta \bar{\psi}\psi)(\delta S_G) \rangle - B \langle (\delta \bar{\psi}\psi)^2 \rangle}{\langle (\delta S_G)^2 \rangle - B \langle (\delta \bar{\psi}\psi)(\delta S_G) \rangle}. \quad (4.2)$$

As one can see, we require as input the already determined mixing parameter B , as well as the susceptibilities and mixed susceptibilities of the QCD operators $\bar{\psi}\psi$ and S_G . As susceptibilities are usually much more difficult to determine, the error on the mixing parameter s is much larger using this condition. Moreover, the value for the mixing parameter we obtain from Eq. (4.2) is $s = -0.8(1)$, which is very different from the previously obtained value. We conclude that with

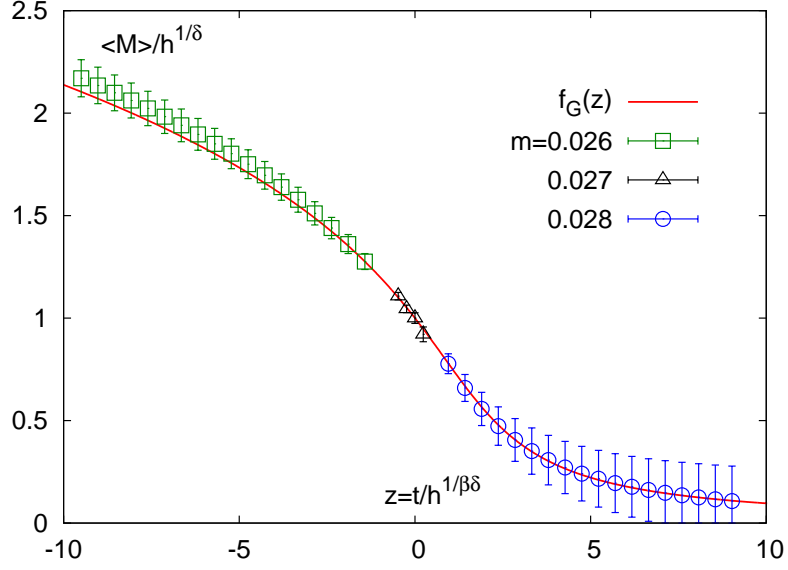


Figure 3: The rescaled order parameter M as function of the scaling variable z .

our ansatz for M we cannot at the same time obtain a very flat behavior for $M(t)$ at $t > 0$ and demand that $M(t)$ vanishes at $t = 0$. This is most likely due to the finite volume effects that are still present in the 24^3 -lattices close to the critical point. We note, that we can obtain a good fit to the magnetic equation of state as described in the next section with both values of s . However, as long as M does not vanish at the critical point, one is forced to keep the leading order contribution from the regular part of the free energy. This will contribute a constant value to M and lead to the desired behavior of the order parameter.

5. Magnetic equation of state

Close to the critical point, where all regular contributions to the free energy become negligible, it follows from (2.2) that the singular part of the free energy can be expressed as a function of the single scaling parameter $z = t/h^{1/\delta}$ (by setting the scale parameter b to $b = h^{-y_h}$). For the order parameter (magnetization), which is the derivative of the free energy with respect to the symmetry breaking field h , one then obtains

$$M(t, h) = h^{1/\delta} f_G(z). \quad (5.1)$$

This relation is known as the magnetic equation of state. The scaling function $f_G(z)$ is unique to the universality class. In the following we use the parameterization as derived in Ref. [10]. In order to obtain the last two missing normalization constants t_0 and h_0 , we fit our data for the order parameter M in the range of $0.026 \leq am \leq 0.028$ to the magnetic equation of state. Using $s = 0.048$, $am_c = 0.0268$ and $\beta_c = 5.1372$ we obtain $t_0 = 0.0210(9)$ and $h_0 = 0.0005(1)$. In Fig. 3 we plot the rescaled order parameter $M/h^{1/\delta}$ as a function of the scaling parameter z . We find good scaling behavior within the range of $-10 \leq z \leq 10$.

6. Outlook

In our future work we will address the question whether the good scaling behavior of our constructed order parameter can also be observed in corresponding susceptibilities. Of special interest will be not only the chiral susceptibility but also the mixed susceptibility that contains the response to the variation of a small chemical potential ($\partial^2 \ln Z / \partial \mu \partial h \equiv \partial M / \partial \mu$). From this susceptibility we will be able to determine the curvature of the critical surface that is defined by the extension of the critical line in the quark mass plane towards non-zero chemical potentials.

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