PROCEEDINGS OF SCIENCE

Towards a parameter-free determination of critical exponents and chiral phase transition temperature in QCD

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In order to quantify the universal properties of the chiral phase transition in (2+1)-flavor QCD, we make use of an improved, renormalized order parameter for chiral symmetry breaking which is obtained as a suitable difference of the 2-flavor light quark chiral condensate and its corresponding light quark susceptibility. Having no additive ultraviolet as well as multiplicative logarithmic divergences, we use ratios of this order parameter constructed from its values for two different light quark masses. We show that this facilitates determining in a parameter-independent manner, the chiral phase transition temperature T_c and the associated critical exponent δ which, for sufficiently small values of the light quark masses, controls the quark mass dependence of the order parameter at T_c. We present first results of these calculations from our numerical analysis performed with staggered fermions on $N_\tau = 8$ lattices.

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1. Introduction

One of the outstanding questions in the study of the phase diagram of strong-interaction matter is whether or not, the effective restoration of the axial anomaly has an influence on the universal properties of the Quantum Chromodynamics (QCD) chiral phase transition. It has been argued [1] that a first order phase transition may occur in QCD with two light quarks, if the axial anomaly is effectively restored in the limit of vanishing up and down quark masses. Moreover in the case of three light quark flavors, the chiral phase transition should be first order irrespective of the temperature dependence of the chiral anomaly.

More recently, it has been shown that in the case of two light flavors, it still would be possible to have a second order phase transition belonging to the 3-dimensional $U(2) \times U(2)$ universality class even, when the axial $U(1)_A$ symmetry gets restored in the chiral limit [2]. This is in contrast to universal critical behavior in the 3-dimensional, $O(4)$ universality class which, one would expect to control the thermodynamics of QCD in the limit of vanishing two light quark masses (2- or (2+1)-flavor QCD), if the axial anomaly does not get restored. Here we aim at a first principle lattice QCD analysis of universal critical behavior in QCD with two light, degenerate up and down quarks and a heavier strange quark mass tuned to its physical value. This does build on earlier studies of the magnetic equation of state in (2+1)-flavor QCD using staggered fermion discretization schemes [3–5].

Even when the chiral phase transition in QCD belongs to the 3-dimensional, $O(4)$ universality class, it is an open question to which extent this is reflected in the thermodynamic properties of QCD with its physical spectrum of light and strange quark masses. In order to address this question, a detailed analysis is needed regarding the temperature and quark mass dependence of e.g. the chiral order parameter and its susceptibility in a narrow temperature interval in the vicinity of the chiral phase transition temperature. This will allow us to disentangle the universal critical behavior, which eventually shows up as divergence of higher order derivatives of the free energy, and the non-critical universal correction-to-scaling as well as regular contributions to thermodynamic quantities. It will also allow us to quantify the size of the scaling regions relevant for different physical observables [6, 7] and thus, will provide crucial input to the interpretation of experimentally measured observables, e.g. higher order cumulants of net-baryon number fluctuations and the correlations between different conserved charges [8].

2. Scaling behaviour and scaling functions

2.1 Theoretical background

We give here, some background for our study of the universal structure of thermodynamic observables in the vicinity of the chiral phase transition in $(2+1)$-flavor QCD. The relevant quantities of interest are the 2-flavor light quark chiral condensate, M_ℓ and the corresponding chiral susceptibility χ_ℓ, which is obtained as the derivative of the light quark chiral condensate with respect to the light quark mass m_ℓ,

$$M_\ell = \frac{m_s}{f_K^4} \left\langle \bar{\psi}\, \psi \right\rangle , \qquad \chi_\ell = m_s \frac{\partial M_\ell}{\partial m_\ell} , \tag{1}$$

where factors of the strange quark mass, m_s, are introduced as multiplicative renormalization factors and the kaon decay constant, f_K, is used to obtain dimensionless quantities. The chiral condensate M_ℓ still requires additive renormalization in order to arrive at an order parameter for chiral symmetry breaking that is well defined in the continuum limit. The ultraviolet divergent contributions to M_ℓ may be eliminated by subtracting a suitable fraction of χ_ℓ. We therefore introduce as an order parameter for chiral symmetry breaking, the difference

$$M(T,H) = M_\ell(T,H) - H\,\chi_\ell(T,H)\ , \tag{2}$$

with H given as the ratio of light and strange quark masses, $H \equiv m_\ell/m_s$. It is obvious from the definition of χ_ℓ given in Eq. 1 that terms linear in m_ℓ are explicitly eliminated in $M(T.H)$. In the vicinity of the chiral limit this order parameter thus receives only light quark mass corrections that are proportional to H^3. We also note that we treat the strange quark mass just like f_K as an external parameter, that is tuned to its physical value by demanding that the mass of the pseudoscalar meson, $\eta_{\bar{s}s}$, is fixed to its physical value. The corresponding line of constant physics has been introduced in [9]. This version of a renormalized order parameter has been introduced in [10] and has been used previously to analyze critical behavior in lattice QCD calculations [5, 6, 11]. In the vicinity of the chiral critical point, $(T,H) = (T_c, 0)$, the temperature and quark mass dependence of this version of an order parameter is controlled by a scaling function, which is given by the difference of the commonly introduced order parameter scaling function, $f_G(z)$ and the corresponding susceptibility scaling function, $f_\chi(z)$. Near the critical point, these scaling functions control the universal critical behavior of the unrenormalized order parameter M_ℓ and its susceptibility, respectively,

$$M_\ell(T,H) = h^{\frac{1}{\delta}}\, f_G(z) + M_{\ell,\,sub-lead}(T,H)\ , \tag{3}$$

$$\chi_\ell(T,H) = \frac{1}{\delta}\, h^{\frac{1}{\delta}-1}\, f_\chi(z) + \chi_{\ell,\,sub-lead}(T,H)\ . \tag{4}$$

Here δ is the critical exponent, controlling the dependence of the order parameter as function of the symmetry breaking parameter H at $T = T_c$, *i.e.* $M(T_c, H) = h^{1/\delta}$, with $h = H/h_0$ and h_0 denoting a non-universal constant. Close to the critical point, the T and H dependence of M is controlled by a single scaling variable,

$$z = t\, h^{-1/\beta\delta}, \qquad \text{where} \quad t = \frac{1}{t_0}\left[\frac{T}{T_c} - 1\right], \quad h = \frac{H}{h_0}\ , \tag{5}$$

with t_0 denoting another non-universal constant. In addition to the leading non-analytic (so-called singular) behavior, the order parameter receives corrections arising from sub-leading universal corrections-to-scaling as well as analytic, non-universal terms. We denote both of them as sub-leading corrections. The leading, singular behavior of the order parameter M is then described by,

$$M(T,H) = h^{1/\delta} f_{G\chi}(z) + \text{ sub} - \text{lead.}\ , \quad \text{with} \ \ f_{G\chi}(z) = f_G(z) - f_\chi(z)\ . \tag{6}$$

Using the relation $f_\chi(z) = \delta^{-1}\left(f_G(z) - z f'_G(z)/\beta\right)$, with β denoting a critical exponent, we have

$$f_{G\chi}(z) = \left(1 - \frac{1}{\delta}\right) f_G(z) + \frac{z}{\beta\delta}\, f'_G(z)\ , \tag{7}$$

and in particular, $f_{G\chi}(0) = 1 - 1/\delta$.

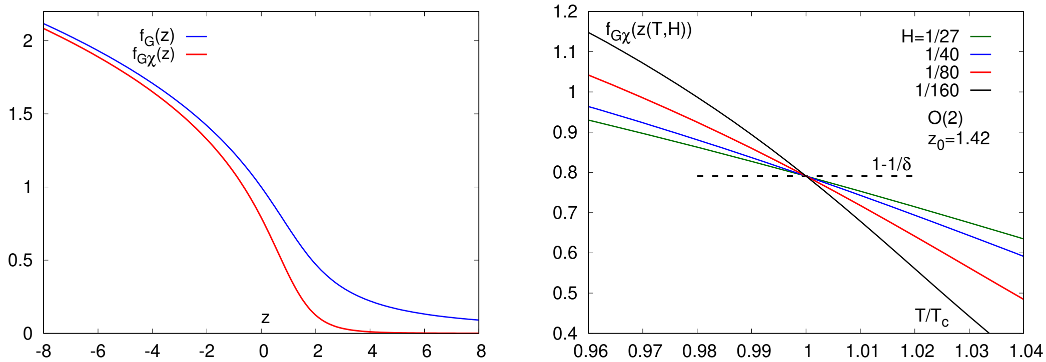

Figure 1: *Left:* The 3-d, $O(2)$ scaling functions $f_G(z)$ and $f_{G\chi}(z)$ as function of scaling variable z. *Right:* The 3-d, $O(2)$, scaling function $f_{G\chi}(z)$ versus T/T_c for an arbitrary non-universal parameter value, $z_0 = 1.42$.

The universal scaling functions $f_G(z)$ and $f_\chi(z)$ have been determined for several universality classes. For a recent parametrization, see for instance [12]. These scaling functions differ in detail, but show qualitatively similar behavior. E.g. the value of $f_G(z)$ and as such also of $f_{G\chi}(z)$ at $z = 0$ directly gives the critical exponent δ and both scaling functions have a unique intersection point at $z = 0$ when plotted versus T for different values of H. In Fig. 1 (left), we show the scaling functions $f_G(z)$ and $f_{G\chi}(z)$ for the 3-dimensional $O(2)$ universality class, which is most relevant for the current scaling analysis performed by us at a single finite lattice cut-off corresponding to lattices with temporal extent $N_\tau = 8$. In the right hand part of Fig. 1, we show $f_{G\chi}(z)$ as function of T/T_c for several values of H. The choice for the latter corresponds to light-to-strange quark mass ratios used previously also in a determination of the chiral phase transition temperature in $(2+1)$-flavor QCD [13]. To draw this figure, we used for the non-universal scale parameter $z_0 = h_0^{1/\beta\delta}/t_0$, the value 1.42, which has been determined in a previous scaling analysis of the order parameter M [5]. However, obviously the qualitative features seen in Fig. 1 (right) do not depend on this particular choice.

2.2 Universal order parameter ratios

From Eq. 6, one obtains the rescaled order parameter

$$M(T,H)/H^{1/\delta} = h_0^{-1/\delta} f_{G\chi}(z) + \text{sub} - \text{lead.}\,, \tag{8}$$

which allows to determine the chiral phase transition temperature from the unique intersection point, once the sub-leading corrections are sufficiently small. Its construction, however requires known knowledge of the relevant universality class, *i.e.* the critical exponent δ. To avoid the need for this input, we construct ratios of the chiral order parameter evaluated for H-values that differ by a factor c, like

$$R(T,H,c) = \frac{M(T,cH)}{M(T,H)}\,. \tag{9}$$

Obviously also these ratios, evaluated for different values of H, have a unique intersection point at T_c once the sub-leading corrections become negligible. We may use these ratios to obtain directly the critical exponent δ at this intersection point. We introduce

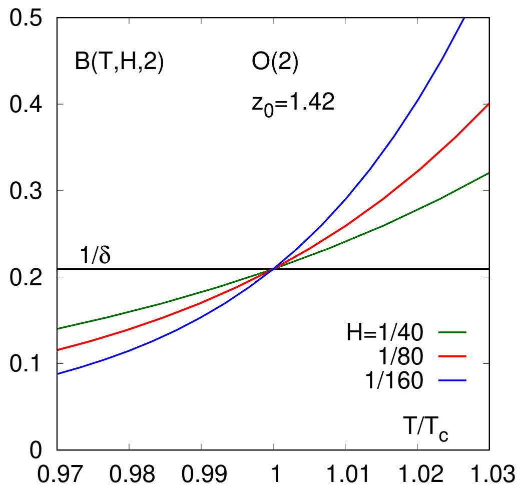

Figure 2: Logarithm of the ratio of order parameters, $B(T, H, c)$, as defined in Eq. 10 versus T/T_c. Shown is the result obtained in the 3-dimensional $O(2)$ universality class for $c = 2$ and the non-universal scale $z_0 = 1.42$.

$$B(T, H, c) \quad = \quad \frac{\ln R(T, H, c)}{\ln(c)} \ . \tag{10}$$

This ratio is shown in Fig. 2 for the 3-dimensional $O(2)$ universality class using the scaling functions shown in Fig. 1. In the chiral limit one finds at T_c,

$$\lim_{H\to 0} B(T_c, H, c) = \frac{1}{\delta} \ . \tag{11}$$

In the following we will present first results for the ratio $B(T, H, c)$ obtained in simulations of (2+1)-flavor QCD on lattices with temporal extent $N_\tau = 8$.

3. Computational setup

The preliminary results for the logarithm of the order parameter ratio $B(T, H, 2)$ discussed in the next section have been obtained from lattice QCD calculations in $(2 + 1)$-flavor QCD using the HISQ action and the $O(a^2)$ improved Symanzik gauge action. Our computational setup is identical to that used previously in the determination of the chiral phase transition from simulations with smaller than physical light quark masses [13] as well as the recent determination of the chiral phase transition temperature at non-vanishing chemical potential [5]. These calculations have been performed on lattice of size $N_\sigma^3 \times 8$ with light to strange quark mass ratios $1/160 \leq H \leq 1/20$ corresponding to pion masses 55 MeV $\leq m_\pi \leq$ 160 MeV. The strange quark mass has been fixed to its physical value, demanding that the strange η meson mass defined in terms of kaon and pion masses, $M_{\bar{s}s} = \sqrt{2m_K^2 - m_\pi^2}$, is kept fixed [9].

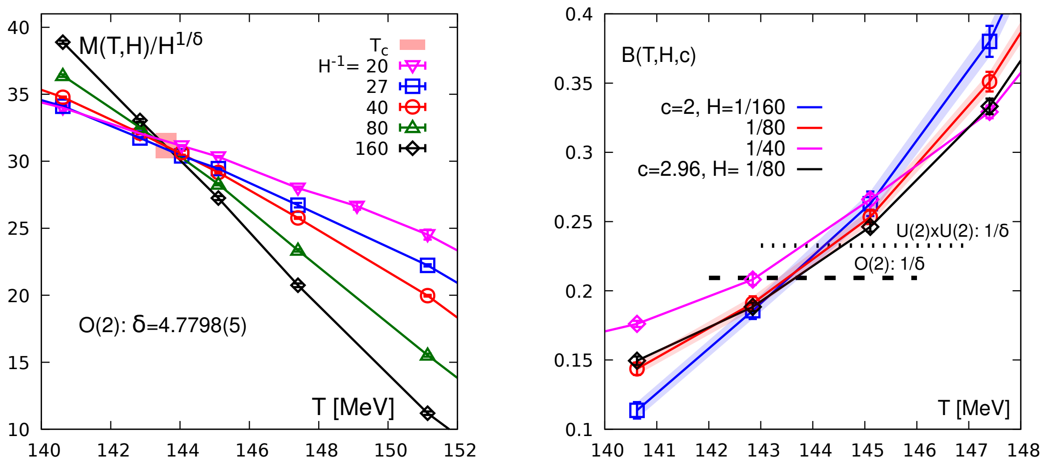

Figure 3: *Left:* Rescaled order parameter versus temperature for several values of H. The shaded rectangle corresponds to the values of $(T_c, h_0^{-1/\delta})$ determined previously from scaling fits [5]. *Right:* The logarithm of ratios of the chiral order parameter versus temperature as introduce in Eq. 10. The dashed and dotted lines give the values for $1/\delta$ in the $O(2)$ and $U(2) \times U(2)$ [2] universality classes, respectively.

In previous work the spatial lattice extent N_σ has been increased with decreasing m_π, *i.e.* $4 \leq N_\sigma \leq 7$, insuring that the inverse of the pion correlation length in units of the spatial lattice extent stays approximately constant, $m_\pi L \simeq (3-4)$.

For our analysis of the rescaled order parameter and the order parameter ratios we used the set of data for $H = 1/27, 1/40, 1/80$ and $1/160$ at several values of the temperature, tabulated in [5]. Data for $H = 1/20$ are taken from [5]. These data are generally taken at temperature values separated by $(2-3)$ MeV. In order to arrive at precision determination of the unique crossing point in the rescaled order parameter, small separations of the T-values is needed. Further, more smaller separations in the set of H values is needed to control the quark mass dependence of the chiral order parameter. We started on this program by adding new data at $T = 144.05$ MeV and at additional H-values, $H = 1/32.2$ and $1/16.1$. The current statistics at these new sets of (T, H) values is about $O(20K)$ gauge configurations, separated by 5 and 10 RHMC time units, respectively.

4. Results

In Fig. 3 (left), we show results for the rescaled order parameter $M/H^{1/\delta}$ taken from [5]. Here we used for the critical exponent δ, the value in the 3-dimensional $O(2)$ universality class, $\delta = 4.7798$. The slope of the rescaled order parameter rises with decreasing H and the existence of an intersection point is clearly visible. In fact, the location of this intersection point, is seen to agree well with the previous determination of T_c *i.e.* $T_c^{N_\tau=8} = 143.7(2)$ MeV [5]. Also the value of $M/H^{1/\delta}$ at this intersection point,

$$M(T_c, H)/H^{1/\delta} = h_0^{-1/\delta}(1 - 1/\delta) \tag{12}$$

agrees well with the previously determined value, $h_0^{-1/\delta} = 39.2(4)$ [5], which has been obtained from fits to the rescaled order parameter in the temperature interval $T \in [140\,\text{MeV} : 148\,\text{MeV}]$.

We note however, again that this analysis starts with assuming a second order critical point in the 3-dimensional $O(2)$ universality. In order to avoid such an apriori input into the analysis, we may turn to an analysis of ratios of the order parameter M as introduced in Eq. 10.

In Fig. 3 (right) we show result for the logarithm of ratios of the chiral order parameter versus temperature for several sets of H-value, (H_1, H_2) with $H_2 = cH_1$ and $H_1 = 1/40, 1/80, 1/160$. While results for $B(T, H, c)$ with $cH \leq 1/40$ give a unique intersection point that is in agreement with a critical exponent δ in the $O(2)$ universality class, this is not the case once larger values of cH are involved in the order parameter ratios entering the definition $B(T, H, c)$. In Fig. 3 (right), this is the case for $B(T, 1/80, 80/27)$, and also for $B(T, 1/40, 2)$. This suggests that the quark ratio $H = 1/27$, corresponding to the physical value of light and strange quark masses and larger than $1/27$ ratios are too large and clearly not in the scaling region where contributions from regular terms can be neglected. Clearly, more detailed information on the H-dependence of the rescaled order parameter, $M/H^{1/\delta}$, is needed to quantify the parameter range in which, a unique crossing point can be established that would then also allow for a clear-cut distinction between different universality classes.

5. Conclusion and Outlook

We have shown that, the rescaled order parameter evaluated as function of T for different values of the light-to-strange quark mass ratio $H = m_\ell/m_s$ exhibits the feature of having a unique intersection point, if the light quark mass or respectively H, is small enough so that contributions from sub-leading terms can be neglected. Taking ratios of order parameters evaluated for different values of H allows for a determination of the critical exponent δ without making apriori assumption about the underlying universality class. However in order to arrive at the point, where these calculations reach a sufficient accuracy to allow for quantitative determination of δ thereby enabling a clear distinction between universality classes relevant for the analysis of the chiral phase transition, one needs to collect more information on the H dependence of the rescaled order parameter close to the chiral limit. Furthermore, a more detailed analysis of finite volume and cut-off effects will be needed that were not subject of the discussion presented here. In fact, this is work in progress.

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References

[1] R. D. Pisarski and F. Wilczek, *Remarks on the Chiral Phase Transition in Chromodynamics*, Phys. Rev. D **29** (1984) 338.

[2] A. Pelissetto and E. Vicari, *Relevance of the axial anomaly at the finite-temperature chiral transition in QCD*, Phys. Rev. D **88** (2013) 105018 [arXiv:1309.5446 [hep-lat]].

[3] S. Ejiri, F. Karsch, E. Laermann, C. Miao, S. Mukherjee, P. Petreczky, C. Schmidt, W. Soeldner and W. Unger, *Magnetic equation of state in (2+1)-flavor QCD*, Phys. Rev. D **80** (2009) 094505 [arXiv:0909.5122 [hep-lat]].

[4] A. Bazavov, T. Bhattacharya, M. Cheng, C. DeTar, H. T. Ding, S. Gottlieb, R. Gupta, P. Hegde, U. M. Heller and F. Karsch *et al.*, *The chiral and deconfinement aspects of the QCD transition*, Phys. Rev. D **85** (2012) 054503 [arXiv:1111.1710 [hep-lat]].

[5] H. T. Ding, O. Kaczmarek, F. Karsch, P. Petreczky, M. Sarkar, C. Schmidt and S. Sharma, *Curvature of the chiral phase transition line from the magnetic equation of state of (2+1)-flavor QCD*, Phys. Rev. D **109** (2024) 114516, [arXiv:2403.09390 [hep-lat]].

[6] A. Y. Kotov, M. P. Lombardo and A. Trunin, *QCD transition at the physical point, and its scaling window from twisted mass Wilson fermions*, Phys. Lett. B **823** (2021) 136749 [arXiv:2105.09842 [hep-lat]].

[7] J. Braun, Y. r. Chen, W. j. Fu, F. Gao, C. Huang, F. Ihssen, J. M. Pawlowski, F. Rennecke, F. R. Sattler and Y. y. Tan, *et al.*, *Soft modes in hot QCD matter*, arXiv:2310.19853 [hep-ph].

[8] A. Bazavov, D. Bollweg, H. T. Ding, P. Enns, J. Goswami, P. Hegde, O. Kaczmarek, F. Karsch, R. Larsen and S. Mukherjee, *et al.*, *Skewness, kurtosis and the fifth and sixth order cumulants of net baryon-number distributions from lattice QCD confront high-statistics STAR data*, Phys. Rev. D **101** (2020) 074502 [arXiv:2001.08530 [hep-lat]].

[9] A. Bazavov *et al.* [HotQCD], *Equation of state in (2+1)-flavor QCD*, Phys. Rev. D **90** (2014) 094503 [arXiv:1407.6387 [hep-lat]].

[10] W. Unger, *The chiral phase transition of QCD with 2+1 flavors : a lattice study on Goldstone modes and universal scaling*, PhD thesis (2010) Bielefeld University

[11] L. Dini, P. Hegde, F. Karsch, A. Lahiri, C. Schmidt and S. Sharma, *Chiral phase transition in three-flavor QCD from lattice QCD*, Phys. Rev. D **105** (2022) 034510 [arXiv:2111.12599 [hep-lat]].

[12] F. Karsch, M. Neumann and M. Sarkar, *Scaling functions of the three-dimensional Z(2), O(2), and O(4) models and their finite-size dependence in an external field*, Phys. Rev. D **108** (2023) 014505 [arXiv:2304.01710 [hep-lat]].

[13] H. T. Ding *et al.* [HotQCD], *Chiral Phase Transition Temperature in (2+1)-Flavor QCD*, Phys. Rev. Lett. **123** (2019) 062002 [arXiv:1903.04801 [hep-lat]].