O(N) universality and the chiral phase transition in QCD

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We discuss universal scaling properties of (2+1)-flavor QCD in the vicinity of the chiral phase transition at vanishing as well as non-vanishing light quark chemical potential ($\mu_l$). We provide evidence for $O(N)$ scaling of the chiral order parameter in (2+1)-flavor QCD and show that the scaling analysis of its derivative with respect to the light quark chemical potential provides a unique approach to the determination of the curvature of the chiral phase transition line in the vicinity of $\mu_l/T = 0$.

§1. Introduction

It is well understood that the phase structure of QCD at non-zero temperature crucially depends on the quark mass values. While in the case of three degenerate quark masses (3-flavor QCD) a first order transition occurs for sufficiently small values of the quark mass, it is expected that the transition in 2-flavor QCD is continuous and belongs to the universality class of $O(4)$ symmetric, 3-dimensional spin models. Several studies of the QCD phase diagram as function of two degenerate light ($m_u, m_d$) and a strange ($m_s$) quark mass suggest that the region around the 3-flavor chiral limit, where the QCD transition becomes first order, is indeed small and does not include the point of physical light and strange quark masses. Our current understanding of the location of the region of 1\textsuperscript{st} order transitions that is separated by a line of 2\textsuperscript{nd} order transitions from the crossover region and its positioning relative to the physical point is presented in the Columbia plot shown in Fig. 1.

While numerical calculations in 3-flavor QCD gave evidence for the existence of a first order transition, many of the details of the transition in 2- or (2+1)-flavor QCD with light up and down quarks are still poorly constrained through lattice calculations. Earlier attempts to verify $O(4)$ scaling in numerical studies of 2-flavor QCD using standard staggered fermions were not very successful in establishing the expected universal scaling properties.

Fig. 1. The phase diagram of 3-flavor QCD.
We present here a new analysis of scaling properties using $O(a^2)$ improved staggered fermion and gauge actions. We perform this analysis for (2+1)-flavor QCD. Implicitly we thus also analyze whether the region of first order chiral transitions ends in a tri-critical point for a strange quark mass value below its physical value or above. We will use the scaling analysis of the chiral order parameter to determine the curvature of the chiral phase transition line at non-vanishing values of the light quark chemical potential $\mu_l$, i.e. the first (Taylor) expansion coefficient of the transition line in powers of $(\mu_l/T)^2$ around $\mu_l/T = 0$.

§2. $O(N)$ scaling of the chiral condensate

In the vicinity of a critical point regular contributions to the logarithm of the partition function become negligible. The universal critical behavior of the order parameter $M$ of, e.g. 3-dimensional $O(N)$ spin models, is then controlled by a scaling function $f_G$ that arises from the singular part of the logarithm of the partition function,

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

(2.1)

with $z = t/h^{1/\beta}$ and scaling variables $t$ and $h$ that are related to the temperature, $T$, and the symmetry breaking (magnetic) field, $H$,

$$t = \frac{1}{t_0} \frac{T - T_c}{T_c} , \quad h = \frac{H}{h_0} .$$

(2.2)

Here $\beta$ and $\delta$ are critical exponents, unique for the universality class of the second order phase transition which the system undergoes in the limit $(t, h) \to (0,0)$. The form of the scaling function $f_G(z)$ is well known from numerical simulations of 3-dimensional $O(N)$ symmetric spin models.

In QCD symmetry breaking arises due to a non-vanishing light quark mass, $H \equiv m_l/m_s$, and the corresponding order parameter is the chiral condensate, which we write as

$$M \equiv M_b = N^4_\tau m_s \langle \bar{\psi} \psi \rangle_l ,$$

(2.3)

where $m_s$ denotes the strange quark mass in lattice units and $N_\tau$ is the temporal extent of the 4-dimensional lattice, $N^3_\sigma \times N_\tau$. One may improve the operator $M_b$ by subtracting a fraction of the strange quark condensate. This eliminates additive linear divergent terms proportional to the light quark masses. Such a subtraction is, in fact, mandatory, if one wants to take the continuum limit at finite quark mass before taking the chiral limit. This ordering of limits, indeed is needed in order to recover the correct $O(4)$ scaling behavior from calculations performed with staggered fermions, which only preserve a global $O(2)$ symmetry for any non-zero value of the lattice spacing. We will be less ambitious here and discuss the chiral limit on lattices with fixed temporal extent, $N_\tau = 4$. In this case, we can only expect to find $O(2)$ rather than $O(4)$ scaling behavior. However, the scaling functions, $f_G(z)$, are very similar for both universality classes and it thus will be difficult to distinguish $O(2)$ and $O(4)$ scaling through an analysis of the order parameter alone. Moreover, given the large scaling violations observed in earlier studies with staggered fermions.
already the observation of scaling in terms of a generic $O(N)$ scaling function at non-zero values of the lattice cut-off is a major step forward.

We show in Fig. 2(left) results from a calculation of chiral condensates in (2+1)-flavor QCD. The bare strange quark mass ($m_s$) has been chosen such that the physical value of the strange pseudo-scalar mass, $m_{s\bar{s}} \equiv \sqrt{2m_K^2 - m_{\pi}^2}$, is reproduced. The light quark mass has been varied in a range $1/80 \leq m_l/m_s \leq 2/5$, which for the light pseudo-scalar Goldstone meson corresponds to a regime $75 \text{MeV} \leq m_{ps} \leq 420 \text{MeV}$. The lattice size has been varied from $16^3 \times 4$ for the heavier quark masses to $32^3 \times 4$ for the lightest quark masses. This insures that finite volume effects remain small in the entire light quark mass regime, i.e. in units of the spatial extent $N_\sigma$ we always have $m_{ps} N_\sigma \geq 3$.

From Fig. 2(left) it is obvious that the chiral condensate scales with the square root of the quark mass in the low temperature, chiral symmetry broken phase, 

$$\langle \bar{\psi} \psi \rangle = a(T) + b(T) \sqrt{m_l/m_s} + \mathcal{O}\left(\frac{m_l}{m_s}\right).$$

This is characteristic for Goldstone-modes in three dimensional $O(N)$ symmetric spin models. In fact, this also is the dominant term characterizing the scaling function $f_G(z)$ in the symmetry broken phase, i.e. for $z < 0$.

Results for the chiral condensate may be put on the universal scaling curve by using the reduced temperature and rescaled symmetry breaking field introduced in Eq. 2. Of course, this is expected to be possible only close to criticality where contributions from regular terms and corrections to scaling are small. The scaling analysis shown in Fig. 2(right) has therefore only been performed for the three lightest quark mass values, $m_l/m_s \leq 1/20$ and for temperatures close to $T_c$. From this one determines the three free parameters, $t_0$, $h_0$ and $T_c$. As expected results for heavier quarks, also shown in Fig. 2(right), show deviations from the universal scaling behavior. Contributions from corrections to scaling become significant for $m_l/m_s \gtrsim 1/5$, i.e. $m_{ps} \gtrsim 300$ MeV. This is in contrast to calculations with Wilson fermions, where indications for $O(4)$ scaling have been reported for even large values of the pseudo-scalar meson mass.

The scaling analysis of the order parameter provides two non-universal parameters that are unique for QCD, the chiral phase transition temperature, $T_c$, and the scale parameter $z_0 = h_1^{1/3\beta}/t_0$. In the continuum limit both quantities are functions of the strange quark mass only. Of course, $T_c$ as well as $z_0$ are cut-off dependent and a proper continuum extrapolation is needed to extract their values in the continuum limit. From our analysis on lattices with temporal extent $N_\tau = 4$ we find $z_0 \simeq 7.5$. A preliminary analysis on lattices with temporal extent $N_\tau = 8$ suggests that this value drops by almost a factor 2. A more detailed analysis of the approach to the continuum limit thus is needed. We stress, however, that $z_0$ is a physical parameter of QCD. It gives the slope of the quark mass dependence of the pseudo-critical temperature, which can be determined from the location of a peak in the chiral
Fig. 2. The light quark chiral condensate in lattice units versus the ratio of the square root of the light and strange quark masses (left) and its scaling form (right). The right hand figure has been obtained using fits for \( m_l/m_s \leq 1/20 \) and \( |T - T_c|/T_c \leq 1.03 \) only.

susceptibility,

\[
\chi_M(t, h) = \frac{\partial M}{\partial H} = \frac{1}{h_0} h^{1/\delta-1} f_{\chi}(z),
\]

\[
f_{\chi}(z) = \frac{1}{\delta} \left( f_G(z) - \frac{z}{\beta} f_G'(z) \right).
\]

The scaling functions \( f_G'(z) = df_G/\delta z \) and \( f_{\chi}(z) \) are shown in the right hand part of Fig. 3. The scaling function \( f_{\chi}(z) \) has a maximum at \( z_p \). The dependence of the pseudo-critical temperature, \( T_p \), on the quark mass is given by the condition that \( z = t / h^{1/\delta} = z_p \), i.e.

\[
\frac{T_p(H) - T_c}{T_c} = \frac{z_p}{z_0} H^{1/\delta}.
\]

For the 3-d \( O(2) \) universality class the peak in the chiral susceptibility is located at \( z_p \approx 1.56 \). Using this and expressing the symmetry breaking field \( H \) in terms of pion and kaon masses rather than quark masses, \( H = m_l/m_s \approx 0.52 (m_{ps}/m_K)^2 \), we find

\[
\frac{T_p(m_{ps})}{T_c} = 1 + \frac{1.06}{z_0} \left( \frac{m_{ps}}{m_K} \right)^{2/\delta}.
\]

This allows to estimate the phase transition temperature in the chiral limit. With \( m_s/m_K \approx 0.27 \) one finds with our current estimates for \( z_0 \) that the transition temperature in the chiral limit is about 7% smaller than the crossover temperature at physical values of the quark masses. Of course, this still needs to be analyzed closer to the continuum limit.

§3. Curvature of the critical line in the \( T-\mu_B \) phase diagram

For non-vanishing light quark chemical potential, \( \mu_l \), the second order chiral phase transition persists to exist in the \( T-\mu_l \) plane. For small values of the chemical
potential, $\mu_l/T > 0$, the curvature of the phase transition line can be determined by making use of the scaling analysis of the order parameter. In this case the reduced temperature variable, $t$, also depends on the chemical potential as it couples to the quark number operator, which does not break chiral symmetry. To leading order it contributes quadratically,

$$ t = \frac{1}{t_0} \left( \frac{T - T_c}{T_c} + \kappa \left( \frac{\mu_l}{T} \right)^2 \right). $$

The condition for criticality, $t = 0$, fixes the shape of the transition line for small values of $\mu_l/T$. In the scaling regime the order parameter $M$ depends on temperature and quark mass only through the scaling variable $z$. The derivative of $M$ with respect to $T$ thus is, up to a constant, identical to the second derivative of $M$ with respect to the chemical potential $\mu_l$. This derivative too is related to the scaling function $f_G'(z)$ which we have introduced in Eq. 2.6 and which is shown in Fig. 4(right).

$$ M_2 \equiv \left. \frac{\partial^2 M}{\partial (\mu_l/T)^2} \right|_{\mu_l=0} = \frac{2\kappa}{t_0} h^{(\beta - 1)/\beta} f_G'(z), $$

We note that $M_2$ has properties similar to the chiral susceptibility. It diverges in the chiral limit at $z = 0$ and the peak position in $f_G'(z)$ can be used to define a pseudo-critical temperature at non-zero values of the light quark mass.

Once the scale parameters $t_0$, $h_0$, $T_c$, needed to project the chiral order parameter onto the $O(N)$ scaling curve, are known, we can use this information to determine the curvature of the critical line, $\kappa$, by calculating $M_2$ and by matching the scaling curve to the data using an appropriate scaling factor $\kappa$. Such a scaling analysis is shown in Fig. 4(left). From this we find for the curvature of the phase transition line in the chiral limit the preliminary result $\kappa \approx 0.035$ which is in good agreement with earlier determinations of the curvature of the pseudo-critical line at non-zero values of the quark mass performed with different numbers of flavors. We note that the current analysis suggests that the curvature of the transition line, expressed in terms of $\mu_B \sim 3\mu_l$, is smaller than the experimentally determined freeze-out curve, which is well parametrized by

$$ \frac{T}{T_{\text{freeze-out}}} \simeq 1 - 0.023 \left( \frac{\mu_B}{T} \right)^2 + \mathcal{O} \left( \frac{\mu_B}{T} \right)^4. $$

\footnote{Some caution is needed when translating $\mu_l$ to $\mu_B$ and comparing lattice results with experimental findings. Lattice calculations have been performed for vanishing strange quark chemical potential (in some cases even for 2-flavor QCD), while the freeze-out conditions in a heavy ion collision refer to a system with $\mu_s/\mu_B \approx 0.16$.}
Frithjof Karsch

Fig. 4. The second derivative of the order parameter with respect to the light quark chemical potential (left). The $O(2)$ scaling curve $f'_2(z)$, shown together with $f_2(z)$ in the right hand part of the figure, has been rescaled to match the data.

§4. Conclusions

We have discussed universal properties of the chiral condensate of (2+1)-flavor QCD in the limit of vanishing light quark masses. It agrees well with expected $O(N)$ scaling predictions. We showed how this can be used to calculate the curvature of the second order chiral phase transition line in the vicinity of $\mu_B/T = 0$.

At present this analysis is limited to rather coarse lattices. Calculations closer to the continuum limit are needed to get control over the scale parameter $z_0$ and the phase transition temperature in the chiral limit.

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