Sensitivity of the Polyakov loop to chiral symmetry restoration

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In the heavy, static quark mass regime of QCD, the Polyakov loop is well known to be an order parameter of the deconfinement phase transition; however, the sensitivity of the Polyakov loop to the deconfinement of light, dynamical quarks is less clear. On the other hand, from the perspective of an effective Lagrangian written in the vicinity of the chiral transition, the Polyakov loop is an energy-like operator and should hence scale as any energy-like operator would. We show here that the Polyakov loop and heavy-quark free energy are sensitive to the chiral transition, i.e. their scaling is consistent with energy-like observables in 3-d O(N) universality classes.

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1. Introduction

The QCD Lagrangian with two mass-degenerate light quarks $m_l$ possesses an exact global $Z_3$ symmetry in the quenched limit, i.e. in the infinite quark mass limit. At low temperature where the symmetry is respected, quarks are confined into bound states; above a critical temperature $T_d$, the $Z_3$ symmetry breaks spontaneously, and quarks become deconfined. The average Polyakov loop$^1$ $\langle P \rangle = \langle \text{Re} P \rangle$ serves as a natural order parameter for this deconfinement transition. At the other end of the spectrum, where $m_l = 0$, the Lagrangian has an SU(2)$_L \times$ SU(2)$_R$ symmetry that spontaneously breaks below a critical temperature $T_c$. In this limit, the light quark chiral condensate $\langle \bar{\psi} \psi \rangle$ serves as an appropriate order parameter.

$^1$ Note that $\langle \text{Im} P \rangle = 0$ at all values of $T$ and all quark masses as the Euclidean QCD action is invariant under $U_\mu(x, \tau) \rightarrow U_\mu(x, \tau)$. 

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At physical $m_l$ both symmetries are broken explicitly, and neither $\langle P \rangle$ nor $\langle \bar{\psi} \psi \rangle$ is zero. Still, these quantities will change substantially as a function of temperature, and the inflection points of these changes have been used to define pseudo-critical temperatures. In the quenched limit [1] and also at larger-than-physical quark mass values [2], inflection points in the temperature dependence for $\langle P \rangle$ and $\langle \bar{\psi} \psi \rangle$ have been found at similar temperatures. This seeming coincidence of inflection points is often taken as evidence for the coincidence of chiral and deconfinement transitions. However, studies with (almost) physical light quark masses and, in particular, studies with improved fermion actions, performed closer to the continuum limit, in general show that the QCD transition is a smooth crossover, and no coincidence of inflection points is found [3, 4, 5], challenging this line of evidence for simultaneous chiral and deconfinement transitions.

This way of thinking interprets the rapid change in $\langle P \rangle$ as a remnant of $m_l = \infty$ physics. But in the chiral limit, there is no obvious symmetry whose breaking can be related to deconfinement; in that sense, there is no a priori reason to interpret $\langle P \rangle$ in the chiral limit in this way. Another possibility is that the behavior of $\langle P \rangle$ is instead sensitive to the chiral transition in this regime. Under this assumption, $\langle P \rangle$ should inherit its behavior from the chiral transition as an energy-like operator.

In this study we explore this idea analytically and numerically. In particular we analyze the temperature and quark mass dependence of the Polyakov loop and heavy-quark free energy in the chiral limit.

2. The Polyakov loop and chiral symmetry restoration

For lattice QCD in a Euclidean space-time volume $N^3 \sigma \times N \tau$, the Polyakov loop and its spatial average are given by

$$P_\vec{x} \equiv \frac{1}{3} \text{tr} \prod_\tau U_4(\vec{x}, \tau), \quad P \equiv \frac{1}{N^3} \sum_\vec{x} P_\vec{x},$$

respectively. Here $U_4(\vec{x}, \tau)$ is the SU(3)-valued link variable originating at space-time point $(\vec{x}, \tau)$, pointing in the Euclidean time direction. $P$ can be related to the heavy-quark free energy by

$$F_q(T, H) = -T \ln \langle P(T, H) \rangle = -T \frac{1}{2} \lim_{|\vec{x} - \vec{y}| \to \infty} \ln \langle P_\vec{x} P_\vec{y}^\dagger \rangle.$$  \hspace{1cm} (2)

We have made explicit in this equation the dependence of $P$ and $F_q$ on the temperature $T$ and symmetry-breaking parameter $H \equiv m_l / m_s$. For the remainder of these proceedings we will not explicitly write these dependencies to keep the notation light. $P$ requires a multiplicative renormalization,

$$P = e^{-c(g^2)N \tau} P_{\text{bare}},$$

$$\hspace{1cm} (3)$$
i.e. the renormalized \( P \) appears in eq. (2). Therefore derivatives of the free energy such as

\[
\frac{\partial F_q}{\partial H} = - \frac{1}{\langle P \rangle} \frac{\partial \langle P \rangle}{\partial H} \quad \text{and} \quad T_c \frac{\partial F_q}{\partial T} = - \frac{T_c}{\langle P \rangle} \frac{\partial \langle P \rangle}{\partial T},
\]

are independent of the renormalization, which in the continuum limit drops out in the ratio.

### 2.1. The Polyakov loop as an energy-like operator

From the perspective of Wilson’s renormalization group [6, 7], thermodynamics in the vicinity of a critical point can be described by an effective Hamiltonian, which is defined in a multi-dimensional space of operators (observables). These operators may be invariant under the global symmetry that gets broken at the critical point or may break this symmetry explicitly. In the former case the operator is said to be energy-like, while in the latter case it is magnetization-like. In this study we are concerned with the spontaneous breaking of the global \( \text{SU}(2)_L \times \text{SU}(2)_R \) chiral symmetry in \((2+1)\)-flavor QCD, which in the continuum is expected to belong to the 3-d \( O(4) \) universality class. The light quark chiral condensate is a typical magnetization-like operator for this phase transition, i.e. it contributes to the Hamiltonian as a symmetry-breaking operator with \( H \sim m_l \) as a coefficient, and in this regard \( H \) parameterizes the extent of symmetry breaking. On the other hand the Polyakov loop is purely gluonic, hence it is invariant under chiral transformations of the quark fields; therefore \( \langle P \rangle \) as well as the heavy-quark free energy \( F_q \) obtained from it are energy-like observables.

In the vicinity of a phase transition, energy-like observables can be written as the sum of a regular (analytic) part, which is a Taylor series in the symmetry-breaking parameter \( H \) and the reduced temperature \( t \equiv (T - T_c)/T_c \), and a singular (non-analytic) part, which is described by a universal scaling function of the scaling variable \( z = z_0 t H^{-1/\delta} \). This scaling variable depends on universal critical exponents \( \beta \) and \( \delta \) and is rescaled by a non-universal constant \( z_0 \). The scaling behavior of an arbitrary energy-like observable in the 3-d \( O(N) \) universality class is given in Ref. [8]. In particular we can write

\[
F_q / T = AH^{(1-\alpha)/\beta \delta} f_f(z) + f_{\text{reg}}(T, H),
\]

where \( A \) is another non-universal constant, \( f_f(z) = df_f(z)/dz \) is the derivative of the scaling function \( f_f(z) \) that characterizes the singular part of the logarithm of the partition function, \( \alpha \) is another critical exponent, and

\[
f_{\text{reg}} = \sum_{i,j} \alpha_{i,2j} t^i H^{2j} \equiv \sum_j p_{2j}^c(T) H^{2j}.
\]
We take eq. (5) as the starting point for our analysis. For example from this and eq. (2) we can get \( \langle P \rangle \) by
\[
\langle P \rangle = \exp \left( -AH^{(1-\alpha)/\beta \delta} f_f'(z) - f_{\text{reg}} \right).
\] (7)

Making use of the relation between \( f_f(z) \) and the scaling function of the order parameter \( f_G(z) \),
\[
f_G(z) = - \left( 1 + \frac{1}{\delta} \right) f_f(z) + \frac{z}{\beta \delta} f_f'(z),
\] (8)
we obtain near \( T_c \)
\[
\frac{\partial F_q/T}{\partial H} = -AH^{(\beta-1)/\beta \delta} f'_G(z) + \frac{\partial f_{\text{reg}}}{\partial H}.
\] (9)

Furthermore, one finds the \( T \)-derivative of \( F_q/T \) to be
\[
T_c \frac{\partial F_q/T}{\partial T} = Az_0^H - \alpha/\beta \delta f''_f(z) + T_c \frac{\partial f_{\text{reg}}}{\partial T}.
\] (10)

### 2.2. Polyakov loop observables in 3-d O(2) systems

As mentioned, the continuum limit universality class is expected to be \( O(4) \), but this study works at fixed \( N_\tau \) using the staggered fermion discretization scheme, so the relevant universality class is 3-d \( O(2) \). The critical exponents, taken from Ref. [9], are
\[
\beta = 0.349, \quad \delta = 4.780, \quad \text{and} \quad \alpha = 2 - \beta(1 + \delta) = -0.0172.
\] (11)

Our parametrization of the 3-d, \( O(2) \) scaling functions is based on data obtained in Ref. [9]. We used \( f_G \), given in that paper in the Widom-Griffiths form, and replaced this in the form \( f_G(z) \). We use the same ansatz, with a Taylor series for small \( z \) and the asymptotic forms for \( z \to \pm \infty \). After finding expansion parameters for \( f_G(z) \), we can determine the corresponding expansion parameters for \( f_f(z) \). The only missing coefficients are, in the notation of Ref. [8], \( c^+_0 \) and \( c^-_0 \), which control the asymptotic behavior of \( f_f(z) \) and are of particular interest for the analysis of energy-like observables in the limit \( H = 0 \),
\[
f_f(z) = |z|^{2-\alpha} \begin{cases}
  c^+_0 + c^+_1 z^{-2\delta}, & z \to \infty \\
  c^-_0 + c^-_2 (-z)^{-\delta}, & z \to -\infty.
\end{cases}
\] (12)

We have calculated \( c^+_0 \) and \( c^-_0 \) using eqs. (58) and (61) of Ref. [8]. For these we find \( c^+_0 = 2.728(30) \) and \( c^-_0 = 2.447(40) \). With \( A^\pm = (2 - \alpha) z_0^{1-\alpha} c^\pm_0 \),
the resulting universal ratio $A^+/A^- = c_0^+/c_0^- = 1.115(30)$ agrees well with $A^+/A^- = 1.12(5)$ calculated in Ref. [10]. The coefficients of the sub-leading corrections in eq. (12) are known universal numbers, $c_1^+ = -R \chi/2 = -0.678(2)$ [10] and $c_2^- = -1$.

From eq. (12) one finds at fixed temperature and for small $H$

$$F_q/T \sim \begin{cases} a^-(T) + Ap_s^-(T) H & , \ T < T_c \\ a_{r,0}^+ + Aa_1 H^{(1-\alpha)/\beta\delta} & , \ T = T_c \\ a^+(T) + p^+(T) H^2 & , \ T > T_c \end{cases}$$

with $a^\pm(T) = Aa^\pm_s(T) + f_{reg}(T,0)$ as well as $p^+(T) = Ap^+_s(T) + p^2_s(T)$ receiving contributions from both the singular and regular terms. For $T < T_c$ the dominant quark mass dependence arises from the singular term only. In particular, we have

$$a^\pm_s(T) = (2 - \alpha) z_0^{1-\alpha} c_0^\pm t |t|^{-\alpha}$$

$$p^s_s(T) = (2 - \alpha - \beta\delta) (-z_0 t)^{1-\alpha-\beta\delta}$$

(14)

To leading order $H$-dependent corrections to $F_q/T$ and $\langle P \rangle$ are proportional to $H$ for all $T < T_c$. The linear dependence on $H$ reflects the contribution of Goldstone modes to the $O(N)$ scaling functions in the symmetry-broken, low-temperature phase. This linear dependence on $H$ is also consistent with the quark mass dependence of heavy-light bound states [11, 12], which dominate the hadronic contributions to $\langle P \rangle$ at low $T$ as

$$\langle P \rangle \approx 4 e^{-\Delta(m_l)/T}, \quad \Delta(m_l) = \lim_{m_h \to \infty} (M_{hl} - m_h),$$

(15)

where $\Delta(m_l)$ is the static limit for the mass of a heavy-light bound state $M_{hl}$ with divergent heavy quark mass $m_h$ removed [11]. As can be shown in heavy-quark chiral perturbation theory, this heavy-light binding energy depends linearly on $m_l$, i.e. $\Delta(m_l) - \Delta(0) \sim m_l^2$ [13]. At low $T$ the resulting linear quark mass dependence of $\langle P \rangle$ and $F_q$, arising from the thermodynamics of a heavy-light hadron gas, is thus consistent with the behavior from the singular part of $O(N)$ scaling functions valid near $T_c$.

As $\alpha < 0$, the first two terms in the regular part, $a_r(T) = a_{r,0}^+ + a_r^1 t$, dominate the temperature dependence and slope of $F_q/T$ and $\langle P \rangle$ at the critical point. For instance

$$\frac{F_q(T,0)}{T} = a_{r,0}^+ + t \left(a_r^1 + A^{\pm}|t|^{-\alpha}\right).$$

(16)
Although at $T_c$ the contribution to the slope is entirely given by the regular term $a_{1,0}$, close to $T_c$ this contribution gets to a large extent canceled by the singular contributions, $A^\pm |t|^{-\alpha}$. This is the origin of the well known spike in specific-heat like observables (2nd derivatives of the logarithm of the partition function with respect to $T$) in $O(N)$ universality classes. As $|\alpha|$ is quite small, the correction from the singular part varies little in a large temperature range, e.g. $|t|^{-\alpha}$ equals 0.92 for $t = 0.01$ and rises to 0.96 for $t = 0.1$. The singular part thus contributes an almost constant term to the slope of $F_q(T,0)/T$ at $T_c$, and the change in slope that arises from the singular contribution is difficult to detect.

In order to examine the sensitivity of $F_q/T$ and $\langle P \rangle$ to chiral symmetry restoration it thus seems easier to first analyze their dependence on $H$ rather than $T$. Results for $\partial (F_q/T)/\partial H$ will be given in Section 4, followed by results for $F_q/T$ and $\langle P \rangle$, while results for the $H$-derivative of $\langle P \rangle$, the mixed susceptibility $\chi_{mP}$, are given in Ref. [14].

### 3. Computational setup and data analysis

We analyze properties of (2+1)-flavor QCD where $m_s$ is fixed to its physical value and $m_l$ is varied in the range $H = m_l/m_s = 1/160 - 1/20$. The analysis is performed on sets of gauge field configurations generated using highly improved staggered quarks (HISQ) [15] and the tree-level improved Symanzik gauge action. We utilize gauge field ensembles that were generated previously by the HotQCD collaboration [16, 17, 18, 19]. Additionally, we have generated further configurations for $H = 1/40$ and $H = 1/80$.

The bare coupling $\beta = 6/g^2$ for physical and smaller-than-physical $m_l$ is taken in the range 6.26-6.50, which is chosen so temperatures lie in the

Table 1. Summary of parameters used in this study and corresponding statistics, reported in average molecular dynamic time units (TU) per parameter combination.

| $m_s/m_l$ | $N_\sigma$ | avg. # TU | $m_s/m_l$ | $N_\sigma$ | avg. # TU |
|-----------|------------|-----------|-----------|------------|-----------|
| 20        | 32         | 99 000    | 80        | 56         | 35 000    |
| 27        | 32         | 1 500 000 | 80        | 40         | 33 000    |
| 40        | 40         | 110 000   | 80        | 32         | 73 000    |
|           |            |           | 160       | 56         | 17 000    |

2 The appearance of this spike in $\partial (F_q/T)/\partial T$ along with a detailed analysis of its features is presented in Ref. [14].

3 Distinguishing singular and regular contributions by just analyzing the temperature dependence of $F_q(T,0)/T$ or $\langle P \rangle$ would require an analysis at very small values of $H$ in a tiny temperature interval. This, in fact, has been done in studies of 3-d, $O(2)$ spin models [9] but is out of reach for current studies in QCD.
vicinity of the chiral pseudo-critical temperature. For \( H = 1/20 \) we also use data from calculations on lattices at smaller couplings, \( \beta = 6.05, 6.125, \) and 6.175 \cite{12}, which allows to establish contact to the low temperature regime. To set the scale we use the recent parametrization of lattice QCD results for the kaon decay constant, \( f_K a(\beta) \) \cite{20}. In particular, this defines our temperature scale, \( T/f_K = 1/N_\tau f_K a(\beta) \), with \( f_K = 156.1/\sqrt{2} \) MeV \cite{21}. Additive renormalization constants \( c(g^2) \) are based on Table V of Ref. \cite{4}. We fit these constants with a univariate spline, which is necessary to determine renormalization constants for a few \( \beta \) not listed in that table. The results from the interpolation are taken as our \( c(g^2) \).

Lattice sizes, quark masses, and statistics are summarized in Table 1. All calculations were performed on lattices with \( N_\tau = 8 \). For \( H = 1/80 \) we have results for aspect ratios \( N_\sigma/N_\tau = 4 - 7 \). We see in Fig. 1 no significant volume dependence of \( \langle P \rangle \) in the entire temperature range. Results on different size lattices agree within errors, which are about 1%. We thus can safely neglect any finite volume corrections to our results for \( \langle P \rangle \). This is quite different for \( \langle |P| \rangle \), which shows a strong volume dependence and converges to \( \langle P \rangle \) only in the infinite volume limit.

4. Results

In Fig. 2 (left) we show \( \partial(F_q/T)/\partial H \) rescaled with the appropriate power of \( H \) expected from the O(2) scaling ansatz. The good scaling behavior suggests that \( \partial(F_q/T)/\partial H \) will indeed diverge as \( H^{(3-1)/\beta \delta} \) in the chiral limit and that \( H \)-dependent contributions to \( F_q/T \) arising from regular terms are
Fig. 2. (Color online) Scaling and temperature dependence of $F_q/T$ and its $H$-derivative. Fits are described in the text. Data with filled symbols are not included in the fits. Left: Rescaled derivative of $F_q/T$ with respect to $H$ as function of $z$. Middle: Derivative of $F_q/T$ with respect to $H$ as function of $T$. Right: $F_q/T$ as function of $T$. The chiral limit result for $H = 0$ obtained from these fits is shown as grey bands. The solid gold line shows the heavy-light meson contribution calculated in the hadron-gas approximation [12]. Images taken from Ref. [14].

small compared to those coming from the singular part. This motivates an $H$-independent fit ansatz for $f_{reg}$, i.e. we use $f_{reg}(T,H=0)$ in all our fits.

A fit to $\partial (F_q/T)/\partial H$ thus only involves the singular term of eq. (9). We performed this 3-parameter fit for all data sets by either including or leaving out the data for $H = 1/27$. These fits are shown in Fig. 2 (middle): the corresponding fit parameters, $A, T_c, z_0$, are given in Ref. [14]. In particular, we find that $T_c$ and $z_0$ obtained from these fits agree well with earlier results for chiral susceptibilities in $(2+1)$-flavor QCD [19].

Data for $F_q/T$ are shown in Fig. 2 (right). They have been fitted to eq. (5) using only the constant and linear $H$-independent terms in the regular part as fit parameters and keeping fixed the three non-universal constants, determined in the previous step, in the singular part. The $T$-range and data used in the fit are shown in the inset. The resulting fit parameters $a_{0,0}^0$ and $a_{1,0}^0$ are also given in Ref. [14]. In this figure we also show the heavy-light meson contribution to $F_q/T$ calculated in the hadron-gas approximation [11, 12]. As mentioned earlier, chiral perturbation theory also gives a linear dependence on $H$ at low temperature [13].

Once we have determined all five fit parameters for $F_q/T$, we can plug them into eq. (7) to arrive at a parameter-free description of the $T$ and $H$ dependence of $\langle P \rangle$. The thus determined curves are shown in Fig. 3 (left). As seen in the inset, they agree well with $\langle P \rangle$ data near $T_c^{\text{exp}} = 144(2)$ MeV [19], which suggests the behavior of $\langle P \rangle$ is explained well by chiral scaling in this region and serves as a consistency check of our approach.

Turning back to Fig. 2 (middle), it is apparent that $\partial (F_q/T)/\partial H$ decreases with $H$ at high $T$ and increases at low $T$. This is consistent with an approach towards zero at high $T$ and a non-vanishing, strongly temperature-
dependent constant at low $T$ in the chiral limit. Such a pattern is in accordance with the expected quadratic dependence on $H$ for $T > T_c$ and the leading linear dependence for $T < T_c$ given in eq. (13). For $T < T_c$ the next-to-leading dependence, $H^{3/2}$, will come with a negative coefficient; correspondingly there is a change from a convex (at high $T$) to concave (at low $T$) $H$-dependence evaluated at fixed temperature in Fig. 3 (right). Although errors are large for the results obtained with the smallest light quark mass, $H = 1/160$, it is evident that $\partial(F_q/T)/\partial H$ has maxima at $T \sim 145 - 150$ MeV which are close to $T_c^{N_\tau=8}$. With decreasing $H$ they approach $T_c^{N_\tau=8}$, and the peak height increases.

5. Conclusions

We examined the $m_l$ dependence of $\langle P \rangle$ and $F_q$. With this work we did not aim at presenting continuum-extrapolated results but rather wanted to establish evidence for the influence of chiral symmetry restoration. The $m_l$ derivative of $F_q$ diverges in the chiral limit consistent with the expected behavior for energy-like observables in the 3-$d$, O(2) universality class. The data for $\langle P \rangle$ are described well by O(2) scaling near $T_c$.

Finding evidence for critical behavior in the temperature derivatives of $F_q$ and $\langle P \rangle$ is challenging. A clear singular structure will only build up at very small values of the quark masses.

As the critical exponent $\alpha$ is also negative and small in the O(4) universality class, we expect similar behavior for $F_q(T,H)/T$ and $\langle P \rangle$ will also persist in the continuum limit.
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