

Imprint of chiral symmetry restoration on the Polyakov loop and the heavy quark free energy

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The Polyakov loop expectation value $\langle P \rangle$ is an order parameter of the deconfinement transition in the heavy quark mass regime, whereas its sensitivity to the deconfinement of light, dynamical quarks is not apparent. From the perspective of an effective Lagrangian in the vicinity of the chiral transition, the Polyakov loop, P, is an energy-like observable, and $\langle P \rangle$ should hence scale like the energy density. Using $N_f = 2 + 1$ HISQ configurations at finite lattice spacing, we show that near the chiral transition temperature, the scaling behavior of $\langle P \rangle$ and the heavy quark free energy F_q is consistent with energy-like observables in the 3-d, O(N) universality class. We extend this analysis to other Polyakov loop observables, including the response of the heavy quark free energy, F_q , to the baryon chemical potential, which is expected to scale like a specific heat.

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1. Introduction

The Polyakov loop and its spatial average are defined in lattice QCD by

$$
P_{\vec{x}} \equiv \frac{1}{3} \operatorname{tr} \prod_{\tau} U_4\left(\vec{x}, \tau\right), \quad \text{and} \quad P \equiv \frac{1}{N_{\sigma}^3} \sum_{\vec{x}} P_{\vec{x}}, \tag{1}
$$

where the space-time volume is $N_{\sigma}^3 \times N_{\tau}$ and $U_4(\vec{x}, \tau) \in SU(3)$ is the link variable originating at the site (\vec{x}, τ) and pointing in the Euclidean time direction. P can be related to the heavy-quark free energy by^{[1](#page-1-0)}

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

where T denotes the temperature and $H = m_l/m_s$ is the ratio of the light and strange quark masses m_l and m_s . In the quenched limit, $\langle P \rangle$ is an order parameter signaling the deconfinement of static quarks above a critical temperature T_d , where a global \mathbb{Z}_3 symmetry is spontaneously broken.

At finite quark mass this symmetry is broken explicitly, and it is unclear whether it makes sense to associate large changes in $\langle P \rangle$ with the deconfinement of light quarks in particular. Still, there is a clear T-dependence for $\langle P \rangle$ at all quark masses, which is often viewed as a remnant of $m_l = \infty$ physics, including its interpretation in terms of deconfinement. This viewpoint is perhaps motivated in part by a coincidence of inflection points for $\langle P \rangle$ and the chiral condensate in the quenched limit [\[1\]](#page-7-0) and a seeming coincidence at larger-than-physical light quark masses [\[2\]](#page-8-0), although the latter coincidence disappears closer to the continuum limit [\[3](#page-8-1)[–6\]](#page-8-2).

One aim of this project therefore was to understand how to interpret the T-dependence of $\langle P \rangle$. There has been much effort investigating the order of the chiral phase transition, and in this context it is natural to examine to what extent the behavior of $\langle P \rangle$ and related observables such as F_q is determined by chiral scaling. For example the response of F_q to the baryon chemical potential μ_B ,

$$
\chi_{Q,\mu_B^2} \equiv -\frac{\partial^2 F_q/T}{\partial \hat{\mu}_B^2} \Big|_{\hat{\mu}_B = 0}, \quad \hat{\mu}_B \equiv \mu_B/T \tag{3}
$$

shows, for larger-than-physical pion mass using the p4-action [\[7\]](#page-8-3) and recently for HISQ quarks at physical mass [\[8\]](#page-8-4), a peak near the QCD crossover. It is similarly interesting to see whether the peak in this observable, which is also derived from the Polyakov loop, can be understood through chiral scaling as well.

In these proceedings we summarize our findings in Ref. [\[9\]](#page-8-5), that at physical and smaller m_l , the Polyakov loop and related observables such as F_q are influenced by the chiral transition. Data used for this part of the project that are presented in the figures can be found online in Ref. [\[10\]](#page-8-6). We also report our progress analyzing χ_{Q,μ_B^2} .

2. Chiral scaling of Polyakov loop observables

QCD thermodynamics in a neighborhood of the chiral critical point at $m_l = 0$ and critical temperature T_c can be described by some effective Lagrangian. Any operator appearing in this

¹We have made explicit in this equation the dependence of P and F_q on the temperature T and H . We will sometimes not explicitly write these dependencies to keep the notation light.

Lagrangian may either break the global $SU(2)_L \times SU(2)_R$ chiral symmetry explicitly or respect it. In the former case, the operator comes with a symmetry-breaking coupling, and we call the operator magnetization-like^{[2](#page-2-0)}; in the latter case it is an energy-like operator. Since P is trivially invariant under chiral rotations, it is an energy-like operator, *i.e.* it has the same scaling function as the energy density. Near the critical point, energy-like observables can be expressed as the sum of a regular part, which is an analytic function in the symmetry-breaking parameter H and the reduced temperature $t \equiv (T - T_c)/T_c$, and a singular part, which is determined by a universal scaling function of the scaling variable $z = z_0 t H^{-1/\beta \delta}$. Here β and δ are universal critical exponents, and z_0 is a non-universal constant that sets the scale of z .

In the continuum limit with two light flavors, the chiral phase transition is expected to fall in the $O(4)$ universality class $[11]$, and while this is not known with absolute certainty, recent lattice calculations present evidence favoring this scenario [\[12,](#page-8-8) [13\]](#page-8-9). Therefore in this study we used scaling functions belonging to the 3-d, $O(N)$ universality class. We used HISQ fermions without performing a continuum limit extrapolation; therefore due to taste violations, the relevant universality class is [3](#page-2-1)-d, $O(2)$ with critical exponents³ [\[14\]](#page-8-10)

$$
\beta = 0.349
$$
, $\delta = 4.780$, and $\alpha = 2 - \beta(1 + \delta) = -0.0172$. (4)

Since F_q/T is an energy-like observable, its scaling behavior can be expressed as [\[15\]](#page-8-11)

$$
F_q/T = AH^{(1-\alpha)/\beta\delta} f'_f(z) + f_{\text{reg}}(T, H),\tag{5}
$$

where A is another non-universal constant, $f'_{f}(z)$ is the z-derivative of the scaling function f_{f} characterizing the singular part of the logarithm of the partition function, and

$$
f_{\text{reg}} = \sum_{i,j} a_{i,2j}^r \ t^i H^{2j} \equiv \sum_j p_{2j}^r (T) H^{2j}.
$$
 (6)

Note that we consider above the infinite volume scaling ansatz since we perform our analysis on data obtained from simulations with the largest volumes. The strategy is to start with the scaling behavior^{[4](#page-2-2)} eq. [\(5\)](#page-2-3) and derive the other observables from this. For instance from eq. (5) and eq. [\(2\)](#page-1-1) one finds

$$
\langle P \rangle = \exp\left(-AH^{(1-\alpha)/\beta\delta}f'_f(z) - f_{\text{reg}}\right). \tag{7}
$$

Also making use of the relation between f_f and the order parameter scaling function f_G ,

$$
f_G(z) = -\left(1 + \frac{1}{\delta}\right) f_f(z) + \frac{z}{\beta \delta} f'_f(z) ,
$$
 (8)

we obtain the quark mass dependence near the critical point

$$
\frac{\partial F_q/T}{\partial H} = -AH^{(\beta - 1)/\beta \delta} f'_G(z) + \frac{\partial f_{\text{reg}}}{\partial H}.
$$
\n(9)

³The O(2) critical exponents β and δ are close to those of O(4), and importantly α < 0 for both universality classes.

²We are borrowing nomenclature from spin systems.

⁴In principle one could have taken $\langle P \rangle$ as the starting point.

Equation [\(9\)](#page-2-4) is especially interesting for us; since $(\beta - 1)/\beta \delta < 0$, this quantity will diverge in the chiral limit, meaning that the singular contribution will dominate for sufficiently small H . Finally for the temperature dependence, we find

$$
T_c \frac{\partial F_q}{\partial T} = A z_0 H^{-\alpha/\beta \delta} f_f''(z) + T_c \frac{\partial f_{\text{reg}}}{\partial T}.
$$
 (10)

In order to carry out fits to the above functional forms, we need some detailed information about the scaling function f_f . We do this using expansions of f_f about $z = 0$ and $z = \pm \infty$, using the notation of Ref. [\[15\]](#page-8-11) and fitting to the 3-d, $O(2)$ data of Ref. [\[14\]](#page-8-10). Inserting this expansion into eq. [\(5\)](#page-2-3) we obtain at fixed T for small H

$$
\frac{F_q}{T} \sim \begin{cases}\na^-(T) + Ap_s^-(T) H & , T < T_c \\
a_{0,0}^r + A a_1 H^{(1-\alpha)/\beta\delta} & , T = T_c , \\
a^+(T) + p^+(T) H^2 & , T > T_c\n\end{cases}
$$
\n(11)

where $a^{\pm}(T) = A a_s^{\pm}(T) + f_{\text{reg}}(T, 0)$ and $p^+(T) = A p_s^+(T) + p_2^r$ $\binom{r}{2}(T)$ receive contributions from both singular and regular terms. Below the critical temperature, the dominant quark mass dependence arises from the singular term only^{[5](#page-3-0)}. We find

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

\n
$$
p_s^-(T) = (2 - \alpha - \beta \delta) (-z_0 t)^{1-\alpha-\beta\delta},
$$

\n
$$
p_s^+(T) = (2 - \alpha - 2\beta \delta) c_1^+(z_0 t)^{1-\alpha-2\beta\delta}.
$$
\n(12)

Again we follow the notation of Ref. [\[15\]](#page-8-11) with c_0^{\pm} $_{0}^{\pm}$, c_{1}^{+} $_1^+$, and a_1 denoting coefficients appearing in the parameterization of the scaling function f_f .

In the chiral limit, F_q and its temperature derivative become

$$
\frac{F_q(T,0)}{T} = a_{0,0}^r + t \left(a_{1,0}^r + A^{\pm} |t|^{-\alpha} \right) , \qquad (13)
$$

with $A^{\pm} = (2 - \alpha)z_0^{1-\alpha} c_0^{\pm}$ $_{0}^{\pm}A$, and

$$
T_c \frac{\partial (F_q(T,0)/T)}{\partial T} = a_{1,0}^r \left(1 + R^{\pm} |t|^{-\alpha}\right) , \qquad (14)
$$

with $R^{\pm} = (1-\alpha)A^{\pm}/a_{1,0}^{r}$. The temperature derivative of an observable scaling as an energy density is expected to scale as a specific heat; correspondingly we will call these observables C_V -like, and we expect eq. [\(14\)](#page-3-1) to exhibit C_V -like characteristics.

Similarly the baryon chemical potential μ_B is an energy-like coupling. We can include μ_B along with temperature in a general energy-like coupling, which we also label t:

$$
t \equiv \frac{1}{t_0} \left(\frac{T - T_c}{T_c} + \kappa \hat{\mu}_B^2 \right),\tag{15}
$$

⁵This linear term in *H* is consistent with what one expects from a heavy-light resonance gas [\[4,](#page-8-12) [16\]](#page-9-0) and heavy-quark effective theory/chiral perturbation theory [\[17\]](#page-9-1). For more details see Ref. [\[18\]](#page-9-2).

where t_0 and κ are non-universal constants. From eq. [\(15\)](#page-3-2) we see that taking two $\hat{\mu}_B$ derivatives is the same as taking one T derivative, which along with eq. [\(3\)](#page-1-2) leads to the expectation that χ_{Q,μ_B^2} should also be C_V -like. Taking derivatives of eq. [\(5\)](#page-2-3) and utilizing eq. [\(15\)](#page-3-2), one expects

$$
\chi_{Q,\mu_B^2} = 2\kappa z_0 A H^{-\alpha/\beta \delta} f_f^{\prime\prime}(z) + \frac{\partial^2 f_{\text{reg}}}{\partial \hat{\mu}_B^2}.
$$
\n(16)

Comparing eq. [\(16\)](#page-4-0) with eq. [\(10\)](#page-3-3), one sees clearly that the observables should behave qualitatively similarly in the chiral limit.

3. Computational setup and observables

Our study uses $N_f = 2 + 1$ HISQ configurations with m_s at its physical value and m_l varying in the range $H = m_l/m_s = 1/160 - 1/20$. These include gauge field ensembles generated previously by the HotQCD collaboration [\[12,](#page-8-8) [19](#page-9-3)[–21\]](#page-9-4) and some further configurations for $H = 1/40$ and $H = 1/80$. The bare coupling β for $H \le 1/27$ is taken in the range 6.26-6.50, which is chosen so T is near the chiral pseudocritical temperature. For $H = 1/20$ we also use data from calculations on lattices at smaller couplings, $\beta = 6.05, 6.125,$ and 6.175 [\[4\]](#page-8-12), which helps establish contact to the low T regime. We set the scale with f_K [\[22\]](#page-9-5) using a recent parameterization of lattice QCD results for $f_K a(\beta)$ [\[23\]](#page-9-6). We find no significant dependence of $\langle P \rangle$ on spatial volume [\[18\]](#page-9-2) and hence, we use the gauge ensembles with the largest volumes in our analysis. A summary of statistics used to analyze the scaling behavior of $\langle P \rangle$, F_q , and their derivatives is given in Ref. [\[18\]](#page-9-2).

The Polyakov loop requires a multiplicative renormalization,

$$
P = e^{-c(g^2)N_\tau} P^{\text{bare}},\tag{17}
$$

i.e. the renormalized P appears in eq. [\(2\)](#page-1-1). When needed, renormalization constants $c(g^2)$ are obtained from an interpolation of Table V of Ref. [\[5\]](#page-8-13). We note however that derivatives of the free energy such as

$$
\frac{\partial F_q/T}{\partial H} = -\frac{1}{\langle P \rangle} \frac{\partial \langle P \rangle}{\partial H} = \langle P \cdot \Psi \rangle - \langle P \rangle \langle \Psi \rangle \quad \text{and} \quad T_c \frac{\partial F_q/T}{\partial T} = -\frac{T_c}{\langle P \rangle} \frac{\partial \langle P \rangle}{\partial T} \tag{18}
$$

are independent of the renormalization in the continuum limit, since this cancels out in the ratio. Here $\Psi = \frac{1}{2}m_s$ tr D_l^{-1} is an extensive observable written in terms of the dimensionless bare strange quark mass $\hat{m_s}$ and the staggered Dirac matrix D_l . Similarly χ_{Q,μ_B^2} , which can be extracted as [\[8\]](#page-8-4)

$$
\chi_{Q,\mu_B^2} = \frac{1}{9} \left(\frac{\langle \text{Re } P \ (n^2 + n') \rangle}{\langle \text{Re } P \rangle} - \langle n^2 + n' \rangle + \frac{\langle (\text{Re } P + \text{Im } P) \ n \rangle^2}{\langle \text{Re } P \rangle^2} \right),\tag{19}
$$

where the total quark number *n* in the $N_f = 2 + 1$ HISQ formulation is

$$
n = 2n_l + n_s, \t n_f = \frac{1}{4} \text{tr} \, D_f^{-1} \partial_{\hat{\mu}_f} D_f, \t n' = 2\partial_{\hat{\mu}_l} n_l + \partial_{\hat{\mu}_s} n_s,
$$
(20)

should be renormalization independent. To extract χ_{Q,μ_B^2} we used about 2.5 million molecular dynamic time units (MDTU) per temperature for $H = 1/27$ and about 125,000 MDTU for $H = 1/40$, including some newly generated configurations for the latter.

Figure 1: Scaling and T-dependence of $\partial (F_q/T) \partial H$. Data with filled symbols are not included in the fits. Left: Rescaled $\partial (F_a/T)/\partial H$ as a function of z. *Right*: Derivative of $\partial (F_a/T)/\partial H$ as a function of T. The chiral limit result obtained from this fit is shown as grey bands. Solid curves are fits that include $H = 1/27$ data, while hatched curves are fits that exclude this these points. Images taken from Ref. [\[9\]](#page-8-5).

4. Results

In Fig. [1](#page-5-0) (left) we show data for $\partial (F_q/T)/\partial H$ rescaled with the power of H according eq. [\(9\)](#page-2-4). That data for different H largely fall on top of each other suggests that $\partial (F_q/T)/\partial H$ indeed diverges as $H^{(\beta-1)/\beta\delta}$ as $H\to 0$ and that H-dependent contributions to F_q/T originating from f_{reg} are small compared to those coming from the singular part. We therefore employ an H -independent fit ansatz for f_{reg} , *i.e.* we use $f_{\text{reg}}(T, H = 0)$ in every fit. We performed this 3-parameter fit for each data set by either including or leaving out the $H = 1/27$ $H = 1/27$ $H = 1/27$ data; the results are shown in Fig. 1 (right). The fit parameters A, T_c , and z_0 are given in Table I of Ref. [\[9\]](#page-8-5). The parameters T_c and z_0 agree well with earlier results for chiral susceptibilities in $(2+1)$ -flavor QCD [\[12\]](#page-8-8).

Looking back at eq. [\(11\)](#page-3-4), it is instructive to note that below T_c the next most significant term in H, which goes as $H^{3/2}$, will also receive contributions from singular terms only. This term turns out to be negative; therefore one expects $\partial (F_q/T)/\partial H$ to increase with decreasing H toward the chiral limit behavior, $Ap_s^-(T)$. From the hyperscaling relation $\alpha = 2 - \beta(1 + \delta)$, this is proportional to $|t|^{\beta-1}$. Correspondingly in Fig. [2](#page-6-0) (right) one sees an increase with decreasing H below T_c toward the expected chiral limit T -dependence.

Next, following our master equation [\(5\)](#page-2-3) we assume for F_q/T a functional form

$$
\frac{F_q}{T} \approx AH^{(1-\alpha)/\beta\delta} f'_f \left(z_0 \frac{T - T_c}{T_c} H^{-1/\beta\delta} \right) + a'_{0,0} + a'_{1,0}t \tag{21}
$$

keeping the leading *t*-dependence in the regular term. We use the previously determined A, T_c , and z_0 and fit the remaining two regular parameters to the F_q/T data, shown in Fig. [2](#page-6-0) (left). The T range and data used in the fit are shown in the inset. The resulting fit parameters $a_{0,0}^r$ and $a_{1,0}^r$ are also given in Table I of Ref. [\[9\]](#page-8-5). We also show in this figure the heavy-light meson contribution to F_a/T calculated in the hadron-gas approximation [\[4,](#page-8-12) [16\]](#page-9-0).

Once we have determined all five fit parameters for F_q/T , we can plug them into eq. [\(7\)](#page-2-5) to arrive at the T and H dependence of $\langle P \rangle$. The thus determined curves are shown in Fig. [2](#page-6-0) (right). As seen in the inset, they agree well with $\langle P \rangle$ data near $T_c^{N_{\tau}=8} = 144(2)$ MeV [\[12\]](#page-8-8), which suggests

Figure 2: Chiral fits for F_q/T and $\langle P \rangle$. The insets show data in the T range covered by the fit. Both fits include $H = 1/27$ data. The chiral limit results obtained from the fit are shown as a grey band. The solid gold line shows the heavy-light meson contribution calculated in the hadron-gas approximation [\[4\]](#page-8-12). *Left*: *T*-dependence of F_q/T . *Right*: *T*-dependence of $\langle P \rangle$. Images taken from Ref. [\[9\]](#page-8-5).

Figure 3: *Left:* Comparison of C_V at $H = 0$ for the 3-d, O(2) spin model taken from Ref. [\[24\]](#page-9-7) (dashed line) and $-T_c \partial (F_q(T,0)/T)/\partial T$ (solid line). The former curve is shifted vertically by a constant for easier comparison. The inset shows how the spike in $-T_c\partial (F_q/T)/\partial T$ develops in the chiral limit. Image taken from Ref. [\[9\]](#page-8-5). *Right:* Response of F_q/T to μ_B as a function of T. The vertical yellow band indicates $T_c^{N_\tau=8}$ [\[12\]](#page-8-8). The blue band is an interpolation based on results from Ref. [\[8\]](#page-8-4).

the behavior of $\langle P \rangle$ is explained well by chiral scaling in this region and serves as a consistency check of our approach.

In the chiral limit, the T-dependence of both F_q/T and $\langle P \rangle$ exhibit a small kink at T_c . This kink hints toward a characteristic spike found in C_V -like observables in $O(N)$ universality classes, which we examine using eqs. [\(13\)](#page-3-5) and [\(14\)](#page-3-1). Although at T_c the contribution to the slope of F_q/T is entirely given by the regular term $a_{1,0}^r$, near T_c this contribution gets mostly canceled by the singular contributions $A^{\pm} |t|^{-\alpha}$. This is the origin of the spike. In the chiral limit our fit results suggest the appearance of this spike in the T-derivatives of $F_q(T, 0)/T$ as well as $\langle P \rangle$.

The basic features found in our analysis of F_q/T and $\langle P \rangle$ are quite similar to those found in the analysis of 3-d, $O(2)$ symmetric spin models [\[24\]](#page-9-7). Also in that case a large cancellation of contributions arising from regular and singular terms is found; the spike in C_V is concentrated in a temperature interval of about 1% around T_c , where C_V changes by almost a factor 10. In Fig. [3](#page-6-1) (left) we show a comparison of the behavior of C_V in O(2) spin models [\[24\]](#page-9-7) and our result for $-T_c \frac{\partial (F_a/T)}{\partial T}$ at $H = 0$. The inset shows the development of this sharp peak as m_l decreases. Clearly, this feature becomes visible only for H being substantially smaller than the light quark masses $H \approx 10^{-2}$ that are accessible in modern lattice QCD calculations.

Our preliminary results for the susceptibility χ_{Q,μ_B^2} at $H = 1/27$ and $H = 1/40$ are shown in Fig. [3](#page-6-1) (right) along with an interpolation of $H = 1/27$ data from Ref. [\[8\]](#page-8-4). Here we find excellent agreement with their results at physical m_l . At our current statistical power, our results for $H = 1/40$ are consistent with $H = 1/27$. Besides the fact that χ_{Q,μ_B^2} is somewhat noisy, the ability to resolve a clear peak will depend on the relative importance of singular and regular contributions[6](#page-7-1). To try to address these issues, we plan to increase the statistics and lower H , where we expect the apparent peak in this quantity to shift closer to T_c . We hope to eventually carry out a complete scaling analysis as has been done with the other C_V -like observables.

5. Conclusion and outlook

For $N_f = 2 + 1$ HISQ fermions at $N_{\tau} = 8$ near and below physical m_l , we find $\partial_H F_q$ diverges as $H \to 0$ according to the 3-d, O(2) universality class. The Polyakov loop is described well by the 3-d, O(2) scaling function near T_c , and $\partial_T F_a$ behaves qualitatively similarly as C_V in O(2) spin models. We expect this behavior to be consistent with $O(4)$ in the continuum limit. We stress that the lack of an *a priori* reason to associate $\langle P \rangle$ with deconfinement along with its consistency with $O(N)$ scaling cast serious doubt on attempts to interpret it as an indicator for the deconfinement of light degrees of freedom near and below physical m_l .

We are in the process of investigating the chiral behavior of χ_{Q,μ_B^2} , which we expect also to be C_V -like. More statistics are required at $H = 1/40$. We plan to calculate this observable for $H = 1/80$ and smaller in order to also investigate its scaling behavior.

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⁶We encounter this problem with other observables expected to be C_V -like. For example fourth-order conserved charge fluctuations are C_V -like, and for this reason one generally expects to find a peak near T_c ; nevertheless contributions of the regular terms to the fourth-order strangeness fluctuation are significant enough to render it monotonic near T_c [\[25\]](#page-9-8). Similarly the Polyakov loop susceptibility is C_V -like. At finite N_{τ} one finds monotonic behavior near T_c [\[6\]](#page-8-2), which may again be due to significant regular contributions.

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