


Sensitivity of the Polyakov loop and related observables to chiral symmetry restoration

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While the Polyakov loop is an order parameter of the deconfinement transition in the heavy quark mass regime of QCD, its sensitivity to the deconfinement of light, dynamical quarks in QCD is not apparent. On the other hand, the quark mass dependence of the Polyakov loop is sensitive to the appearance of a chiral phase transition. Using lattice QCD calculations in the staggered fermion discretization scheme at finite values of the lattice spacing, $aT = 1/8$, we show here, for the first time, that the Polyakov loop expectation value, and the heavy quark free energy extracted from it, behaves like an energylike observable in the vicinity of the chiral phase transition temperature T_c . Consistent with scaling behavior of energylike observables in the $3d$, $O(2)$ universality class, the quark mass derivatives diverge in the chiral limit at T_c while the temperature derivatives stay finite. The latter will develop a characteristic spike at T_c . This, however, may be resolved only in calculations with quark masses being 2 orders of magnitude smaller than those currently accessible in lattice QCD calculations.

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I. INTRODUCTION

The Lagrangian of quantum chromodynamics (QCD), the theory describing interactions controlled by the strong force, possesses exact global symmetries only in the massless (chiral) and infinite quark mass (pure gauge) limits. The latter case has been extensively exploited in lattice QCD calculations to discuss the deconfinement phase transition in pure gauge theories [1–3] and its imprint in the heavy quark sector of QCD. Also, in the light quark mass region, the rapid change of the Polyakov loop expectation value, $\langle P \rangle$, as function of the temperature, characterized by an inflection point in its T -dependence, is often taken as an indication for the occurrence of deconfinement. However, studies with (almost) physical light up and down quark masses and improved discretization schemes for the QCD Lagrangian, performed closer to the continuum limit, in general show that the QCD transition is a smooth crossover, and no evidence for an inflection point in the vicinity of the chiral transition temperature is found [4–7].

In the limit of vanishing values of the two light quark masses, the chiral flavor symmetry, $SU(2)_L \times SU(2)_R$, gets

restored above a temperature T_c , giving rise to a chiral phase transition [8]. In QCD, the nonzero light quark masses, m_l , are small on the scale of relevant temperatures, e.g., T_c . Thus, the light quark chiral condensate, $\langle \bar{\psi}\psi \rangle$, is a good indicator for the occurrence of a phase transition in the chiral limit of QCD. The maxima in either the quark mass or temperature derivatives of $\langle \bar{\psi}\psi \rangle$ diverge in the chiral limit, and for $m_l > 0$ the positions of these maxima define pseudocritical temperatures that converge to T_c in the chiral limit.

The Polyakov loop is a purely gluonic observable that is trivially invariant under chiral transformations in the fermion sector of the QCD Lagrangian. As far as critical behavior close to a second order phase transition point is concerned, it thus may be expected that $\langle P \rangle$ as well as the heavy quark free energy, $F_q = -T \ln \langle P \rangle$, behave like any other “energylike” operator that may appear in an effective Hamiltonian describing e.g., QCD thermodynamics in the vicinity of the chiral phase transition. One may thus expect that $\langle P \rangle$ as well as F_q/T are sensitive to critical behavior arising from this transition.

Here we present results on the temperature and quark mass dependence of $\langle P \rangle$ and F_q/T close to the chiral limit. We show that both of them reflect properties of energylike observables in the vicinity of T_c and discuss the resulting chiral limit behavior. As we will perform calculations at a nonzero value of the lattice spacing, using the highly improved staggered quark (HISQ) action, the relevant symmetry group for the discussion of universal scaling

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properties is the $O(2)$ rather than $O(4)$ group as it will be the case in the continuum limit of lattice QCD. However, as will become clear in the following, none of the qualitative features that will arise from the energylike behavior of the Polyakov loop in theories with global $O(N)$ symmetry will depend on this difference.

II. POLYAKOV LOOP AND THE HEAVY QUARK FREE ENERGY

For lattice QCD in a finite Euclidean space-time volume $N_\sigma^3 \times N_\tau$, the Polyakov loop, $P_{\vec{x}}$, and its spatial average, P ,

$$P_{\vec{x}}^{\text{bare}} \equiv \frac{1}{3} \text{tr} \prod_{\tau} U_4(\vec{x}, \tau), \quad P \equiv \frac{1}{N_\sigma^3} e^{N_\tau c(g^2)} \sum_{\vec{x}} P_{\vec{x}}^{\text{bare}},$$

are given in terms of $SU(3)$ -valued field variables, $U_4(\vec{x}, \tau)$, defined on the temporal link ($\mu = 4$) originating at a Euclidean space-time point (\vec{x}, τ) . The volume $V = (N_\sigma a)^3$ and inverse temperature $T^{-1} = N_\tau a$ are given in terms of the lattice spacing a . The bare Polyakov loop, P^{bare} , has been renormalized using renormalization constants, $c(g^2)$, determined in Ref. [6] (Table V) for the regularization scheme used also in this work.

The heavy quark free energy, F_q/T , characterizes the behavior of correlation functions between static quark and antiquark sources at infinite distances [9],

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

Here $H = m_l/m_s$ parametrizes the quark mass dependence in terms of the ratio of degenerate light quark masses $m_l \equiv m_u = m_d$ and the strange quark mass m_s . For the analysis of the quark mass dependence of the heavy quark free energy, we calculate the renormalization-scheme-independent mixed susceptibility,

$$\frac{\partial F_q(T, H)/T}{\partial H} = -\frac{1}{\langle P \rangle} \frac{\partial \langle P \rangle}{\partial H} \equiv -\frac{\chi_{mP}}{\langle P \rangle}, \quad (2)$$

with the quark mass derivative of $\langle P \rangle$ given by

$$\chi_{mP} \equiv \frac{\partial \langle P \rangle}{\partial H} = \langle P \cdot \Psi \rangle - \langle P \rangle \langle \Psi \rangle. \quad (3)$$

Here $\Psi \equiv \frac{1}{2} \hat{m}_s \text{tr} M_l^{-1}$ denotes the extensive observable defining a dimensionless combination of the two-flavor light quark chiral condensate in terms of the light quark, staggered fermion matrix M_l ; \hat{m}_s is the bare strange quark mass in lattice units, $m_s/T = \hat{m}_s N_\tau$.

Using fit results for F_q/T and its derivative with respect to the quark mass, we will also be able to determine the derivatives of $\langle P \rangle$ and F_q/T with respect to T . Similar to

the H -derivatives, these derivatives are closely related to each other,

$$T_c \frac{\partial F_q(T, H)/T}{\partial T} = -\frac{T_c}{\langle P \rangle} \frac{\partial \langle P \rangle}{\partial T}. \quad (4)$$

III. POLYAKOV LOOP AND CHIRAL SYMMETRY RESTORATION

Within Wilson's renormalization group approach [10,11], thermodynamics in the vicinity of a critical point can be described by an effective Hamiltonian, which is defined in a multidimensional 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 energylike, while in the latter case it is magnetizationlike. In QCD the two-flavor, light quark chiral condensate is a typical magnetizationlike operator.

The Polyakov loop is invariant under chiral transformations of the quark fields. Its expectation value, $\langle P \rangle$, as well as the heavy quark free energy, F_q/T , thus are energylike observables. We expect that they are sensitive to the chiral phase transition to the extent that they receive nonanalytic (singular) contributions in addition to analytic (regular) terms. In the vicinity of the critical point, i.e., close to $(T, H) = (T_c, 0)$, nonanalytic contributions are universal scaling functions of a scaling variable $z = z_0 t H^{-1/\beta\delta}$ with $t = (T - T_c)/T_c$ and z_0, T_c being nonuniversal constants. Energylike observables receive contributions from the scaling function, $f'_f(z) = df_f(z)/dz$, of the $3d$, $O(N)$ universality class [12], which is the derivative of the scaling function $f_f(z)$ that characterizes the singular part of the logarithm of the partition function. For the heavy quark free energy, we use the scaling ansatz,

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

where A is another nonuniversal constant and the critical exponents are β , δ , and $\alpha = 2 - \beta(1 + \delta)$. The regular contribution is an analytic function, which close to $(T_c, 0)$ can be given as a Taylor series with even powers in H ,

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

Using Eqs. (1) and (5), the Polyakov loop expectation value may be written as

$$\langle P \rangle_{T,H} = \exp(-AH^{(1-\alpha)/\beta\delta} f'_f(z) - f_{\text{reg}}(T, H)). \quad (7)$$

Note that for (T, H) close to $(T_c, 0)$ Eq. (7) reduces to the usual nonexponential scaling ansatz.

Using the known asymptotic behavior of $f_f(z)$ for $z \rightarrow \pm\infty$ [12], we obtain from Eq. (5) for the quark mass dependence of F_q/T at fixed T and for small H ,

$$\frac{F_q(T, H)}{T} \sim \begin{cases} a^-(T) + Ap_s^-(T)H, & T < T_c \\ a_{0,0}^r + Aa_1H^{(1-\alpha)/\beta\delta}, & T = T_c, \\ a^+(T) + p^+(T)H^2, & T > T_c, \end{cases} \quad (8)$$

with $a^\pm(T) = Aa_s^\pm(T) + f_{\text{reg}}(T, 0)$ as well as $p^+(T) = Ap_s^+(T) + p_2^+(T)$ receiving contributions from both the singular and regular terms. For $T \leq T_c$, the dominant quark mass dependence arises from the singular term only. In particular, we have

$$\begin{aligned} a_s^\pm(T) &= (2 - \alpha)z_0^{1-\alpha}c_0^\pm t|t|^{-\alpha}, \\ p_s^-(T) &= (2 - \alpha - \beta\delta)(-z_0t)^{1-\alpha-\beta\delta}, \\ p_s^+(T) &= (2 - \alpha - 2\beta\delta)c_1^+(z_0t)^{1-\alpha-2\beta\delta}, \end{aligned} \quad (9)$$

where we followed the notation of Ref. [12] with c_0^\pm , c_1^+ , and a_1 denoting coefficients appearing in the parametrization of the scaling function $f_f(z)$.

For the $3d$, $O(4)$ universality class these coefficients are given in [12]. As we will present here only, results from calculations for one nonzero value of the lattice spacing, $a = 1/8T$, and do not perform a continuum extrapolation, we will use the critical exponents and scaling functions of the $3d$, $O(2)$ universality class. We extracted these from [13], where the scaling functions are parametrized in the Widom-Griffiths form. We use $a_1 = 0.4734$, $c_0^- = 2.447$, $c_0^+ = 2.728$, $c_1^+ = -0.678$, along with $\beta = 0.349$, $\delta = 4.780$ [13–15].

Making use of the relation between scaling functions, $f_f(z)$ and that of the order parameter, $f_G(z)$ (see e.g., [12]), we obtain in the vicinity of T_c ,

$$\frac{\partial F_q(T, H)/T}{\partial H} = -AH^{(\beta-1)/\beta\delta}f'_G(z) + \frac{\partial f_{\text{reg}}(T, H)}{\partial H}. \quad (10)$$

The derivative of F_q/T with respect to T is given by

$$T_c \frac{\partial F_q(T, H)/T}{\partial T} = Az_0H^{-\alpha/\beta\delta}f''_f(z) + T_c \frac{\partial f_{\text{reg}}(T, H)}{\partial T}. \quad (11)$$

As $\alpha/\beta\delta < 0$ for the $3d$, $O(2)$ as well as $O(4)$ universality classes, the derivatives of $\langle P \rangle$ and F_q/T with respect to T do not diverge at T_c in the limit $H \rightarrow 0$. On the other hand, the corresponding quark mass derivatives, Eq. (10), are expected to diverge when approaching the chiral limit at T_c as well as when approaching T_c from below at $H = 0$. A possible influence of the chiral phase transition on the quark mass dependence of $\langle P \rangle$ and F_q/T is thus much easier to establish than on their temperature dependence.

IV. COMPUTATIONAL SETUP AND DATA ANALYSIS

In this study, we analyze properties of $(2+1)$ -flavor QCD where the strange quark mass has been kept fixed to its physical value and the two degenerate light quark masses are varied in the range $H = 1/20$ to $1/160$, corresponding to a pion mass $160 \text{ MeV} \gtrsim m_\pi \gtrsim 58 \text{ MeV}$ [16]. The analysis is performed on sets of gauge field configurations that had been generated previously by the HotQCD Collaboration [16–19] on lattices of size $32^3 \times 8$ ($H = 1/20, 1/27$), $40^3 \times 8$ ($H = 1/40$), and $56^3 \times 8$ ($H = 1/80, 1/160$) using HISQ [20] and the tree-level improved Symanzik gauge action. These data have previously been used in calculations of pseudo-critical temperatures [21] and the chiral phase transition temperature of $(2+1)$ -flavor QCD [16]. We also have generated additional configurations for $H = 1/40, 1/80$. For the scale setting, we use the kaon decay constant obtained in calculations with the HISQ action, i.e., $f_K = 156.1/\sqrt{2} \text{ MeV}$ [22].

Observables have been calculated on lattices with temporal extent $N_\tau = 8$ and $N_\sigma/N_\tau = 4-7$. For $H = 1/80$, we have results for the entire range of aspect ratios, N_σ/N_τ . An analysis of finite volume effects on $\langle P \rangle$ shows no significant volume dependence of $\langle P \rangle$ in the entire temperature range. Results for different N_σ/N_τ agree within errors of about 1%. We thus can safely neglect any finite volume corrections to our results for $\langle P \rangle$. The statistics used in this study can be found in [15], along with more details for the finite volume dependence of $\langle P \rangle$.

V. RESULTS

In Fig. 1 (left), we show results for the derivative of $F_q(T, H)/T$ with respect to H as function of T . It is apparent that $\partial(F_q/T)/\partial H$ decreases with quark mass at high temperature and increases at low temperature. This is consistent with an approach toward zero at high T and a nonvanishing, strongly temperature dependent constant at low T . Such a pattern is in accordance with the expected quadratic dependence on H for $T > T_c$ and the linear dependence for $T < T_c$ given in Eq. (8). 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 $T \sim 145-150 \text{ MeV}$ which are close to the chiral phase transition temperature on lattices with temporal extent $N_\tau = 8$ determined in [16], $T_c^{N_\tau=8} = 144(2) \text{ MeV}$. With decreasing H , they approach $T_c^{N_\tau=8}$ and the peak height increases.

In Fig. 1 (middle), we show $\partial(F_q/T)/\partial H$ rescaled with the appropriate power of H expected from the $O(2)$ scaling ansatz and plotted versus z . The good scaling behavior suggests that $\partial(F_q/T)/\partial H$ will indeed diverge in the chiral limit and that H -dependent contributions to F_q/T , arising

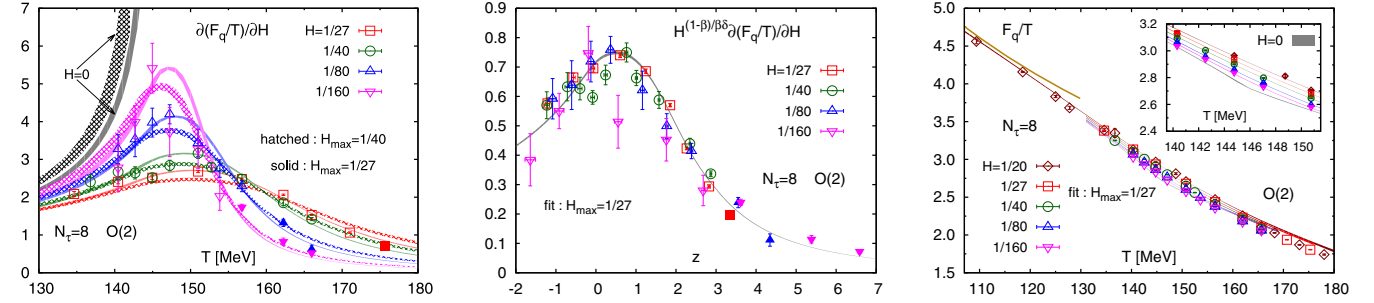


FIG. 1. Derivative of $F_q(T, H)/T$ with respect to H as function of T (left) and the rescaled version for the fit with $H_{\max} = 1/27$ as function of z (middle). Shown are results for several values of m_l , calculated on lattices with temporal extent $N_\tau = 8$. Curves in the left-hand figure show results of fits, with and without the data sets for $H = 1/27$, based on the scaling ansatz given in Eq. (10), with fit parameters given in Table I. Data shown with filled symbols correspond to $z \geq 3$ and have not been included in the fit. The right-hand figure shows F_q/T versus T . Fits are explained in the text. The inset in the right-hand figure shows data in the temperature range covered by the fits. The chiral limit result for $H = 0$ obtained from these fits is shown as gray bands (left, right). The solid gold line in the right-hand figure shows the static-light meson contribution to F_q/T [23].

from regular terms, are small compared to those coming from the singular part. This motivated a fit ansatz for the regular term that is independent of H , i.e., we use $f_{\text{reg}}(T, H = 0)$ in all our fits.

A fit to $\partial(F_q/T)/\partial H$ thus only involves the singular term of Eq. (10). We performed this three-parameter fit for all data sets with $H \leq H_{\max}$ by either including or leaving out the data for $H = 1/27$. These fits are shown in Fig. 1 (left), and the corresponding fit parameters, A , T_c , z_0 , are given in Table I. In particular, we find that T_c , obtained from these fits, as well as the nonuniversal scale parameter z_0 , agree well with earlier fit results for chiral susceptibilities [16] in $(2+1)$ -flavor QCD. The rescaled fits are also shown in Fig. 1 (middle).

Data for $F_q(T, H)/T$ are shown in Fig. 1 (right). They have been fitted to the scaling ansatz Eq. (5) using only the constant and linear H -independent terms in the regular part as fit parameters and keeping fixed the three nonuniversal constants, determined in the previous step, in the singular part. The T -range and data included in the fit are shown in the inset. The resulting fit parameters, $a'_{0,0}$, $a'_{1,0}$, are given in Table I. In this figure, we also show the static-light meson contribution to F_q/T calculated in the hadron-gas approximation [23,24]. In chiral perturbation theory, this also gives a linear dependence on H at low temperature [25].

Once we have determined all five fit parameters for $F_q(T, H)/T$, we can plug them into Eq. (7) to arrive at a

TABLE I. Summary of fit parameters for $F_q(T, H)/T$ and the ratio R^+ introduced in Eq. (13). The parameters for the singular part (A, T_c, z_0) have been obtained from a fit to $\partial(F_q/T)/\partial H$.

H_{\max}	Singular part			Regular part			R^+
	A	T_c	z_0	$a'_{0,0}$	$a'_{1,0}$		
1/27	2.48(2)	145.6(3)	2.24(5)	2.74(1)	-34.4(7)	-0.92(1)	
1/40	2.26(5)	144.2(6)	1.83(9)	2.81(3)	-27(1)	-0.86(1)	

parameter-free description of the T and H dependence of $\langle P \rangle$. The thus determined curves are shown in Fig. 2. As seen in the inset, they agree well with $\langle P \rangle$ data near $T_c^{N_\tau=8}$, which suggests the behavior of $\langle P \rangle$ is explained well by chiral scaling behavior in this region and serves as a consistency check of our approach.

In Figs. 1 (right) and 2 (top), we also show the chiral limit ($H = 0$) results for F_q/T and $\langle P \rangle$. For the former, this is a sum of regular and singular contributions,

$$\frac{F_q(T, 0)}{T} = a'_{0,0} + t(a'_{1,0} + A^\pm |t|^{-\alpha}), \quad (12)$$

with $A^\pm = (2 - \alpha)z_0^{1-\alpha}c_0^\pm A$; see Eq. (9). 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 (second derivatives with respect to T) in the $O(N)$ universality classes. In the chiral limit, our fit results suggest the appearance of such a spike in the temperature derivatives of $F_q(T, 0)/T$ as well as $\langle P \rangle$. For the former, we obtain from Eq. (12),

$$T_c \frac{\partial(F_q(T, 0)/T)}{\partial T} = a'_{1,0}(1 + R^\pm |t|^{-\alpha}), \quad (13)$$

with $R^\pm = (1 - \alpha)A^\pm/a'_{1,0}$. R^+ is given in Table I and $R^+/R^- = c_0^+/c_0^- = 1.12(5)$ is a universal ratio [26]. This makes it evident that already for $|t| = 0.01$ the slope of $-F_q/T$ is about a factor 5 smaller than at T_c .

The basic features found in our analysis of $(2+1)$ -flavor QCD are quite similar to those found in the analysis of $3d$, $O(2)$ symmetric spin models [26]. Also in that case a large cancellation of contributions arising from regular and singular terms is found; the spike in the specific heat, C_V , is concentrated in a temperature interval of about 1% around T_c , and C_V changes by almost a factor 10 in this

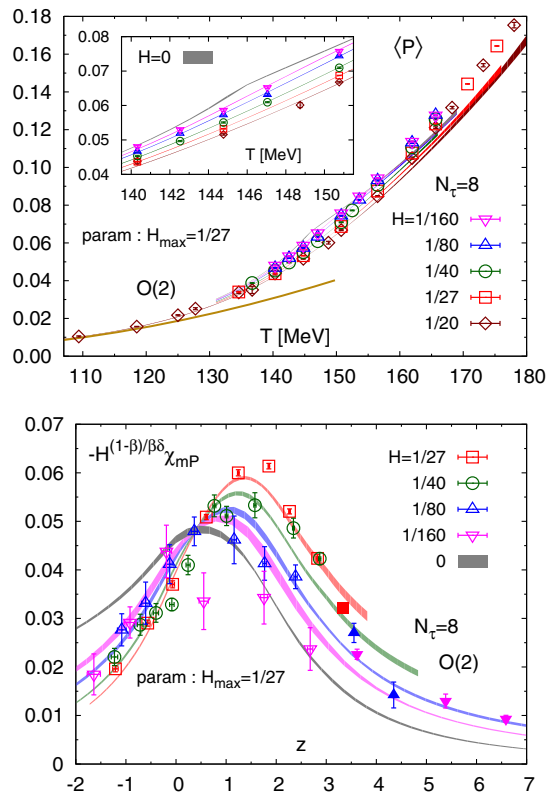


FIG. 2. Top: T dependence of $\langle P \rangle$ obtained on lattices with temporal extent $N_\tau = 8$ for several values of H . The inset shows data in the T range covered by the fit. Curves are based on a fit that used for the singular part parameters for $H_{\max} = 1/27$ given in Table I. The chiral limit result for $H = 0$ obtained from this fit is shown as a gray band. The solid gold line is as described in Fig. 1. Bottom: derivative of $\langle P \rangle$ versus scaling variable z .

temperature interval. In Fig. 3, we show a comparison of the scaling behavior of $-T_c \partial(F_q(T, 0)/T)/\partial T$, obtained for the case of $(2 + 1)$ -flavor QCD, and C_V in $O(2)$ spin

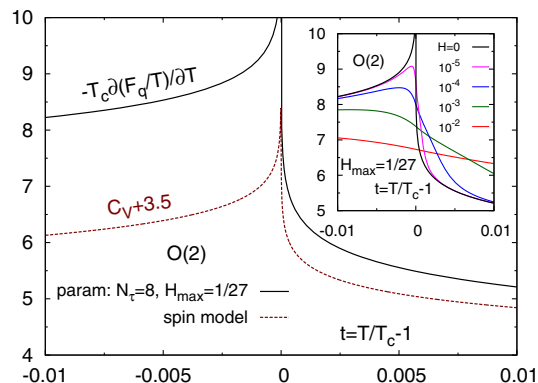


FIG. 3. Comparison of fits to the specific heat at $H = 0$ of the $3d, O(2)$ spin model taken from Ref. [26] (dashed line) and the negative of the temperature derivative of $F_q(T, 0)/T$ (solid line). The former curve is shifted vertically by a constant for easier comparison with the spin model result.

models at $H = 0$ [26]. The inset shows the development of this sharp peak as the quark mass decreases. It makes clear that this feature becomes visible only for H being substantially smaller than the region $H \simeq 10^{-2}$ that is accessible in current lattice QCD calculations.

VI. CONCLUSIONS

We have examined the quark mass dependence of the Polyakov loop expectation value and the heavy quark free energy extracted from it. We provided evidence for the influence of chiral symmetry restoration that manifests in the singular behavior of the quark mass derivatives of $\langle P \rangle$ and F_q/T and arises from the energylike behavior of these observables with respect to chiral transformations. These derivatives diverge at T_c in the chiral limit, consistent with the expected behavior for energylike observables in the $3d, O(2)$ universality class.

We showed that at finite values of the lattice spacing the relative distribution between singular and regular contributions to the energylike variables in QCD seems to be similar to that in the $3d, O(2)$ spin model. In particular, in the chiral limit, the very narrow spike showing up in specific-heat-like observables, which results from a partial cancellation of singular and regular contributions combined with the existence of a quite small, negative critical exponent α , is expected to show up also in the T -derivatives of F_q/T and $\langle P \rangle$.

As the critical exponent α also is negative and small in the $O(4)$ universality class, similar behavior of F_q/T and $\langle P \rangle$ is expected to persist in the continuum limit. However, as $|\alpha|$ is an order of magnitude larger compared to the $O(2)$ case, the spike may become broader and may also be more prominent already for larger quark masses. This may be tested also in effective model calculations.

All data from our calculations, presented in the figures of this paper, can be found in [27].

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Correction: A minor error in the first sentence of the Abstract has been fixed.