Chiral susceptibility in (2 + 1)-flavor QCD

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We calculate chiral susceptibilities in (2 + 1)-flavor QCD for different masses of the light quarks using the functional renormalization group (fRG) approach to first principles QCD. We follow the evolution of the chiral susceptibilities with decreasing masses as obtained from both the light-quark and the reduced quark condensate. The latter compares very well with recent results from the HotQCD Collaboration for pion masses $m_\pi \gtrsim 100$ MeV. For smaller pion masses, fRG and lattice results are still consistent. In particular, the estimates for the chiral critical temperature are in very good agreement. We close by discussing different extrapolations to the chiral limit.

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I. INTRODUCTION

The phase structure of QCD probed with heavy-ion collisions is well described by (2 + 1)-flavor QCD. While the charm, bottom, and top quarks are too heavy to significantly add to the dynamics of the system, the dynamics of the strange and, most importantly, of the light up and down quarks determine the rich phase structure in particular at large densities. Recently, functional methods for first-principles QCD have made significant progress in the description of this regime; see Refs. [1,2] for functional renormalization group studies (fRG) and, e.g., Refs. [3–5] for Dyson-Schwinger studies. Still, in the high-density regime, the systematic error of the current computations grows large. This asks for both systematically improved computations and a better error control. In turn, lattice simulations are obstructed by the sign problem at finite density and either rely on Taylor expansions at vanishing chemical potential [6–10] or on analytic continuations from imaginary to real quark chemical potential [11–17]. In summary, this suggests a two-tier strategy to tackle the high-density regime by direct systematically improved functional computations and a quantitative access to the zero-density limit.

Interestingly, the mass dependence of the phase structure at vanishing density can potentially constrain the phase structure at large density. For instance, low-energy effective theory computations indicate that the chiral phase transition temperature in the limit of massless up and down quarks is a possible upper bound for the transition temperature at the critical endpoint; see Refs. [18–21] for recent works and reviews. Accordingly, the nature of the chiral transition in QCD with three quark flavors is very actively researched. For sufficiently small masses of the three quarks, one expects a finite mass range with a first-order chiral transition [22]. Interestingly, this first-order regime may even extend to the limit of infinitely heavy strange quarks; see, e.g., Refs. [17,23,24]. This intricate question regarding the existence and range of such a regime is tightly connected to the fate of the axial $U_{\mathrm{A}}(1)$ anomaly at finite temperature: depending on the strength of the associated $U_{\mathrm{A}}(1)$ breaking, the phase transition may indeed be of first order; see, e.g., Refs. [19,22,25–27].

For physical masses of the three quarks, the transition in (2 + 1)-flavor QCD from a low-temperature hadronic phase to a high-temperature quark-gluon plasma phase has been found in lattice and functional QCD studies to be a crossover; see, e.g., Refs. [10,28–33] for lattice studies and Refs. [1–5] for functional studies.

In the chiral limit of the light quarks, the critical behavior is controlled by the three-dimensional (3D) $O(4)$ universality class, if the anomalous breaking of the $U_{\mathrm{A}}(1)$ symmetry is sufficiently strong. In turn, if the $U_{\mathrm{A}}(1)$ symmetry is effectively restored sufficiently close to the chiral transition, the critical behavior may no longer be controlled by the 3D $O(4)$ universality class [34–37]. Within a very recent lattice QCD study investigating pion masses in the range of $50 \lesssim m_\pi \lesssim 160$ MeV with a physical strange quark mass, the scaling properties of the chiral susceptibility are now found to be compatible with the 3D $O(4)$ universality class [33]. An extrapolation to the chiral limit of the light quarks leads to $T_c = 132^{+3}_{-6}$ MeV for the chiral critical temperature [33].

The reconstruction of the chiral critical temperature from an extrapolation to the chiral limit is in general a nontrivial task as it is affected by nonuniversal aspects, such as the order of the transition and the dependence of the pseudocritical temperature on the pion mass. Moreover, the definition of a pseudocritical temperature is not unique. Indeed, the strength of the pion-mass dependence of the pseudocritical temperature is different for different definitions. Assuming that the chiral phase transition is of second order in the limit of massless up and down quarks, it follows from universal scaling arguments [38] that the pion-mass scaling of the pseudocritical temperature defined as the position of the peak of the chiral susceptibility is controlled by the critical exponents of the underlying universality class. Unfortunately, the size of the scaling regime is also a nonuniversal quantity. These statements also hold for other definitions of the pseudocritical temperature, and it is also reasonable to expect that the size of the scaling regime is of the same order for different definitions, provided that they rely on properties of the chiral susceptibility.

In low-energy effective theories of QCD, it has been found that the pseudocritical temperature defined as the position of the peak of the chiral susceptibility scales roughly linearly over a wide range of pion masses which appears compatible with scaling arguments at first glance [39–41]. Even more, it was found that the results for the suitably rescaled chiral order parameter fall almost on one line [41] for $m_\pi \gtrsim 75$ MeV, seemingly suggesting scaling behavior. However, a comparison of these results with the corresponding scaling function extracted within the model studies exhibits clear deviations from scaling. A detailed analysis then revealed that the size of the actual scaling regime is very small [41]. More precisely, it has been found that the chiral susceptibility and the chiral order parameter only exhibit scaling behavior for very small pion masses, $m_\pi \lesssim 1$ MeV, see Ref. [41].

Our present first-principles fRG study corroborates these findings in low-energy effective theories; the actual scaling regime in QCD is indeed small, with a conservatively estimated upper bound of $m_\pi \approx 30$ MeV. In addition, our present work shows that the glue dynamics softens the strong dependence of the pseudocritical temperature on the pion mass observed in low-energy effective theories of QCD. In fact, it is found to be in very good agreement with recent lattice QCD results [33]. Moreover, we shall discuss different extrapolations to the chiral limit, leading us consistently to $T_c \approx 142$ MeV for the critical temperature; see also Figs. 2 and 3.

This work is organized as follows. In Sec. II, we briefly discuss the methodological framework of our present study. Our results for the chiral susceptibility as obtained from the light-quark condensate are presented in Sec. III. There, we also show a comparison of these results with those for the susceptibility extracted from the reduced condensate, also used in lattice computations. The results for the reduced condensate are then compared to lattice QCD data [33], including a discussion of the dependence of the pseudocritical temperature on the pion mass. Our conclusions can be found in Sec. IV.

II. CONDENSATES AND FUNCTIONAL QCD

In this section. we discuss different chiral condensates and the associated susceptibilities which we compute to access the mass dependence and scaling of the pseudocritical temperature. We also briefly introduce the fRG approach to QCD used for this computation. The basis for our present study is discussed in detail in Ref. [1].

A. Chiral condensates

In order to obtain the (chiral) susceptibility in $(2+1)$-flavor QCD for various (current) quark masses $m^0_{q_i}$, we have to compute the chiral condensates Δ_{q_i} associated with the three quark flavors q_i. Here, $q_i = u, d, s$ refer to the up, down, and strange quark, respectively. The Δ_{q_i} can be obtained from the logarithmic derivative of the thermodynamic grand potential Ω with respect to the corresponding current quark mass,

$$\begin{aligned}\Delta_{q_i} &= m^0_{q_i}\frac{\partial\Omega(m_q;T,\mu_u,\mu_d,\mu_s)}{\partial m^0_{q_i}} \\ &= m^0_{q_i}\frac{T}{V}\int_0^{\frac{1}{T}}\mathrm{d}\tau\int_V \mathrm{d}^3x\langle\bar{q}_i(\tau,\vec{x})q_i(\tau,\vec{x})\rangle. \qquad (1)\end{aligned}$$

Here, T is the temperature, and V is the spatial volume. The logarithmic derivative with respect to the current quark mass is taken since Δ_{q_i} then carries the same scaling properties as the grand potential Ω. Consequently, it is not sensitive to details of the setup that typically change the precise value of the current quark mass, in particular the renormalization scheme; see Ref. [1] for a discussion. In the present work, we only consider the zero-density limit, and therefore we set the quark chemical potentials to zero, $\mu_u = \mu_d = \mu_s = 0$. Thus, the quark condensates are only functions of the temperature and the current quark masses from here on. Moreover, we use identical current masses for the two light quarks, $m^0_u = m^0_d = m^0_l$. This allows us to define the light quark condensate $\Delta_l = \Delta_u = \Delta_d$.

The computation of the quark condensates via the expectation value in the last line of Eq. (1) requires renormalization and hence the result depends on the renormalization procedure. Both the necessity for renormalizing the operator and the renormalization scheme dependence is removed when considering finite difference of chiral condensates. Two possible choices are the *renormalized* and the *reduced* condensate. Both are commonly used in lattice QCD studies and have also been studied in functional approaches to QCD. The fRG approach naturally provides a renormalized finite expression for the condensate Δ_{q_i} as it is based on a finite free energy and hence the current mass derivative in Eq. (1) is finite; for more details, see Sec. II B and Ref. [1]. For our study of the chiral phase transition, the condensate Δ_l is therefore the key observable in the present work since it has the smallest systematic error within the truncation used for the computation.

The renormalized condensate associated with the light-quark flavors can be defined as

$$\Delta_{l,R}(T) = \frac{1}{\mathcal{N}_R}(\Delta_l(T) - \Delta_l(0)). \tag{2}$$

The normalization constant $\mathcal{N}_R$ is at our disposal; in the following, it is chosen independent of the current masses and is typically used to render $\Delta_{l,R}(T)$ dimensionless. Note that, by including a m_l^0-dependence of the form $\mathcal{N}_R \sim m_l^0/m_s^0$, we recover the definition of the renormalized condensate conventionally employed in lattice QCD studies; see, e.g., Ref. [42].

The reduced condensate $\Delta_{l,s}$ is a combination of the light-quark condensate Δ_l and the strange quark condensate Δ_s,

$$\Delta_{l,s} = \frac{1}{\mathcal{N}_{l,s}}\left(\Delta_l(T) - \left(\frac{m_l^0}{m_s^0}\right)^2 \Delta_s(T)\right), \tag{3}$$

where the definition of the m_l^0-independent normalization constant $\mathcal{N}_{l,s}$ is again irrelevant for our discussion of the susceptibilities below. Instead, if we choose $\mathcal{N}_{l,s}$ to be m_l^0 dependent, $\mathcal{N}_{l,s} = (\Delta_l(0) - (m_l^0/m_s^0)^2\Delta_s(0))^2$, we arrive at the standard lattice definition of the reduced condensate; see, e.g., Ref. [42]. Alternatively, we could simply choose $\mathcal{N}_{l,s} \sim m_l^0/m_s^0$, which yields the observable defined in Ref. [33] (up to numerical factors) to compute susceptibilities.

The subtraction in Eq. (3) renders the reduced condensate finite as in the case for the renormalized condensate. However, the systematic error of results of such a light-strange quark mixture is a combination of that in the strange and in the light quark sector and requires a quantitative treatment of both. Consequently, it is affected by larger systematic errors in our present fRG study than the light-quark condensate Δ_l.

The corresponding susceptibilities are readily obtained from all three condensates. We define them as follows,

$$\chi_M^{(i)}(T) = -\frac{\partial}{\partial m_l^0}\left(\frac{\Delta_i(T)}{m_l^0}\right), \tag{4}$$

where $(i) = (l), (l,R), (l,s)$. We shall refer to these susceptibilities as light-quark susceptibility, renormalized susceptibility, and reduced susceptibility, respectively. Leaving an overall normalization aside, it follows from the definition of the light-quark condensate Δ_l and the renormalized condensate $\Delta_{l,R}$ that the associated susceptibilities only differ by a temperature-independent shift. From our discussion above, it moreover follows that our definition of the reduced susceptibility matches the one used in lattice studies [33].

By multiplying the magnetic susceptibilities (4) with $(m_l^0)^2$, they also carry the scaling properties of the grand potential, and there is no dependence on the renormalization procedure left. This is in one-to-one correspondence to the lack of renormalization scheme dependence of Δ_l defined by the logarithmic m_l^0-derivative of the grand potential, and to that of the renormalized and reduced condensates. However, for the sake of a straightforward comparison with the lattice results from Ref. [33], we have not included these factors in Eq. (4). Moreover, for a comparison of the susceptibilities for different pion masses (or current quark masses) as well as for a comparison with results from other methods, it is convenient to normalize the magnetic susceptibilities $\chi_M^{(i)}(T)$ with the respective peak value for the physical pion mass $m_\pi \approx 140$ MeV,

$$\bar{\chi}_M^{(i)} = \max_T \chi_M^{(i)}(T)|_{m_\pi = 140\ \mathrm{MeV}}, \tag{5}$$

where again $(i) = (l), (l,R), (l,s)$. Thus, we have $\chi_M^{(i)}(T)/\bar{\chi}_M^{(i)} = 1$ at the peak position in case of the physical pion mass. The size and evolution of the increasing peak toward the chiral limit give a rough estimate for the "distance" to criticality.

B. Functional renormalization group approach

In this work, we use the fRG approach for the computation of the light-quark and reduced susceptibilities from first principles. In this approach, quark, gluon, and hadron correlation functions of QCD are computed from functional relations that are derived from the flow equation for the *finite* effective action Γ. Accordingly, the finite effective action is easily accessible in this approach and is self-consistent. In particular, it automatically encodes the same RG scheme as the correlation functions.

The thermodynamic grand potential Ω is then given by the effective action evaluated on the equations of motion (EoM), i.e., the ground state: $\Omega = (T/V)\Gamma|_{\mathrm{EoM}}$. Hence, the fRG approach provides a finite thermodynamic grand potential Ω. This leads to a finite quark condensate Δ_{q_i} within the RG scheme used for the computation of the correlation functions; see Eq. (1).

The computation of the susceptibilities in our fRG study requires the computation of the light-quark and reduced quark condensates for various temperatures and quark masses. To this end, we have to follow the RG flow from the classical QCD action in the ultraviolet to the long-range (infrared) limit where the dynamics is effectively described by hadronic degrees of freedom rather than quarks and gluons. To facilitate the description of the transition between the degrees of freedom in the ultraviolet and infrared limit, we employ *dynamical hadronization* techniques [1,43–46]; see Refs. [1,44,47–51] for their application to QCD. The chiral susceptibilities can then be obtained with two different—formally equivalent procedures—from Eq. (1), both of which are detailed below around Eq. (6) as their comparison provides an important self-consistency and reliability check for our present truncation.

Our present study has been done within the *fQCD Collaboration* [52] and is a follow-up of a recent work [1] within this collaboration. It also builds on previous advances made within this collaboration; see, e.g., Refs. [2,48–51,53–55]. Therefore, we refrain from showing the flow equations required to compute the light-quark and reduced quark condensate because of the size of this set of equations. All these equations are derived, documented, and discussed in detail in Ref. [1].

We only would like to discuss two aspects of our computation which are particularly relevant for the estimate of the systematic error of our results.

First, we only take into account the sigma-pion channel in the computation of the order-parameter potential and do not allow for an effective $U_{\mathrm{A}}(1)$ restoration at, e.g., high temperatures. Thus, we tacitly assume that the chiral transition falls into the 3D $O(4)$ universality class. This assumption is based on the fact that Fierz-complete finite-temperature studies of the chiral transition indeed indicate that the sigma-pion interaction channel is by far most dominant close to the chiral phase transition at vanishing baryon density [2]. A discussion of whether this dominance is strong enough relative to $U_{\mathrm{A}}(1)$-restoring channels for keeping QCD in the 3D $O(4)$ universality class is beyond the scope of the present work. However, a recent lattice study suggests that this may indeed be the case and that the transition is of second order in the chiral limit [33].

Second, in order to compute the chiral order-parameter potential, we employ a Taylor expansion about the renormalization group (RG) scale-dependent minimum of the effective action. An inclusion of a finite pion mass into the flow equations then tends to stabilize this expansion [56,57]. However, it becomes numerically unstable for (very) small pion masses.

In the present work, we employ an error estimate to evaluate the self-consistency and reliability of our results in case of small pion masses. To this end, we compute the light-quark susceptibility with two different methods. Within the first method, we directly perform the derivative of the condensate Δ_l with respect to the light-quark current mass:

$$\chi_M^{(l)}(T) = \left(\frac{T}{V}\right)^2 \int_{x,y} \langle \bar{q}_l(x) q_l(x) \bar{q}_l(y) q_l(y) \rangle - \left(\frac{\Delta_l}{m_l^0}\right)^2. \quad (6)$$

This expression can be computed directly from the grand potential Ω for a *given* current quark mass m_l^0. Indeed, it is directly related to the screening mass of the σ-meson; see Refs. [1,57] for details.

Within the second method, the light-quark susceptibility $\chi_M^{(l)}$ is simply obtained by computing the light-quark condensate as a function of the temperature and the light quark mass m_l^0, and then taking a numerical derivative of this dataset with respect to m_l^0. Note that we also compute the reduced condensate in this way.

Evidently, both methods should give the same results for the light-quark susceptibility, provided that no approximations are involved. Therefore, deviations give access to the reliability of the underlying approximations. In particular, a comparison of the results from both methods allows us to some extent to test the convergence of the expansion of the effective potential. In fact, the first method simply amounts to a direct computation of the mass of the σ-meson, which is obtained by suitably combining the renormalized four-meson coupling and the minimum of the order-parameter potential. The latter is computed directly from a corresponding flow equation. The computation of the susceptibility via the mass derivative of the condensate also requires initially the computation of the minimum of the potential. However, when we now take a derivative of the latter with respect to the quark mass, we implicitly also take derivatives of the meson couplings with respect to the quark mass since the minimum is a function of the quark mass and also of a set of couplings, e.g., the four-meson coupling and the eight-meson coupling. The latter are nothing but the expansion coefficients of the order-parameter potential and also depend on the quark mass. As derivatives with respect to the quark mass effectively correspond to derivatives with respect to the source of the σ field (in the path integral), a derivative of a meson coupling with respect to the quark mass tests the effect of higher-order couplings and therefore provides an implicit test whether our results are converged with respect to the expansion of the effective potential. A comparison of results from the two methods is depicted in Fig. 1. From this, we conclude that our present approximation is trustworthy for pion masses $m_\pi \gtrsim 30$ MeV. In particular, the peak positions obtained from the two methods are in very good agreement with each other in this pion-mass regime. In fact, they only differ by about 1 MeV. Based on this comparison, we consider it sufficient to show in the following only those results for the

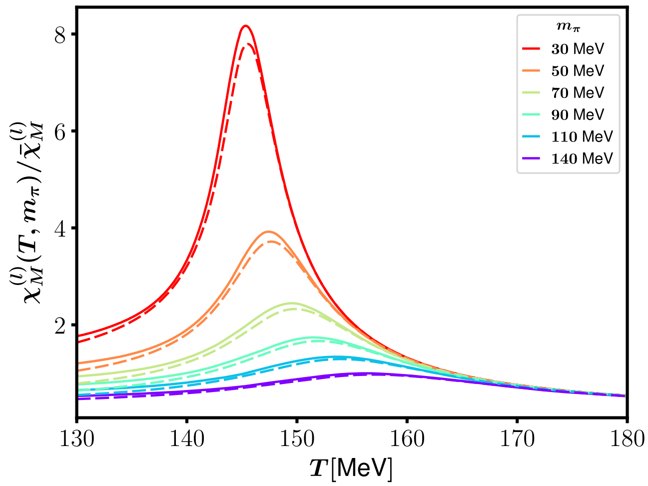

FIG. 1. Light-quark susceptibility for different pion masses as obtained from two independent methods within our present truncation. The dashed lines correspond to the results obtained via the relation (6). The solid lines are associated with the results computed by taking a derivative of our numerical dataset for the light-quark condensate with respect to m_l^0. The normalization is given by the maximum of the susceptibility at the physical pion mass; see Eq. (5). We observe that the results from the two methods agree very well for $m_\pi \gtrsim 30$ MeV. This is particularly true for the respective peak positions; see the main text for details.

light-quark susceptibility which have been obtained by taking a derivative of our numerical dataset for the light-quark condensate with respect to m_l^0. As the light-quark condensate is part of the reduced condensate, we may assume that the uncertainty for the pseudocritical temperatures extracted from the reduced susceptibilities is the same as in the case of the light-quark susceptibilities. However, the systematic error is likely to be bigger in this case, as already indicated in Sec. II A. Regarding smaller pion masses, we add that an extension in this direction (including the chiral limit) is possible but requires either an expansion of the effective action about a scale-independent point [53] or the use of, e.g., recently developed techniques to access the full order-parameter potential [58].

We would like to close this section by adding that a variation of the regularization scheme can in principle also be used to assess the truncation underlying our present work. However, it should also be noted that a mild regulator dependence of a given set of observables is only a necessary condition for considering a given truncation as reliable. In the present work, we do not perform an analysis of regulator dependences but only resort to earlier studies of this aspect. To be specific, the regulator dependence of chiral observables in first-principles fRG studies of QCD in the vacuum limit has been found to be small [51]. As we argued in Ref. [1], the results for the vacuum case extracted from our present study are consistent with those reported in Ref. [51]. Therefore, we may cautiously expect the regular dependence to be mild in our present work. Regarding the study of critical behavior, we would like to point out that the regulator dependence of critical exponents as well as their dependence on the order of the expansion of the order-parameter potential has been analyzed in detail for $O(N)$ models in, e.g., Refs. [59,60]. A scaling analysis within the quark-meson model in Ref. [41] has been found to be consistent with the findings presented in Ref. [59] regarding the employed order of the potential. In particular, the critical exponents are found to agree on the 1% level with the current world's best estimates. The dependence of nonuniversal quantities, such as the critical temperature, on the regularization scheme as well as on the order of the expansion of the effective potential has been tested explicitly within the quark-meson model in the local potential approximation in Ref. [61]. There, it was found that the results for the critical temperature are almost converged for the order of the expansion considered in our present work. Based on these observations and our self-consistency check for the susceptibility, we consider our numerical results to be meaningful. Nevertheless, even a weak dependence on the order of the expansion and the regularization scheme may already be sufficient to explain the small deviation of our present result for the slope of the pseudocritical temperature as a function of the pion mass from the one found in lattice QCD studies; see our discussion in the subsequent section.

III. RESULTS

Let us now discuss the susceptibilities associated with the light-quark and reduced condensate for various temperatures and pion masses. To this end, we shall keep the strange quark mass fixed at its physical value and only vary the light-quark mass. As already discussed in the previous section, the renormalized condensate only differs from the light-quark condensate by a temperature-independent shift. This implies that the peak positions of these two susceptibilities are the same for a given pion mass. Therefore, we shall not further discuss the renormalized susceptibility in this section.

Susceptibilities as introduced in the previous section are of great interest as their maxima can be used to define pseudocritical temperatures. From general scaling arguments [38], it then follows that the pseudocritical temperatures extracted from the light-quark and reduced susceptibility scale as

$$T_{\rm pc}^{(i)}(m_\pi) \approx T_{\rm c} + c_{(i)} m_\pi^p, \tag{7}$$

at least within the scaling regime. Here, $(i) = (l), (l, s)$. The chiral critical temperature is given by $T_{\rm c}$ in Eq. (7). The quantity $c_{(i)}$ is a nonuniversal constant depending on the susceptibility under consideration, whereas the exponent p can be related to the universal critical exponents β and δ, $p = 2/(\beta\delta)$. The relation (7) follows from the fact that the

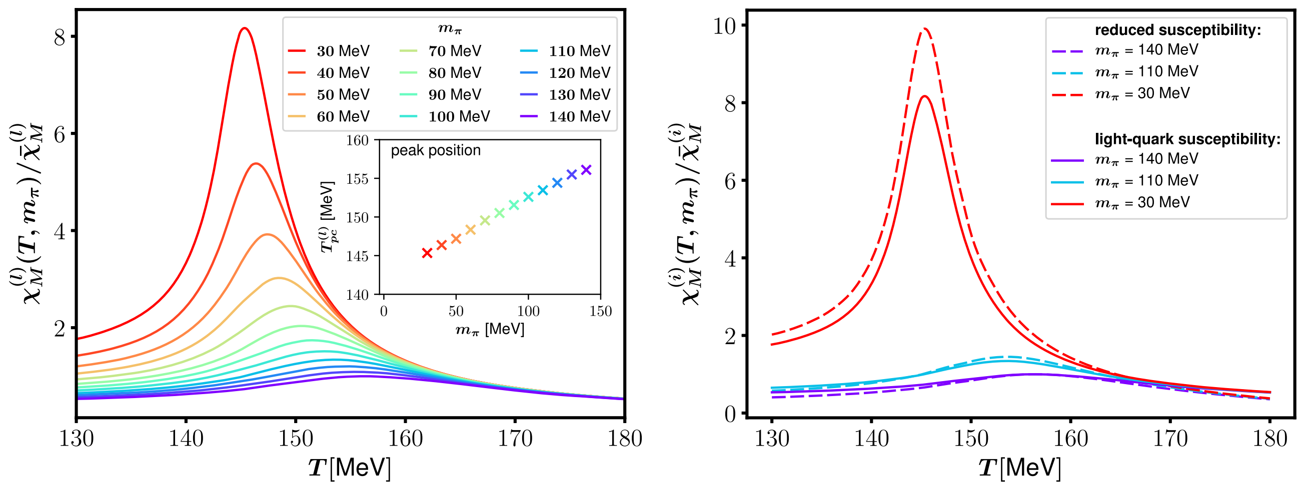

FIG. 2. Left panel: Light-quark susceptibility $\chi_M^{(l)}$ as a function of the temperature. The inset shows the peak positions of the depicted susceptibilities as a function of the pion mass. Right panel: Comparison of the light-quark susceptibility $\chi_M^{(l)}$ and the reduced susceptibility $\chi_M^{(l,s)}$ as a function of the temperature. The normalizations are the maxima of the respective susceptibilities at the physical pion mass; see Eq. (5).

position of the peak of the susceptibility as a function of the scaling variable $z = t/h^{1/(\beta\delta)}$ is constant in the scaling regime. Here, $t = (T - T_c)/T_0$ is the reduced temperature with T_0 being a suitably chosen normalization factor and $h = H/H_0$ is the symmetry breaking field normalized by a suitably chosen normalization H_0. In the present case, H can be identified with the current mass of the light quarks m_l^0, which, in turn, is directly related to the pion mass via $m_\pi^2 \sim m_l^0$.

For example, employing the critical exponents of the 3D $O(4)$ universality class [62–64], we have $p \approx 1.08$. Based on previous fRG studies of critical exponents [60,65–67], however, we expect p to be slightly smaller in our present study. In any case, this suggests an almost linear dependence of the peak positions of the susceptibilities on the pion mass, at least within the scaling regime. Note that the size of the latter is not universal but depends on the details of the theory under consideration.

In Fig. 2 (left panel), we show our results for the light-quark susceptibilities $\chi_M^{(l)}(T)$ as a function of the temperature T, where we have normalized the susceptibilities with $\bar{\chi}_M^{(l)}$, i.e., the value of $\chi_M^{(l)}(T)$ for $m_\pi = 140$ MeV evaluated at its maximum; see Eq. (5). As expected, we find that the susceptibility increases when the pion mass is decreased. Indeed, by decreasing the pion mass, we approach the chiral limit associated with a diverging susceptibility at the chiral phase transition temperature T_c.

Our results for the pseudocritical temperature indeed appear to depend almost linearly on the pion mass; see Fig. 2 (left panel). Fitting the scaling relation (7) to our numerical results for $T_{pc}^{(l)}(m_\pi)$ for $m_\pi = 30, 35, 40, \ldots, 140$ MeV, we obtain $T_c \approx 141.4^{+0.5}_{-0.5}$ MeV, $c_{(l)} \approx 0.19^{+0.05}_{-0.05}$ MeV^{1-p}, and $p \approx 0.88^{+0.05}_{-0.05}$. At this point, we would like to remind the reader that the renormalized susceptibility obeys the same temperature dependence as the light-quark susceptibility. Therefore, the pseudocritical temperatures extracted from these two susceptibilities are identical.

The deviation of our estimate for the exponent p from the value associated with the 3D $O(4)$ universality class [62–64] already suggests that QCD is not within the scaling regime, not even for the smallest pion masses considered in the present work. As already mentioned in Sec. I, this is in line with studies of low-energy effective theories of QCD. There, it has been found that deviations from scaling are still sizeable, even if the pseudocritical temperature scales approximately linearly for large pion masses and also the suitably rescaled chiral susceptibilities for pion masses $m_\pi \gtrsim 75$ MeV appear to fall approximately on one line [41]. Even worse, from a practical standpoint, actual scaling behavior of the chiral susceptibility and the chiral order parameter has only been observed for very small pion masses, $m_\pi \lesssim 1$ MeV [41]. Given these results from low-energy QCD model studies and the fact that the exponent p is close to 1 for the 3D $O(4)$ universality class anyhow, a linear fit for the pseudocritical temperature may be considered reasonable. Performing such a linear fit, we obtain $T_c \approx 142.4^{+0.1}_{-0.1}$ MeV from the extrapolation to $m_\pi = 0$, in very good agreement with our estimate for T_c presented above.

Let us now consider the ratio

$$D_{(l)}(m_\pi) = \frac{T_{pc}^{(l)}(m_\pi) - T_c}{T_c}, \tag{8}$$

which is an estimate for the relative dependence of the pseudocritical temperature on the pion mass. For the physical pion mass, $m_\pi = 140$ MeV, this ratio in our present first-principles fRG study is about a factor of 3 smaller than typical values for $D_{(l)}$ found in low-energy QCD model studies [39,40]. For example,

$$D_{(l)}^{\mathrm{QM}}(m_\pi = 140\ \mathrm{MeV}) \approx 0.28 \qquad (9)$$

was reported in Ref. [40] for the quark-meson (QM) model. In our present QCD study, we instead find

$$D_{(l)}^{\mathrm{QCD}}(m_\pi = 140\ \mathrm{MeV}) \approx 0.10, \qquad (10)$$

where we have employed the value for T_c obtained from an extrapolation of the pseudocritical temperature $T_{\mathrm{pc}}^{(l)}$ to the limit $m_\pi = 0$. The observed significant difference for the nonuniversal quantity $D_{(l)}$ as obtained from model studies and our first-principles fRG study deserves a comment. First of all, the parameters in low-energy models are tuned at a given UV cutoff scale to fix a given set of low-energy observables. A change of the current quark mass then in principle requires adapting these parameters following a given prescription which is not unique; see, e.g., the discussion in Ref. [19]. In our present study, such an adaption of parameters is not required. Related to this aspect, the UV cutoff scale in low-energy models is generally chosen to be (significantly) greater than the chiral symmetry breaking scale. However, it has been found by comparisons of RG flows of the quark-meson model with those of QCD that the UV cutoff scale in models is generally chosen too large from a QCD standpoint; see Refs. [69–71]. In fact, these comparisons reveal that the gluodynamics significantly affects the RG flow of the effective potential almost down to the symmetry breaking scale. Since the latter eventually determines the scaling of low-energy observables, it also leaves its imprint in the pion-mass dependence of the pseudocritical temperature. Second, it should also be emphasized that the chiral critical temperature in our present study is obtained from an extrapolation of our results for finite pion masses. Thus, our estimate for the critical temperature naturally suffers from an uncertainty associated with the extrapolation which affects our estimate for $D_{(l)}$. Moreover, while the linear behavior of $T_{\mathrm{pc}}^{(l)}(m_\pi)$ is basically determined by universality, the comparison of our results to the lattice QCD for large pion masses in Fig. 3 indicates that we presently may still underestimate the slope of $T_{\mathrm{pc}}^{(l)}(m_\pi)$ also at small pion masses.

Next, we turn to the reduced susceptibility $\chi_M^{(l,s)}$ as defined in Eq. (4). In Fig. 2 (right panel), we show a comparison of the light-quark susceptibility and the reduced susceptibility for three pion masses. As expected, the qualitative behavior of the reduced susceptibility is the same as the one found for the light-quark susceptibility. More specifically, the susceptibilities increase for decreasing pion mass, indicating the approach to a singularity in the chiral limit. Fitting the relation (7) to our numerical results for $T_{\mathrm{pc}}^{(l,s)}(m_\pi)$ for $m_\pi = 30, 35, 40, \ldots, 140$ MeV, we obtain $T_c \approx 141.6^{+0.3}_{-0.3}$ MeV, $c_{(l,s)} \approx 0.17^{+0.03}_{-0.03}$ MeV^{1-p}, and $p \approx 0.91^{+0.03}_{-0.03}$. Thus, the critical temperature T_c is in excellent agreement with the one extracted from our

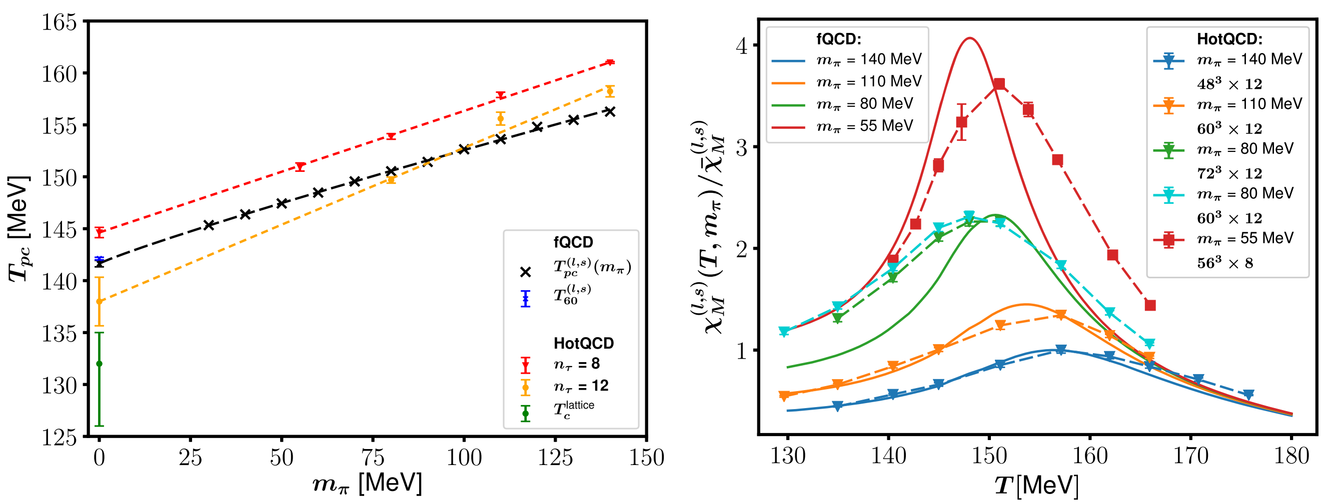

FIG. 3. Left panel: Comparison of our fRG results for the pseudocritical temperature as a function of the pion mass to those from the HotQCD Collaboration [33]. The various dashed lines represent fits to the numerical data; see the main text for details. The estimates for the critical temperature T_c have been obtained from an extrapolation of the fits to $m_\pi \to 0$. The temperatures $T_{60}^{(l,s)}$ and T_c^{lattice} are the extrapolated results for the chiral critical temperature obtained from a definition of the pseudocritical temperature which does not involve the peak position of the susceptibility; see the main text for details. Right panel: Susceptibility as obtained from the reduced condensate as a function of the temperature. The normalization $\bar{\chi}_M^{(l,s)}$ is the maximum of the susceptibility at the physical pion mass; see Eq. (5). The lattice QCD data have been taken from Refs. [33,68].

TABLE I. Selection of peak positions of the reduced susceptibility for various pion masses as obtained from our present fRG computation and a recent lattice QCD study [33].

		m_π (MeV)								
		30	40	55	70	80	100	110	120	140
$T_{\rm pc}$ (MeV)	fQCD (reduced)	145.3	146.4	148.0	149.6	150.5	152.7	153.6	154.8	156.3
	HotQCD ($N_\tau = 12$) [33]	⋯	⋯	⋯	⋯	$149.7^{+0.3}_{-0.3}$	⋯	$155.6^{+0.6}_{-0.6}$	⋯	$158.2^{+0.5}_{-0.5}$
	HotQCD ($N_\tau = 8$) [33]	⋯	⋯	$150.9^{+0.4}_{-0.4}$	⋯	$153.9^{+0.3}_{-0.3}$	⋯	$157.9^{+0.3}_{-0.3}$	⋯	$161.0^{+0.1}_{-0.1}$

analysis of the light-quark susceptibilities, as it should be. With respect to the exponent p, we note that it also deviates clearly from the expected $O(4)$ value. However, we observe that it is consistent within fit errors with the value for p which we obtained from our analysis of the light-quark susceptibility. Overall, we therefore cautiously conclude that QCD is not within the scaling regime for the range of pion masses considered here, providing us with $m_\pi \approx 30$ MeV as a conservative estimate for the upper bound of this regime. An actual determination of the size of the scaling regime is beyond the scope of present work as it requires studying very small pion masses.

In analogy to the definition (8), we can also define the relative dependence $D_{(l,s)}(m_\pi)$ of the pseudocritical temperature on the pion mass in case of the reduced susceptibility. For $m_\pi = 140$ MeV, we then find that this quantity is only slightly smaller than the corresponding quantity associated with the light-quark susceptibility.

In Fig. 3 (right panel), we finally compare our fRG results for the reduced susceptibility to very recent results from the HotQCD Collaboration [33]. We observe excellent agreement between the results from the two approaches for pion masses $m_\pi \gtrsim 100$ MeV. The deviations of the results from the two approaches for smaller pion masses may at least partially be attributed to cutoff artifacts in the lattice data. Note that cutoff effects are expected to shift the maxima to smaller temperatures. We refer to Ref. [20] for a respective discussion.

It is also worthwhile to compare the peak positions of the reduced susceptibilities extracted from the lattice QCD data with those from our fRG study; see Table I and Fig. 3 (left panel). As discussed above, the peak position can be used to define a pseudocritical temperature. For the presently available pion masses on the lattice, we find that the results from the two approaches for this pseudocritical temperature are in very good agreement. Moreover, we observe that at least a naive linear extrapolation of the HotQCD results for the peak position yields $T_{\rm c} \approx 144.6^{+0.5}_{-0.5}$ MeV for $N_\tau = 8$ and $T_{\rm c} \approx 138.0^{+2.3}_{-2.3}$ MeV for $N_\tau = 12$, which is consistent with our estimate for $T_{\rm c}$. However, as argued in Ref. [33], the strong pion-mass dependence of the so-defined pseudocritical temperature potentially complicates the chiral extrapolation of lattice QCD data. Therefore, an alternative definition of the pseudocritical temperature has been introduced in Ref. [33]. In the following, we shall refer to this pseudocritical temperature as $T_{60}^{(l,s)}$. Its implicit definition reads [33]

$$\chi_M^{(l,s)}(T_{60}^{(l,s)}, m_\pi) = 0.6 \max_T \chi_M^{(l,s)}(T, m_\pi). \tag{11}$$

Here, it is tacitly assumed that $T_{60}^{(l,s)}$ is determined at a temperature to the left of the maximum of the susceptibility, implying $T_{60}^{(l,s)} < T_{\rm pc}^{(l,s)}$. For $m_\pi \to 0$, $T_{60}^{(l,s)}$ then converges to $T_{\rm c}$. Moreover, the so-defined pseudocritical temperature is expected to exhibit only a mild dependence on the pion mass and should hence be close to the chiral phase transition temperature $T_{\rm c}$ for the range of pion masses of interest in the present work. In Ref. [33], this definition of the pseudocritical temperature has been used to extrapolate to the chiral limit, resulting in $T_{\rm c}^{\rm lattice} = 132^{+3}_{-6}$ MeV. Employing this definition of the pseudocritical temperature to analyze our fRG results for the reduced susceptibility, we indeed observe an extremely weak dependence of $T_{60}^{(l,s)}$ on the pion mass. To be specific, we find that it increases by less than 1 MeV when the pion mass is increased from $m_\pi = 30$ MeV to $m_\pi = 140$ MeV. An extrapolation to the chiral limit yields $T_{\rm c} \approx 142.4$ MeV, which agrees nicely with our estimates for $T_{\rm c}$ presented above, as it should be. Thus, from our fRG study, we eventually conclude

$$T_{\rm c} \approx 142 \text{ MeV} \tag{12}$$

for the chiral phase transition temperature.

IV. CONCLUSIONS

In this work, we have studied the magnetic susceptibility in (2 + 1)-flavor QCD within a first-principles fRG calculation. Specifically, we have presented results for the susceptibilities associated with the light-quark condensate and the reduced condensate.

The chiral pseudocritical temperatures have been determined from the peak positions of the susceptibilities. Interestingly, we found that its dependence on the pion mass in the present QCD study is milder than in low-energy QCD model studies. From an extrapolation to the chiral limit, we obtained $T_{\rm c} \approx 142$ MeV for the chiral phase transition temperature.

Our results for the susceptibilities and the scaling of the corresponding pseudocritical temperature indicate that QCD is not within the scaling regime for the considered pion masses $m_\pi \geq 30$ MeV. As discussed in detail, this conclusion is at least in accordance with low-energy QCD model studies [41]. There, a qualitatively similar behavior of the susceptibilities and the pseudocritical temperature has been observed for the same pion mass range as considered here. However, the actual size of the scaling regime turned out to be significantly smaller. A detailed analysis of this issue within our present first-principles fRG approach is deferred to future work as it requires to study (very) small pion masses.

We have also compared our results for the reduced susceptibility with very recent results from the HotQCD Collaboration [33] and found that the results from both approaches are in very good agreement for pion masses $m_\pi \gtrsim 100$ MeV. For smaller pion masses, the lattice and fRG results are still consistent with each other. Following the analysis of the HotQCD Collaboration, we have also estimated the phase transition temperature in the chiral limit based on scaling properties of the susceptibility in the temperature regime below the temperature defined by the peak of the susceptibility. As it should be, this provides us with the same value for the chiral phase transition temperature as in the case of an extrapolation of the peak positions of the light-quark and reduced susceptibility.

As a next step, it will be important to further extend our present study. For example, we plan to improve the stability of our numerical calculations for very small pion masses to eventually reach the chiral limit by employing recent developments for the solution of fRG equations [58] as well as the stability-enhancing expansion about a fixed expansion point [53]. Moreover, an analysis of the effect of the breaking of the $U_{\mathrm{A}}(1)$ symmetry and effective $U_{\mathrm{A}}(1)$ restoration at high temperatures is in order; for a first flow study in the vacuum, see Ref. [72]. A detailed analysis of the latter issue requires the study of Fierz-complete truncations of the effective action. First steps into this direction have been taken [73], suggesting that effective $U_{\mathrm{A}}(1)$ restoration already sets in closely above the chiral phase transition temperature, in accordance with recent lattice QCD studies [74]. An understanding of the effect of this almost coincidence of chiral and $U_{\mathrm{A}}(1)$ restoration on the critical behavior is indeed an intriguing and not yet fully resolved problem in QCD.

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