

Finite density QCD phase structure from strangeness fluctuations

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Charting the phase diagram of quantum chromodynamics (QCD) at large density is a challenging task due to the complex action problem in lattice simulations. Through simulations at imaginary baryon chemical potential μ_B we observe that, if the strangeness neutrality condition is imposed, both the strangeness chemical potential μ_S/μ_B and the strangeness susceptibility χ_2^S take on constant values at the chiral transition for varying μ_B . We present new lattice data to extrapolate contours of constant μ_S/μ_B or χ_2^S to finite baryon chemical potential. We argue that they are good proxies for the QCD crossover because, as we show, they are only mildly influenced by criticality and by finite volume effects. We obtain continuum limits for these proxies up to $\mu_B = 400$ MeV, through a next-to-next-to-leading order (N²LO) Taylor expansion based on large-statistics data on $16^3 \times 8$, $20^3 \times 10$ and $24^3 \times 12$ lattices with our 4HEX improved staggered action. We show that these are in excellent agreement with existing results for the chiral transition and, strikingly, also with analogous contours obtained with the hadron resonance gas (HRG) model. On the $16^3 \times 8$ lattice, we carry out the expansion up to next-to-next-to-next-to-next-to-leading order (N⁴LO), and extend the extrapolation beyond $\mu_B = 500$ MeV, again finding perfect agreement with the HRG model. This suggests that the crossover line constructed from this proxy starts deviating from the chemical freeze-out line near $\mu_B \approx 500$ MeV, as expected but not yet observed.

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I. INTRODUCTION

The phase structure of strongly interacting matter has been the subject of intense research in decade-long experimental programs at the SPS and LHC (CERN), SIS18 (GSI) and RHIC (BNL) accelerator facilities. There is clear evidence that heavy-ion collision experiments reach high enough temperatures for the quark gluon plasma phase to be created [1]. In this large temperature phase quarks are deconfined and chiral symmetry is approximately restored (up to the small explicit breaking due to finite quark masses). The transition from hadronic to quark matter for zero quark-antiquark asymmetry (i.e., zero baryon

chemical potential μ_B) and physical quark masses is a smooth crossover, as was shown using finite-size scaling in lattice QCD simulations [2], located at around $T = 156\text{--}158$ MeV [3,4]. At larger chemical potentials, a rich phase diagram is conjectured. In particular, the search for the critical end point of QCD has received special attention, both by theory and experiment [5].

One way to locate the QCD crossover temperature on the lattice is by finding a peak in the susceptibility of the pseudo-order parameter, namely the chiral susceptibility [6,7], as a function of the temperature. In the limit of vanishing quark masses (the so-called chiral limit), this susceptibility is associated to the second order chiral transition and follows the critical behavior of the three dimensional $O(4)$ universality class [8]. The connection between QCD and the three-dimensional $O(4)$ spin model has been intensively studied on the lattice [9,10], but also with Dyson-Schwinger equations (DSE) [11,12] and the functional renormalization group (FRG) [13]. On the

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lattice, the crossover temperature as a function of the baryon chemical potential has been calculated by means of Taylor expansion [3,14] and analytic continuation from purely imaginary μ_B [4,14–17], based on the location of the peak of the chiral susceptibility, providing results up to around $\mu_B = 300$ MeV [3,4]. The theoretical community distinguishes between crossover lines depending on the handling of the strange quark. Two frequently used options are the theoretically simpler choice of vanishing strangeness chemical potential ($\mu_S = 0$) and the strangeness neutrality ($n_s = 0$), which is motivated by the experimental setup of heavy ion collisions. The latter case is more involved for theory, because μ_S has to be tuned to meet the neutrality condition. The differences between the two setups have been often emphasized and quantified by the lattice community [15,18].

An experimental proxy of the crossover temperature (valid at small-enough chemical potentials) is given by the temperature of chemical freeze-out, namely the stage of a heavy-ion collision where the chemical composition of the resulting hadronic medium is fixed (up to final-state decay processes). Since this can by definition only happen in the hadronic phase, the chemical freeze-out temperature naturally represents a lower bound on the QCD transition temperature. Still, due to the rapid drop in scattering rates at the crossover, it is expected to be very close to the actual crossover temperature, especially for large collision energies [19]. Indeed, recent estimates at LHC energies show a freeze-out temperature that agrees with the crossover determined on the lattice within errors [20]. As the chemical potential increases, the freeze-out curve approaches the nuclear liquid-gas transition [21] and is thus no longer expected to follow the crossover line, but rather to deviate downward and separate from it. In the range of chemical potentials where lattice QCD calculations for the crossover line exist, this deviation has not yet been observed [4,17,22].

Determining the crossover line up to large density and where it deviates from the freeze-out line is crucial for our understanding of the phase structure of QCD, as well as for the interpretation of experimental measurements, which provide snapshots of fluctuation observables taken at freeze-out conditions. The freeze-out curve can also serve as a lower bound on the critical point location [23], at least if one assumes that the chiral critical end point is also a deconfinement critical endpoint. Moreover, the critical end point should be located on the analytic continuation of the crossover line.

In order to extend the lattice QCD phase diagram to higher chemical potentials (so that a possible deviation from the freeze-out curve can be observed) it is useful to study other proxies for the crossover temperature, instead of the theoretically cleaner definition based on the chiral susceptibility. One unfortunate aspect of the chiral susceptibility is that it suffers from sizable finite-volume effects.

On the one hand, this makes extrapolations to large chemical potentials very difficult, as signal-to-noise ratios in Taylor coefficients deteriorate exponentially with the volume. On the other hand, this volume dependence is unsurprising, since this observable effectively uses light quarks (with a large Compton wavelength) to probe the medium. Recently, in Ref. [22] finite-volume effects have been compared for observables based on light quarks and infinitely heavy (static) quarks, and indeed it was observed that the values of static quark observables have much smaller finite-volume corrections. However, observables based on static quarks have different undesirable properties. First, compared to the chiral pseudo-order parameter (the chiral condensate) the Polyakov-loop (which is used to define the static quark free energy) is noisier. Second, the slope of the static quark free energy is small and weakly dependent on the temperature. As a consequence, the static quark entropy has an extremely broad peak. Indeed, it was estimated that, while at $\mu_B = 0$ the width of the chiral transition is around ~ 15 MeV [4], the width of the deconfinement transition is much larger, around ~ 35 MeV [24]. In a way, the Polyakov loop and related observables are less sensitive to the QCD crossover.

Thus, light quark observables have a larger volume dependence, while infinitely heavy quark observables have a smaller volume dependence, but are also less sensitive to the crossover. It is then natural to ask what happens if one probes the medium at the scale of the intermediate mass quark: the strange quark.

In this work we observe that two strangeness-related quantities are remarkably constant along the chiral transition line, at imaginary as well as real chemical potentials, as long as the strangeness neutrality condition is satisfied. The first is the strangeness susceptibility χ_2^S , defined as the second derivative of the QCD pressure with respect to the strange quark chemical potential, or the grand canonical variance of strangeness,

$$\chi_2^S = \frac{\partial^2(p/T^4)}{\partial(\mu_S/T)^2}, \quad (1)$$

where p is the pressure, T is the temperature and μ_S is the strangeness chemical potential. The second is the strangeness chemical potential needed to reach strangeness neutrality, normalized by the baryon chemical potential, namely μ_S/μ_B .

The strangeness susceptibility has some technical aspects that are advantageous in lattice calculations. First, unlike static quark quantities, the slope of χ_2^S near T_c is large enough to make the calculation of $\chi_2^S \approx \text{const}$ curves practical. Second, due to the larger strange quark mass, the associated remnant of the sign problem is milder, as compared to quantities dominated by light quarks, making it possible to extrapolate to larger chemical potentials. Third, like the static quark quantities, and unlike light-quark-based quantities, the strangeness susceptibility

has a remarkably mild volume dependence (at least at $\mu_B = 0$). The ratio μ_S/μ_B is directly determined by the strangeness density and enjoys the same advantages as the strangeness susceptibility. Thus, if we can successfully argue that the conditions $\chi_2^S, \mu_S/\mu_B = \text{const}$ are good proxies for the crossover, this will allow us to chart the phase diagram to an unprecedentedly large chemical. We note that the observation that $\mu_S/\mu_B \approx \text{const}$ along the crossover line is not new, as was already shown in Ref. [25] for real chemical potentials from a Taylor expansion.

The observation upon which this work is based, that both the strangeness susceptibility χ_2^S and the ratio μ_S/μ_B are remarkably constant at the crossover temperature as the chemical potential is increased, is an empirical statement based on lattice data at zero and purely imaginary chemical potentials. Using strange quarks, instead of light quarks to probe the hot and dense QCD medium allows us to use a smaller volume, and thus higher statistics.

In this work we employ data from three different lattices, all with aspect ratio $LT = 2$ and $N_\tau = 8, 10, 12$. By means of a two-dimensional Taylor expansion in μ_B, μ_S we obtain a controlled extrapolation of the different contours, and provide the continuum limit of our two proxies of the chiral transition up to $\mu_B \approx 400$ MeV. We observe mild cutoff dependence, especially in μ_S/μ_B . We also find finite volume effects to be small, by comparing finite density results in two volumes, with $LT = 2$ and $LT = 3$. Remarkably, we find that the corresponding results from the hadron resonance gas (HRG) model agree with our results for both observables and at all chemical potentials. The extreme statistics we accumulated on our $16^3 \times 8$ lattice allows us to obtain, for this single lattice spacing, the proxies for the QCD transition up to $\mu_B \approx 550$ MeV. In this case, the $\mu_S/\mu_B = \text{const.}$ curve detaches from the parametrized chemical freeze-out line from Ref. [26] above $\mu_B = 400$ MeV, while remaining in perfect agreement with the HRG model prediction.

The structure of the paper is as follows. In the next section, we present phenomenological arguments for why the strangeness susceptibility may be a good proxy for the crossover line. This argumentation has two steps. First, we show directly using lattice QCD data (at real and several different purely imaginary chemical potentials, as well as several volumes) that, at small chemical potentials, constant values of the strangeness susceptibility or of the ratio μ_S/μ_B indeed coincide with the peak of the chiral susceptibility. We also show that, unlike the chiral susceptibility, χ_2^S has a very weak volume dependence, which is practically useful if one wants to accumulate the extreme statistics needed for a very high order Taylor expansion. Second, we show (using a phenomenological calculation) that the critical fluctuations of strangeness are suppressed when strangeness neutrality is imposed on the system. This means that such a correspondence should break down much more

slowly when approaching the critical point than for other observables: e.g. no such suppression of critical fluctuations takes place for the chiral susceptibility. In Sec. III we first discuss our lattice setup, then present our results for the finite μ_B extrapolations of the contours and finally their continuum limit. We compare our results with other relevant lines in the phase diagram, such as the chiral crossover and the chemical freeze-out line from heavy ion collisions phenomenology. Finally, we summarize our results and discuss their relevance in mapping the phase diagram of QCD in Sec. IV.

II. STRANGENESS FLUCTUATIONS NEAR THE PHASE BOUNDARY

We start by arguing that the lines with a constant strangeness susceptibility χ_2^S , or with a constant μ_S/μ_B , are good proxies for the crossover line on the QCD phase diagram. We have two arguments: the first is empirical and based on lattice simulations at imaginary chemical potential; the second is phenomenological and applies in the vicinity of a supposed critical end point.

A. Strangeness fluctuations as proxies for the QCD crossover

Our initial observation is based on lattice QCD data sets perviously used in Refs. [4,27,28]. These simulations use lattices of size $48^3 \times 12$ with the 4stout improved staggered action [29]. Here we do not present new simulation results, but rather use different visualizations of already published results to make a point.

We show the chiral susceptibility as a function of the strangeness susceptibility and of the ratio μ_S/μ_B , for several different imaginary chemical potentials in Fig. 1. With the exception of the low-temperature regime for μ_S/μ_B , the different imaginary chemical potentials neatly fall on the same curve, and the position of the peaks is independent of μ_B . The observed lattice data point to apparently universal values for these strangeness-related variables, defined by the peak of the chiral susceptibility: $\chi_2^S = \text{const} \approx 0.3$ and $\mu_S/\mu_B = \text{const} \approx 0.25$. Note that Fig. 1 shows a broad range of imaginary chemical potentials, $\mu_B/T = 0 \dots i \cdot 2.75$. The largest chemical potential is close to $\mu_B/T = i\pi$, where the Roberge-Weiss critical point is located [30]. The fact that we observe this apparent collapse even close to this point indicates that the associated critical region is narrow, and non-singular behavior dominates. We do not have data exactly at $\mu_B/T = i\pi$ because of the numerical challenge posed by setting the strangeness neutrality condition in the presence of critical slowing down.

The observation in the imaginary domain of the chemical potential implies that, after analytic continuation, the curves defined by the peak of the chiral susceptibility, and those defined by proxies ($\chi_2^S = \text{const} \approx 0.3$ and

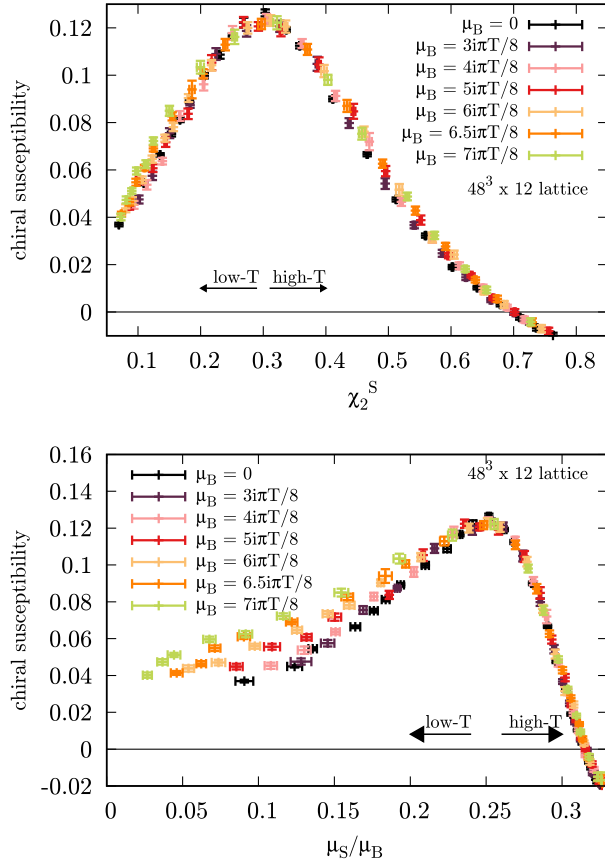


FIG. 1. The chiral susceptibility in the case of strangeness neutrality, as a function of the strangeness susceptibility (top) and the normalized strangeness chemical potential (bottom), on a $48^3 \times 12$ lattice for different imaginary values of the baryon chemical potential.

$\mu_S/\mu_B = \text{const} \approx 0.25$) are bound to agree, at least at small enough real chemical potentials. This is seen in Fig. 2, where we compare the chiral transition curve calculated in Ref. [4] from analytic continuation using a polynomial ansatz and the curves of constant χ_2^S or μ_S/μ_B obtained using the T' -expansion in Ref. [27]. Up to around 300 MeV, all bands agree within error.

Collapse plots similar to Fig. 1 have been presented for the chiral susceptibility versus the chiral condensate in Ref. [4]. In fact, a constant value of the chiral condensate could also be suggested as a proxy of the crossover temperature. However, that choice has some technical/practical disadvantages. One important disadvantage is that definitions of T_c based on the chiral condensate of chiral susceptibility have larger finite volume effects than those based on the strangeness susceptibility (at least at zero chemical potential) [22]. This is shown in Fig. 3, where different proxies for T_c are shown as functions of the aspect ratio LT (the spatial extent of the lattice in temperature units). A smaller simulation volume helps to reach higher chemical potentials, as the signal-to-noise

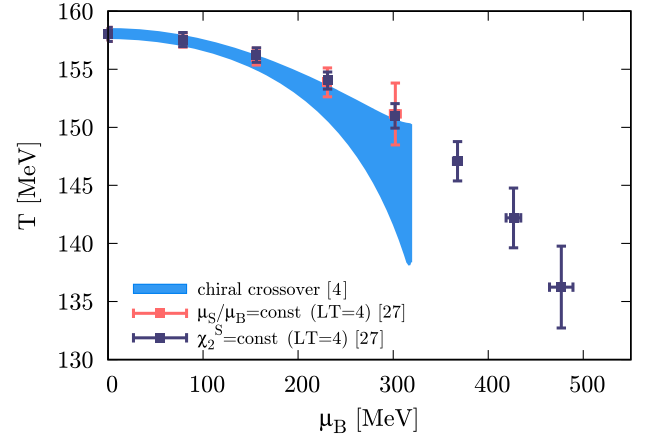


FIG. 2. The contour obtained through the conditions $\chi_2^S = \text{const}$ or $\mu_S/\mu_B = \text{const}$ in continuum extrapolated results in the T' expansion from Ref. [27], compared to the chiral transition line from Ref. [4].

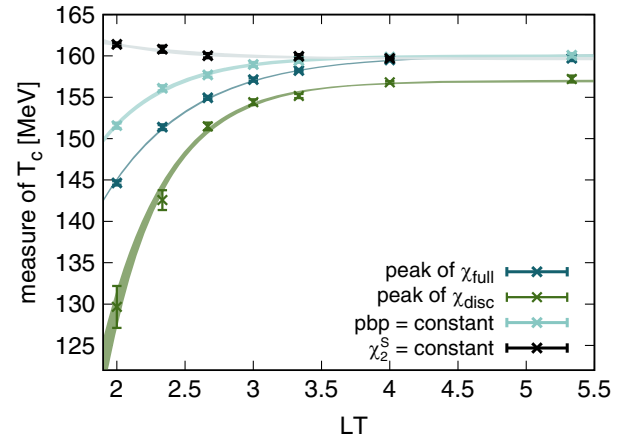


FIG. 3. Different definitions and proxies of the QCD crossover temperature as functions of the lattice volume in temperature units (the aspect ratio) on $N_\tau = 12$ lattices.

ratios of the Taylor coefficients strongly deteriorate with volume [31]. Furthermore, the per-configuration-cost is also smaller for smaller volumes, which makes it possible to gather the very large statistics needed for a high order Taylor expansion.

We remark that similar collapse plots also underlie the rationale for the T' expansion, which is a resummation of the Taylor series designed to converge quickly [27,32,33] in situations where such collapse is a good approximation. This happens if the free energy density is to a good approximation a single-variable function of the combination $T(1 - \kappa\hat{\mu}_B^2)$ [34], with κ a constant, instead of T and μ_B separately. This appears to be a good assumption at small chemical potentials. However, it is also an assumption that should break down at higher chemical potentials if the critical endpoint exists.

B. The (in)sensitivity of strangeness fluctuations to the QCD critical end point

So far our arguments were based on lattice QCD data, and we only argued that a constant value of the strangeness susceptibility or μ_S/μ_B are good proxies for the crossover temperature at small chemical potentials. In general, such contours starting from the pseudo-critical temperature at $\mu_B = 0$ will hit the critical point if: (1) they follow the chiral transition line, and (2) the value of the observable they are based on is not influenced by critical effects.

We already showed Fig. 2 in support of argument (1), and will present more precise, continuum extrapolated lattice results in a smaller physical volume in the next section. As far as argument (2) is concerned, we note that the value of μ_S/μ_B needed for strangeness neutrality is driven by the strangeness density, which does not diverge at the critical point. On the other hand, χ_2^S is a susceptibility, which then could diverge at the critical point. However, we will show in the following that such divergence is strongly suppressed in the case of strangeness neutrality.

In fact, it is possible for fluctuation observables to be insensitive to the critical end point, if they do not couple to the baryochemical potential. That this is the case for e.g. net-pion fluctuations was pointed out a long time ago in the literature [35,36]. This happens because, while the $\pi^+\pi^+$, $\pi^+\pi^-$, and $\pi^-\pi^-$ correlators are all singular at the critical point, due to isospin symmetry, and the pions not coupling to a baryochemical potential, these singular parts cancel in net-pion fluctuations.

This argument can also be applied to fluctuations of strange quarks, as we are going to show in this section. We will use a quark-meson model to show how the coupling to the critical σ mode affects the expected critical contribution to χ_2^S , both for $\mu_S = 0$ (larger effect) and for strangeness neutrality $n_S = 0$ (where it will turn out to be a much smaller effect). This will allow us to exploit, in the $n_S = 0$ case, the empirical argument of $\chi_2^S = \text{const}$ at the chiral transition to estimate the location of the QCD phase boundary up to large μ_B .

Fluctuations of the net baryon number diverge at the critical point as powers of the system's correlation length [35,36]: for example, the second baryon susceptibility diverges as

$$\chi_2^B \sim \xi^\gamma, \quad (2)$$

where ξ is the correlation length, and γ and ν are the critical exponents for the 3D Ising universality class.

In an effective model treatment, this divergence is due to the coupling of baryons to the critical σ field by means of a Yukawa term,

$$\mathcal{L}_{\sigma NN} = G\sigma \bar{N}N. \quad (3)$$

This is conveniently reflected into experimentally available observables, such as event-by-event fluctuations and

correlations of hadrons [35], in particular protons. Correlations between hadron species i, j of order two can be written as

$$\langle \Delta N^i \Delta N^j \rangle = V \int_p \int_k \langle \delta n_p^i \delta n_k^j \rangle, \quad (4)$$

where n_p^i is the occupation number of species i in momentum mode p .

Contributions e.g. to the proton-proton correlator integrated over in Eq. (4) are diagrammatically shown in Fig. 4, where the critical contribution comes from the right diagram due to the exchange of a zero-momentum σ field which becomes massless at the critical point.

The critical contribution to the second order net-proton fluctuations is then driven by the right diagram, which evaluates to [36]

$$V \langle \delta n_p \delta n_k \rangle = \frac{g^2}{m_\sigma^2 T E_p E_k} [n_p^+(1 - n_p^+) - n_p^-(1 - n_p^-)] \times [n_k^+(1 - n_k^+) - n_k^-(1 - n_k^-)], \quad (5)$$

where $E_p = \sqrt{p^2 + m_p^2}$, m_p is the proton mass, m_σ is the diverging σ mass, T the temperature, $n_p^\pm = [\exp\{(E_p \mp \mu_p)/T\}]^{-1}$ are the Fermi-Dirac distributions for proton and antiproton, and the factors $(1 - n)$ account for the Pauli principle.

We now wish to estimate the size of the critical contribution to the strangeness susceptibility $\chi_2^{S(\text{crit})}$. In order to do so, we apply the same line of reasoning to constituent quarks. In this case, the Yukawa coupling term would be analogous to the previous case,

$$\mathcal{L}_{\sigma \bar{q}q} = G\sigma \sum_{i=u,d,s} \bar{q}_i q_i, \quad (6)$$

where we can assume the same coupling G for all three quark flavors thanks to the $SU(3)_f$ symmetry.

This means that the macroscopic correlation between the net numbers of quarks of flavors i, j reads

$$\langle \Delta N^i \Delta N^j \rangle = V \int_p \int_k \langle \delta n_p^i \delta n_k^j \rangle, \quad (7)$$

with, as before,

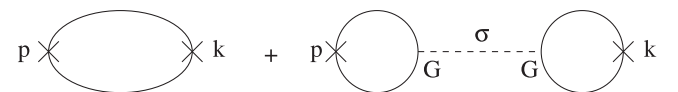


FIG. 4. Diagrams contributing to the second order fluctuations of net-proton number. Figure from Ref. [35].

$$V\langle\delta n_p^i \delta n_k^j\rangle = \frac{G^2}{m_\sigma^2 T} \frac{4m_i m_j}{E_p^i E_k^j} \times [n_p^{i,+}(1 - n_p^{i,+}) - n_p^{i,-}(1 - n_p^{i,-})] \times [n_k^{j,+}(1 - n_k^{j,+}) - n_k^{j,-}(1 - n_k^{j,-})], \quad (8)$$

where the $n_p^{i,\pm}$ are now the Dirac distributions for flavor i , and m_i are the constituent quark masses $m_u = m_d = 340$ MeV or $m_s = 500$ MeV. This expression factorizes into

$$V\langle\delta n_p^i \delta n_k^j\rangle = \frac{G^2}{m_\sigma^2 T} F_p^i F_k^j, \quad (9)$$

where we defined

$$F_p^i = \frac{2m_i}{E_p^i} [n_p^{i,+}(1 - n_p^{i,+}) - n_p^{i,-}(1 - n_p^{i,-})]. \quad (10)$$

Apart from the explicit factor of temperature in Eq. (8), the whole dependence on T, μ_B, μ_S is contained in F_p^i through the quarks' Dirac distributions. The flavor-flavor correlation then reads

$$\langle\Delta N^i \Delta N^j\rangle = \frac{G^2}{m_\sigma^2 T} \int_p F_p^i \int_p F_p^j.$$

In order to estimate the size of the critical contribution to the strangeness susceptibility, consider the ratio,

$$R(T, \mu_B) = \frac{\int_p F_p^u}{\int_p F_p^s}. \quad (11)$$

By rearranging the derivatives with respect to the u, d, s chemical potentials in terms of those related to the conserved charges B, Q, S , the relative size of the critical contributions to χ_2^S and χ_2^B becomes

$$\frac{\chi_2^{S(\text{crit})}}{\chi_2^{B(\text{crit})}}(T, \mu_B) = \frac{4}{9} R(T, \mu_B)^2 + \frac{4}{9} R(T, \mu_B) + \frac{1}{9}. \quad (12)$$

We can estimate this ratio by considering values for $T_c, \mu_{B,c}$ consistent with current predictions [37–41] for the critical point location, at $\mu_S = 0$ or in the strangeness neutral condition, which as we showed roughly fixes the chemical potentials as $\mu_S \simeq 0.25\mu_B$. For all such predictions, where $T = 100$ – 120 MeV and $\mu_B = 600$ – 650 MeV, from Eq. (12) it follows that in the $\mu_S = 0$ case the critical contributions satisfy $\chi_2^{S(\text{crit})} \simeq 0.3\chi_2^{B(\text{crit})}$, while in the strangeness neutral case $\chi_2^{S(\text{crit})} \simeq 0.01\chi_2^{B(\text{crit})}$. This means that, in the latter case, the strangeness susceptibility χ_2^S is almost completely oblivious to the possible presence of a critical point. Because the constituent quark masses are

generated by a finite expectation value of the σ field, their value at the critical point will be lower than in the vacuum. With the reasonable assumption that such expectation value at the critical point is reduced by a factor two [42], we can expect the light constituent quark masses to drop accordingly, and the strange quark mass to be reduced by the same (absolute) amount. In this simplified scenario, i.e. with constituent quark masses $m_u = m_d = 170$ MeV or $m_s = 330$ MeV, we obtain in the strangeness neutral case $\chi_2^{S(\text{crit})} \simeq 0.03\chi_2^{B(\text{crit})}$.

Independently of the constituent quark masses, in the case of a zero *strange quark* chemical potential $\mu_S = 0$ one has $\chi_2^{S(\text{crit})} = 0$, as contributions from the strange quarks and their antiparticles cancel in this Feynman diagram exactly.

III. LATTICE RESULTS AT $LT=2$

We now briefly discuss the simulation setup for the new lattice results we present on the χ_2^S and μ_S/μ_B contours at finite chemical potential.

We use $N_f = 2 + 1$ flavors of rooted staggered fermions with four steps of HEX smearing [43] and the DBW2 action [44], at physical values of the quark masses. We set the scale with the pion decay constant f_π , or with a modified version of the Wilson-flow-based w_0 [45], as introduced in Ref. [46], where this particular lattice action was already used, as well as in Ref. [31]. We employ $16^3 \times 8$, $20^3 \times 10$ and $24^3 \times 12$ lattices to perform continuum extrapolations of the transition line proxies up to $\mu_B = 400$ MeV. We have here the same statistics as in Ref. [46] on the $20^3 \times 10$ and $24^3 \times 12$, while on the $16^3 \times 8$ lattice it is much larger, the same as in Ref. [31]. Additionally, we employ new simulation results on a $24^3 \times 8$ lattice to gauge finite volume effects (with 60 000–70 000 configurations per temperature). Thanks to the larger statistics, we can extrapolate our results on the $16^3 \times 8$ lattice further in μ_B , and provide guidance on where the transition might take place when the density is further increased. On the smaller lattices ($16^3 \times 8$ and $20^3 \times 10$) we use the reduced matrix formalism to calculate the fluctuations, in the same way as we did in Refs. [31,46–48], on the larger lattices we determine the μ_B -derivatives with stochastic sources [49].

A. Extrapolation to finite chemical potential

In this work we take advantage of the extreme statistics we have gathered to build a two-dimensional Taylor expansion in μ_B, μ_S . We obtain results for the lines of constant χ_2^S or μ_S/μ_B up to $\mu_B = 400$ MeV, that we extrapolate to the continuum. This is based on an expansion up to next-to-next-to-leading (N²LO) order in the chemical potentials. In our coarsest lattice $16^3 \times 8$ we are able to employ coefficients up to next-to-next-to-next-to-next-to-leading (N⁴LO) order, i.e. including up to tenth order

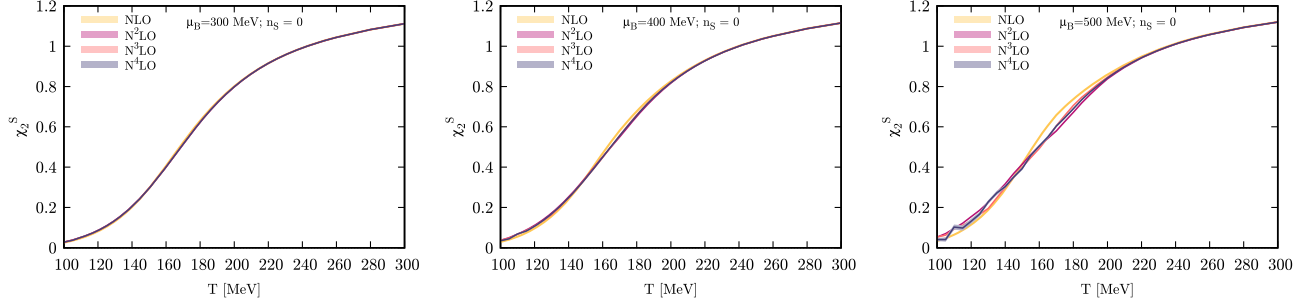


FIG. 5. The extrapolated χ_2^S at different values of μ_B and different orders in the Taylor expansion, on our $16^3 \times 8$ lattice. The strangeness chemical potential μ_S was set for each T, μ_B pair to match the strangeness neutrality condition.

conserved charge fluctuations and correlations, and push the extrapolation above $\mu_B = 500$ MeV.

The results in this work refer to the strangeness neutral case, i.e. a setting of the strangeness chemical potential μ_S such that the strangeness density n_S vanishes. We accomplish this by constructing the two-dimensional Taylor expansion in μ_B, μ_S and, for each T and μ_B , search for the $\mu_S = \mu_S^*$ that corresponds to the strangeness neutral case. This provides the value of μ_S^* over the whole portion of the phase diagram we are able to access with our

extrapolations. This scheme slightly differs from Ref. [50] where $\mu_S^*(\mu_B)$ itself is Taylor expanded. Our direct solution of $-n_S(\mu_S) = 0$ at fixed T and μ_B achieves a faster convergence in the orders of μ_B . Once $\mu_S^*(T, \mu_B)$ is known, we can evaluate $\chi_2^S(T, \mu_B, \mu_S^*)$ at strangeness neutrality, too, as shown in Fig. 5. Notice that, for all studied chemical potentials, the strange susceptibility is a monotonic function of the temperature. This means that the temperature where $\chi_2^S(T, \mu_B, \mu_S^*) = \chi_2^S(T_c, 0, 0)$ is always well defined.

We show in Fig. 6 the extrapolated contours of constant μ_S/μ_B (top) and χ_2^S (bottom) from our $16^3 \times 8$ lattice at different orders in the Taylor expansion, from NLO to N^4 LO, and observe very good convergence. The effects beyond N^2 LO are visible only above $\mu_B \approx 450$ MeV, and a discrepancy between N^3 LO and N^4 LO appears, if at all, above $\mu_B \approx 500$ MeV.

In this work we are after proxies for the QCD transition line. In order to obtain a continuum limit, on each lattice we construct $\chi_2^S = \text{const}$ contours, where the constant is the $\mu_B = 0$ value of χ_2^S at $T_0 = 158$ MeV, i.e. the result we obtained in the continuum in Ref. [4]. We then repeat the procedure for $\mu_S/\mu_B = \text{const}$ contours. The results are shown in Fig. 7, where one can see that the two proxies

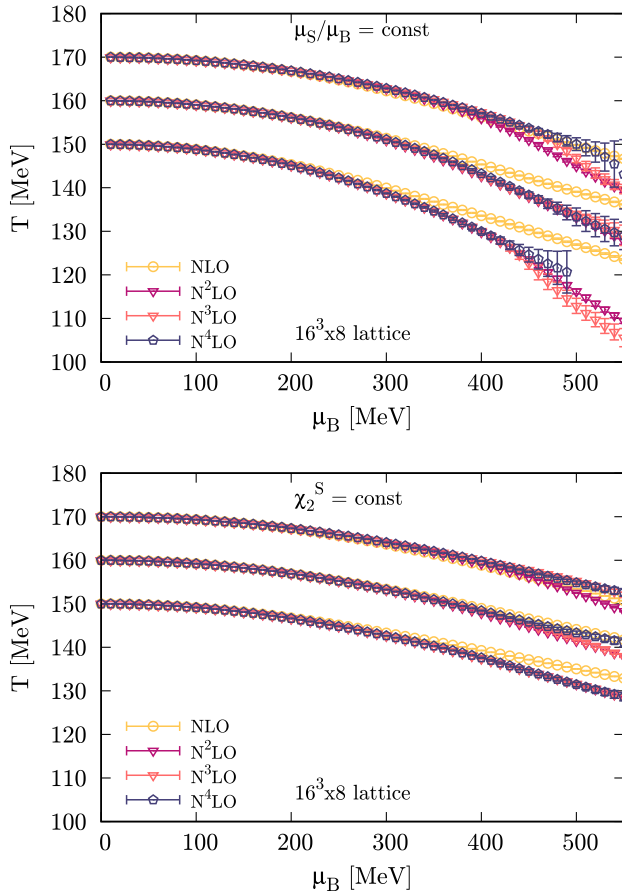


FIG. 6. Contours of constant μ_S/μ_B or χ_2^S , on our $16^3 \times 8$ lattice at different orders in the Taylor expansion.

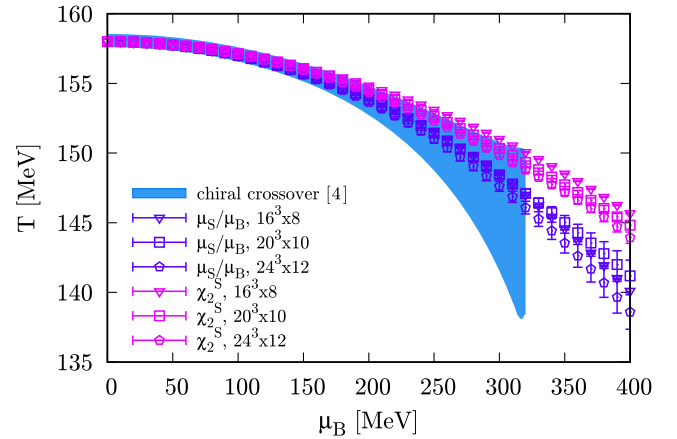


FIG. 7. Contours of constant μ_S/μ_B or χ_2^S from a N^2 LO Taylor expansion, on our $16^3 \times 8$, $20^3 \times 10$ and $24^3 \times 12$ lattices. Constant values are taken at $T_0 = 158$ MeV.

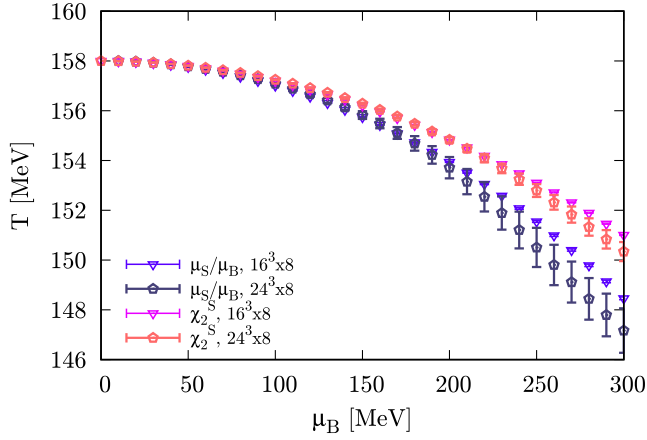


FIG. 8. Contours of constant μ_S/μ_B or χ_2^S from a N^2 LO Taylor expansion, on our $16^3 \times 8$ and $24^3 \times 8$. Constant values are taken at $T_0 = 158$ MeV.

yield slightly different results, although both are in agreement with the current continuum extrapolated result for the QCD crossover [4], and their spread is in fact smaller than the error on such result. This result is based on a N^2 LO Taylor expansion, i.e. including up to $\mathcal{O}(\mu_B^6)$ contributions. We observe that discretization effects are smaller for the $\mu_S/\mu_B = \text{const}$ contours, as no clear N_τ ordering appears, compared to the $\chi_2^S = \text{const}$ contours.

Before carrying out the continuum limits, we wish to assess the size of finite volume effects. We perform the same analysis on a $24^3 \times 8$ lattice, and compare to the $16^3 \times 8$ result in Fig. 8. We see that the results from both volumes are in good agreement in the whole range we can access with the statistics we gathered on our $24^3 \times 8$ lattice. Hence, finite volume effects are smaller than discretization effects, and in particular smaller than the difference in

temperature between the contours based on the different observables.

B. Continuum limit

Finally, we perform the continuum extrapolation of the N^2 LO Taylor expansion results up to $\mu_B = 400$ MeV. In Fig. 9 we show this for the strangeness susceptibility (left) and μ_S/μ_B (right). We first observe, as noticed earlier, that cutoff effects are smaller for the latter, for which the results are almost N_τ -independent. In both panels, the two sets of points and fit bands indicate the results obtained with the two scale settings we employ. These were defined and introduced for this action in Ref. [46]. We consider the difference between the two scale settings as a source of systematic errors, and combine the two results in the following. We also observe that in general the continuum limits based on the two different observables are in good agreement, showing discrepancies around the 1σ level.

Combining the results from Fig. 9 for each μ_B value (and including both scale settings), we obtain the continuum extrapolated proxies for the chiral crossover we show in Fig. 10. Again, we find that these contours are in perfect agreement with the chiral crossover, and the tension between the contours based on the different observables is quite mild. The two contours could in fact be taken together, interpreting their spread as an additional source of systematic error on the QCD crossover. Even so, the error we obtain is much smaller than on the chiral crossover, thanks to the smaller physical volume and the extreme statistics we employed. Additionally, we show the corresponding contours obtained with the HRG model, and strikingly find that they are also in perfect agreement with our continuum extrapolations. These are obtained in the same way as our lattice-based ones: we fix the value of the observables at $T_0 = 158$ MeV, then construct the contours

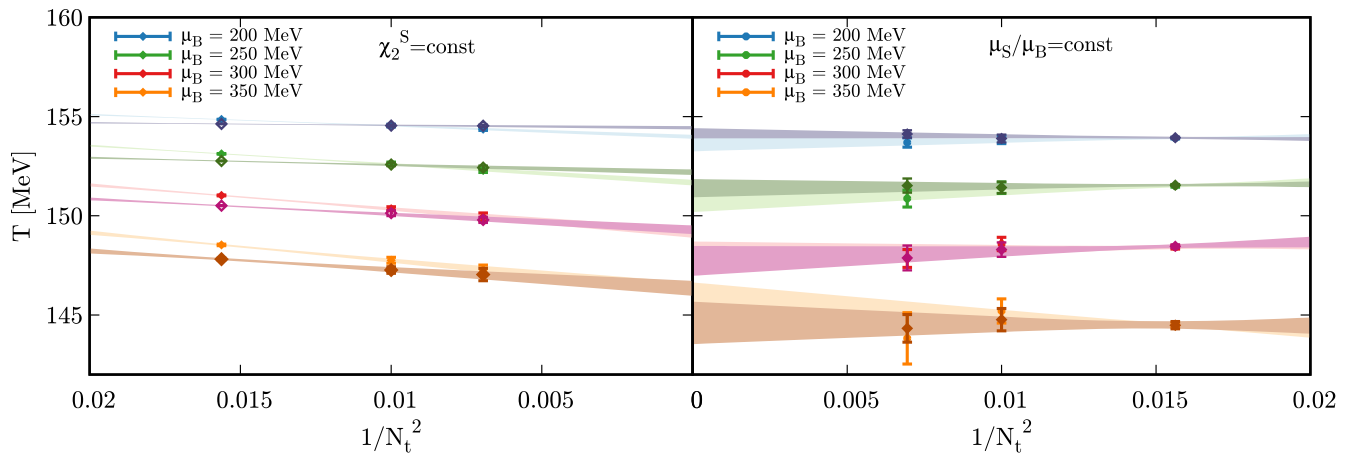


FIG. 9. Continuum limits of the contours of constant χ_2^S (left) and μ_S/μ_B (right) at different values of μ_B . Different points and bands in each plot indicate the two different scale settings we employ, with the lighter and darker bands corresponding to the f_π and the w_1 scales, respectively.

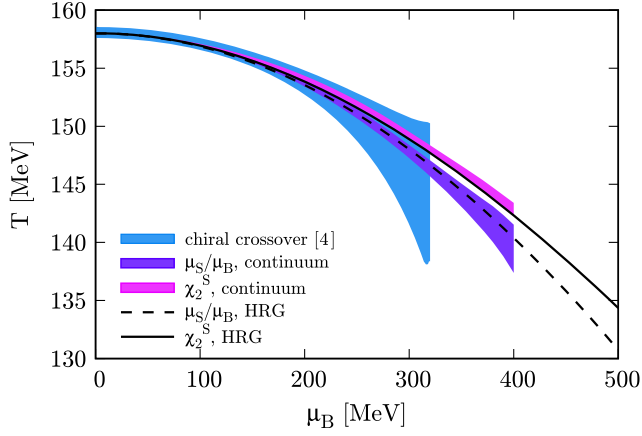


FIG. 10. Contours of constant μ_S/μ_B or χ_2^S from a N²LO Taylor expansion (constant values taken at $T_0 = 158$ MeV), extrapolated to the continuum, compared to the chiral crossover and to HRG results.

at all μ_B values. The agreement we observe means that, although the HRG might (slightly) disagree with lattice results at $\mu_B = 0$, the μ_B dependence is captured correctly by the model. This is highly not trivial, given the simple assumptions the model lies upon. From what we observe, one could take the HRG result itself as a proxy of the QCD crossover, in which case it would be possible to extend its predictions to even larger chemical potential.

IV. SUMMARY AND DISCUSSION

In this work we discussed how observables related to strangeness fluctuations can shed light on the phase structure of QCD at finite density. The starting point of our discussion was the remarkable collapse of the chiral susceptibility when plotted against the strange susceptibility χ_2^S as the chemical potential was varied. This implied that the chiral transition can be associated with a specific value of $\chi_2^S \approx 0.3$. Similar statements are true for our other observable, the μ_S/μ_B ratio, satisfying the strangeness neutrality condition, though the data collapse is only observed at the high temperature side of the transition. In the latter case $\mu_S/\mu_B \approx 0.25$ seems to characterize the transition in a broad range of chemical potentials. Since direct simulations in large volumes are only feasible at zero or imaginary chemical potentials, our initial observation was limited to this domain.

One may wonder at this point, why we can make this statement in the strangeness neutrality context only, and if there are other thermodynamic variables that behave similarly. Obvious candidates would be the normalized baryon density n_B/μ_B or the baryon susceptibility χ_2^B . One of the requirements for a successful proxy variable is that it is monotonic in temperature. The monotonicity of n_B/μ_B and the corresponding data collapse have already been exploited to construct the T' -expansion in Refs. [27,32]. By

the nature of this construction, the χ_2^B is predicted to be nonmonotonic, and this is confirmed by lattice data at imaginary μ_B . Its sensitivity to critical behavior in the vicinity of either the Roberge-Weiss end point or the chiral end point is obvious. Another criterion for a successful proxy, though, is to have a μ_B -independent Stefan-Boltzmann (SB) limit. While n_B/μ_B is a sigmoid in temperature for a broad range of chemical potentials, its high temperature (SB) limit is μ_B -dependent, and one cannot associate a universal value with the “middle of the transition”. The same is true for χ_2^S , unless the strangeness neutrality condition is imposed (or, as an approximation, the fixed ratio $\mu_S = \mu_B/3$ is considered, which corresponds to a vanishing *strange quark* chemical potential $\mu_s = 0$). We argued that the same condition suppresses the coupling of this proxy to the critical fluctuations near the CEP. Considering also the practical advantages of defining the proxy on the scale of the strange mass, we are left with the two proxies, χ_2^S and μ_S/μ_B , both constrained with the phenomenologically relevant strangeness neutrality condition.

Next, we extended the initial observation to real chemical potentials, by comparing to the chiral transition line we have already published in Ref. [4]. To extrapolate the proxies themselves, we evaluated them via the T' -expansion with the continuum extrapolated coefficients of Ref. [27]. We found good agreement with the chiral line, though with large errors. One may argue that this comparison is trivial, since both the proxies and the chiral observables were in agreement at imaginary μ_B , and however sophisticated their analytical continuation may be, they are bound to remain equal. For this reason here we followed a different strategy. First, we argued that the finite volume corrections on our chosen observables are under control even if we reduce the simulation volume to two inverse temperatures ($LT = 2$). The practical advantage of this is the availability of high order baryon fluctuations, since the severity of both the sign and overlap problems is exponential in the volume. Armed with these generalized susceptibilities of baryon and strangeness we could calculate sufficiently high orders of the Taylor expansion, and demonstrate that subsequent orders are negligible up to a given μ_B . This range is $\mu_B \approx 400$ MeV if the highest available coefficient is N²LO, but stretches out to 550 MeV if we can afford the N⁴LO coefficients. This latter range is what we could cover with our extreme statistic ensembles at the coarsest lattice, while the former range applies to the continuum limit (driven down by the much higher cost of the $24^3 \times 12$ lattices). Even with this limitation, we could continuum extrapolate both of our proxies to a broader range of chemical potentials than what is known today as the chiral crossover line.

It is not obvious that the coarsest lattice in the study is close to the continuum limit. With our discretization, we do observe this for the ratio μ_S/μ_B . To highlight the

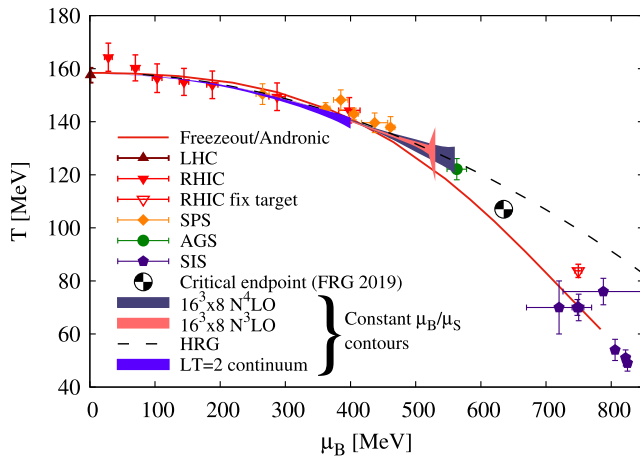


FIG. 11. We show the contours of constant μ_S/μ_B that satisfy the strangeness neutrality condition. On our coarsest lattice we give the $\mathcal{O}(\mu_B^6)$ (N^3 LO) and $\mathcal{O}(\mu_B^8)$ (N^4 LO) extrapolations of the contours up to 550 MeV, where the expansion seems to break down. The continuum limit (available at N^2 LO) is computed up to 400 MeV. These are consistent with each other, but also with the prediction of the hadron resonance gas model. We show in addition freeze-out data from various publications [23,51–54] together with their parametrization of Ref. [26] and a recent functional result on the critical end point’s location [37].

implication of our results for current knowledge of the QCD phase diagram, we show a sketch of the latter covering a broad range in temperature and chemical potential in Fig. 11. The continuum extrapolated contour of constant μ_S/μ_B , starting at T_c at $\mu_B = 0$, is shown together with the same contour for two subsequent orders on the $16^3 \times 8$ lattice. The highest order corresponds to employing up to 10th order fluctuations. χ_{10}^B was first presented in our recent work [31], and the analogous strange derivatives are used in this work for the first time. This unprecedented high order extrapolation allows us to confidently predict strangeness-related observables at finite density at least as far as this lattice size allows.

Quite remarkably, this observable is in agreement with the hadron resonance gas model’s prediction in the entire range where the contour was computed (also shown in Fig. 11). Equally remarkable is the fact that, assuming the validity of the proxies introduced here, the HRG model can predict the crossover. We stress that the only input we used for the HRG-based contour is the starting temperature at $\mu_B = 0$, that we get from lattice QCD to be $T_0 = 158$ MeV.

Given the experimental knowledge of the chemical freeze-out (see data points in Fig. 11) one can estimate the point of divergence between the freeze-out line and the QCD crossover. We stress that we have not demonstrated the validity of our proxies for the entire μ_B range.

However, if we assume that they work, and that finite volume and discretization effects on $16^3 \times 8$ lattice data are under control, we may be guided by the HRG prediction

and predict that the two curves start deviating between 400 and 500 MeV.

Recently, in Ref. [55] a similar conclusion was drawn from an HRG model calculation of the chiral condensate (which, in addition to the usual hadron spectrum also needs sigma terms as QCD input). The chiral condensate-based HRG proxy for the crossover line was found to start deviating from the freeze-out line for $\mu_B > 400$ MeV. An important distinction between Ref. [55] and the present work is that we see the deviation not only in an HRG proxy of the crossover line, but also directly in the high statistics $N_t = 8$ lattice QCD data.

The freeze-out data themselves may also provide a similar insight. Along the parametrization of the freeze-out line from Ref. [26], which we show in Fig. 11 as a red curve, the μ_S/μ_B ratio maintains a near-constant value up to $\mu_B \approx 400$ MeV, before dropping to lower values at higher densities. This drop in the value of μ_S/μ_B might indicate the point of deviation from the cross-over line. On the other hand, it might also signal the breakdown of this proxy. Results from e.g. the PNJL model [56] suggest that the strangeness chemical potential is related to deconfinement through the Polyakov loop. The fact that our proxies follow the chiral transition line so well at finite *imaginary* chemical potentials might be due to the fact that the deconfinement and chiral transition agree in that regime, and does not imply that the same is true at finite *real* chemical potential. There is the possibility that the deconfinement and chiral transitions detach at finite density, and that our proxy would follow the former while the chiral transition remains close to the freeze-out line. In any case, since our continuum extrapolated proxies show quite a good agreement with the freeze-out line up to $\mu_B = 400$ MeV, this detachment is not likely to happen in this range.

Finally, the location of the critical end point, for which first principles theoretical predictions outside of lattice already exist [37–39], is expected to be in the range $\mu_B \sim 600$ –650 MeV. We argued that these proxies are weakly influenced by critical behavior, implying that the critical point is expected to be close to the lines defined by the constant values of χ_2^S or of μ_S/μ_B . While the two proxies may diverge at high μ_B , the range spread by these two contours is still the best estimate for the transition line that lattice QCD can offer today.

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DATA AVAILABILITY

The data that support the findings of this article are openly available [58].

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