Letter

Continuum-extrapolated high-order baryon fluctuations

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Fluctuations play a key role in the study of QCD phases. Lattice QCD is a valuable tool to calculate them, but going to high orders is challenging. Up to the fourth order, continuum results have been available since 2015. We present the first continuum results for sixth-order baryon fluctuations for temperatures between $T = 130$ and 200 MeV and eighth order at $T = 145$ MeV in a fixed volume. Comparison with earlier studies with imaginary chemical potential suggests that the volume effect is under control for $T < 145$ MeV. Our results are in sharp contrast with well-known results in the literature obtained at finite lattice spacing.

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Introduction: Fluctuations and qcd phases. The main goal of the heavy ion program of many accelerator facilities (e.g., at LHC, RHIC, or the upcoming CBM/FAIR) is to create new phases of matter and explore their properties under extreme conditions. Several experimental programs (such as the beam energy scan program at RHIC [1,2]) are designed to search for a hypothetical critical end point in the temperature-baryon density phase diagram. Some of the most important observables in this quest are fluctuations of conserved charges. In the grand canonical ensemble, they are derivatives of the pressure with respect to the chemical potentials coupled to the charges. In this work, we will calculate such fluctuation observables at zero baryochemical potential.

The physics applications of fluctuation observables are numerous. First, the equation of state of the hot-and-dense quark gluon plasma is one of the main inputs of lattice QCD to the phenomenology of heavy ion physics. Fluctuations at zero baryochemical potential μ_B are the basis for extrapolations of the QCD equation of state to nonzero μ_B, both by means of a truncated Taylor expansion [3] as well as via different resummations of the Taylor series [4–6].

Second, fluctuation observables are sensitive to criticality. While first-principle lattice simulations have shown that the chiral transition is a crossover at zero baryon density [7], at larger baryon densities several model calculations predict a critical end point in the 3D Ising universality class [8–11], where the crossover line becomes a line of first-order transitions. One of the proposed experimental signatures of such a critical end point is a nonmonotonic behavior of the fourth-to-second-order baryon number fluctuations as a function of μ_B [12,13]. The extrapolation of this ratio to $\mu_B > 0$ is possible, if a sufficient number of Taylor coefficients (fluctuations) are available at $\mu_B = 0$. Thus, fluctuations at $\mu_B = 0$ are also important for the quest to find the critical end point. An important baseline in this search is given by the hadron resonance gas (HRG) model, a noncritical model that describes thermodynamics below the chiral transition at $\mu_B = 0$ remarkably well. A reasonable minimum criterium for criticality searches, then, is the presence of solid deviations between HRG predictions and equilibrium QCD.

A different type of criticality—in the O(4) universality class—is also expected to be present in QCD, related to chiral symmetry restoration, one of the most important concepts in heavy ion physics. In the limit of zero light quark masses, the $SU(2) \times SU(2)$ chiral symmetry becomes exact, and the crossover transition occurring at physical masses is expected to be replaced by a genuine second-order transition [14–16]. Through the presence of a single scaling variable (a combination of the quark masses, the temperature and the chemical potential), O(4) criticality has imprints on the temperature dependence of higher baryon number fluctuations at $\mu_B = 0$ up to physical values of the quark masses (for a model calculation, see, e.g., Ref. [17]). The presence of such an O(4) scaling regime is likely the reason why lattice QCD calculation sees no sharpening or strengthening of the crossover transition for small chemical potentials [4,18,19]. The complicated interplay of O(4) and Ising criticality motivates more involved theoretical approaches to the phase diagram, based on Lee-Yang zeros [20,21], which have gained popularity in recent years [22–26]. These approaches, too, require reliable determinations of the corresponding fluctuations.

Third, fluctuation observables are very sensitive to the degrees of freedom of a thermodynamic system. This fact has been used before to argue, e.g., the existence of further (yet undiscovered) resonances [27–29] in the hadron spectrum, which was later confirmed by experiment [30].

Finally, fluctuation observables are central in the study of chemical freeze-out in heavy ion collisions. This is an especially interesting avenue of research, since it has the potential of allowing a direct comparison between first-principle QCD predictions and experimental data. While the comparison itself has many caveats, due to experimental effects [31–33], it is obviously worth pursuing.

Current lattice estimates. Conserved charge fluctuations have been a focus of lattice simulations for well over a decade now. Like any other observable, a reliable calculation of these requires a continuum limit extrapolation, via simulations using smaller-and-smaller lattice spacings. Up to second order, they have been known in the continuum since 2012 [34]. Fourth-order fluctuations in the baryon number and strangeness were first continuum extrapolated in 2015 [35]. In that case, a large temperature range was considered, showing good agreement with the hadron resonance gas model at low temperatures, as well as good agreement with perturbative calculations [36,37] at high temperatures. Since then, calculations of the fourth-order coefficients were pushed to very high precision [38]. Thus, up to fourth order, the derivatives in full QCD are known accurately, with the exception of electric charge fluctuations, which suffer from large cutoff effects that make continuum extrapolations difficult [35].

At the sixth and eighth orders, the statistics requirements for the direct determination of the coefficients dramatically blow up; thus, a continuum extrapolation of these coefficients has never been attempted. Because of the high statistics required, all available results on higher fluctuations employ the computationally cheapest discretization: staggered fermions. These suffer from a lattice artifact called taste breaking [39,40], whose effect is to strongly distort the meson spectrum and to some extent also the baryon spectrum at a finite spacing. At low temperatures baryon fluctuations receive their dominant contributions from the $B = 1$ sector of the Hilbert space; this part is also predicted by the HRG model. Since the relative taste breaking effect on baryons is mild, continuum extrapolations are well controlled with most staggered discretizations. The first deviations from HRG in the fluctuation ratios come from the $B = 2$ sector, which in many models dominated by repulsive interactions. Their characteristic scale is $\mathcal{O}(1)$ fm^3 still fitting in our simulation volume [41]. Since mesons mediate this repulsion, the relatively important taste breaking effect on these may have a significant effect on the magnitude of the $B = 2$. In χ_n^B the sectors are represented with a weight of B^n. Thus, higher-order fluctuations are increasingly sensitive to such cutoff effects.

The statistics required for the calculation of higher-order fluctuations can be drastically reduced by introducing a purely imaginary chemical potential, calculating lower-order fluctuations, and fitting their functional dependence on the imaginary chemical potential. The price for this reduction in statistics requirements is that assumptions have to be made on the functional form of the lower-order fluctuations, leading to hard-to-control systematic errors.

So far, three collaborations have presented results up to the eighth order with improved lattice actions. In chronological order: First, the Pisa group presented results on lattices with six time slices of 2stout improved fermions [7,42] in Ref. [43]. Second, the Wuppertal-Budapest Collaboration presented results with 12 time slices of 4stout improved fermions [44] in Ref. [45]. These two calculations took advantage of simulations at imaginary chemical potential. Finally, the HotQCD Collaboration presented results with eight time slices of Highly Improved Staggered Quark (HISQ) fermions [46], using a direct determination at $\mu_B = 0$ (i.e., without imaginary μ_B simulations) in Refs. [6,38]. For the latter calculation, 2 orders of magnitude more statistics were collected, compared to the previous two. It is a testament to the efficacy of the imaginary chemical potential method, then, that the error bars on the imaginary chemical potential calculations of the sixth- and eighth-order coefficients are substantially smaller.

At the current level of precision, discrepancies emerge between the calculations. In particular, the results based on the imaginary chemical potential method are in good agreement with the hadron resonance gas model for low temperatures. On the other hand, the direct calculation shows significant deviations for both observables even at the lowest temperature considered. To shed light on QCD criticality, this discrepancy has to be resolved.

In addition to the different extraction method for the higher-order coefficients (direct at $\mu_B = 0$ vs indirect from $\mu_B^2 \leq 0$), a potentially more significant difference between the two types of calculation lies in how the chemical potential is defined. Due to the extreme cost of the direct method, for fluctuations of order six and higher, the chemical potential in that case was introduced via the so-called linear prescription. In the other two cases, the exponential definition was used. Derivatives with respect to the chemical potential can be shown to be UV finite by virtue of a $U(1)$ symmetry if the chemical potential is introduced like a constant imaginary gauge field [47]. This is the exponential definition. If, instead, a naive linear definition is employed, power-law UV divergences appear in the free energy already in the case of free quarks. By taking enough derivatives with respect to the chemical potential, such power-law divergences disappear. However, this is not the case for logarithmic divergences, the absence of which for the naive linear definition is not proven for the interacting theory. Thus, although the linear definition is computationally cheaper, care should be taken in considering these results.

The linear definition also breaks the exact Roberge-Weiss periodicity [48] of the partition function. Even if one assumes that there are no problems with logarithmic divergences, the loss of Roberge-Weiss periodicity with the linear definition can potentially lead to large cutoff effects, since it effectively means that at a finite spacing, in contrast to the continuum, the free energy gets contributions from Hilbert subspaces not only at integer, but also at noninteger values of the baryon number, which at the very least, is a nonphysical feature at finite spacing.

Lattice calculation of fluctuations up to eighth order. In this paper, we present the first continuum results for baryon fluctuations up to the sixth order for temperatures between $T = 130$ and 200 MeV and up to the eighth order for a temperature of $T = 145$ MeV. Continuum extrapolation is made possible by the introduction of a new discretization, which we call the 4HEX action, that strongly suppresses taste breaking effects compared to all available actions in the literature. Although more costly, we pursue a direct determination at $\mu_B = 0$, in order to avoid possible systematic effects due to a choice of fit ansatz, necessary for the imaginary chemical potential method. Moreover, in order to avoid possible issues with the introduction of the chemical potential, we employ the exponential definition to all orders. Due to the extreme statistics cost of the direct method, this endeavor is only feasible in a volume that is smaller than what is typically used in the field, with an aspect ratio $LT = 2$. Thanks to the availability in the literature of the aforementioned results at finite lattice spacing, but with larger volume, we are able to show that, below $T = 145$ MeV, finite volume effects in our results are under control. At this temperature the simulation volume is 20 fm^3, which is several times larger than the $\mathcal{O}(1)$ fm^3 volume scale of the repulsive core of baryon-baryon interactions. Note also that $T \leq 145$ MeV is the relevant temperature range for the search for the elusive critical end point of QCD.

The novel lattice action we use for this thermodynamics study, 4HEX, is based on rooted staggered fermions with four steps of HEX smearing [49] with physical quark masses and the DBW2 gauge action [50]. This lattice action benefits from dramatically reduced taste breaking effects, compared to all other actions used in the literature. We simulate $16^3 \times 8$, $20^2 \times 10$ and $24^3 \times 12$ lattices to obtain a well-controlled continuum extrapolation. Details on the 4HEX action, the scale setting procedure, and the systematic error estimation can be found in Supplemental Material [51].

We calculate fluctuations of the baryon number at zero strangeness chemical potential:

$$\chi_n^B \equiv \left(\frac{\partial^n (p/T^4)}{\partial(\mu_B/T)^n} \right)_{\mu_S = 0}. \tag{1}$$

We also include results on the strangeness neutral line $n_s \equiv 0$ (see later in Fig. 2), which lead to similar conclusions as in the $\mu_S = 0$ case.

We use the exponential definition of the chemical potential at all orders in μ_B on all our lattices. For the $N_\tau = 8$, 10 lattices, we use the reduced matrix formalism to calculate the fluctuations, in the same way as we did in Refs. [52,53]. For the $N_\tau = 12$ lattice, we use the standard random source method [54].

We show our continuum extrapolated results for χ_4^B/χ_2^B (left) and χ_6^B/χ_2^B (center), together with the corresponding finite lattice spacing results in Fig. 1. The continuum results are obtained together with a spline fit of the temperature dependence. The exact procedure is described in Supplemental Material [51]. The bands include statistical and systematic uncertainties, consisting of different scale settings and different spline fits of the data. The covered temperature range is 130 MeV $\leq T \leq$ 200 MeV. Also shown are the results on the $N_\tau = 8$, 10 lattices for χ_8^B/χ_2^B (right). For this observable, we also include the continuum extrapolation at a single temperature of $T = 145$ MeV. Hadron resonance gas predictions are shown, and they equal 1 in all cases independently from the temperature and the hadron spectrum used.

From Fig. 1, it is apparent how small the cutoff effects of the 4HEX action are, as is the fact that, for $T < 145$ MeV, the fluctuations in continuum QCD are in very good agreement with the HRG results.

We also calculated the expansion coefficients at constant vanishing strangeness. These facilitate the computation of the QCD pressure at finite μ_B while maintaining the experimental constraint of zero strangeness density ($n_S = 0$) through the introduction of a strangeness chemical potential $\mu_S(T, \mu_B)$:

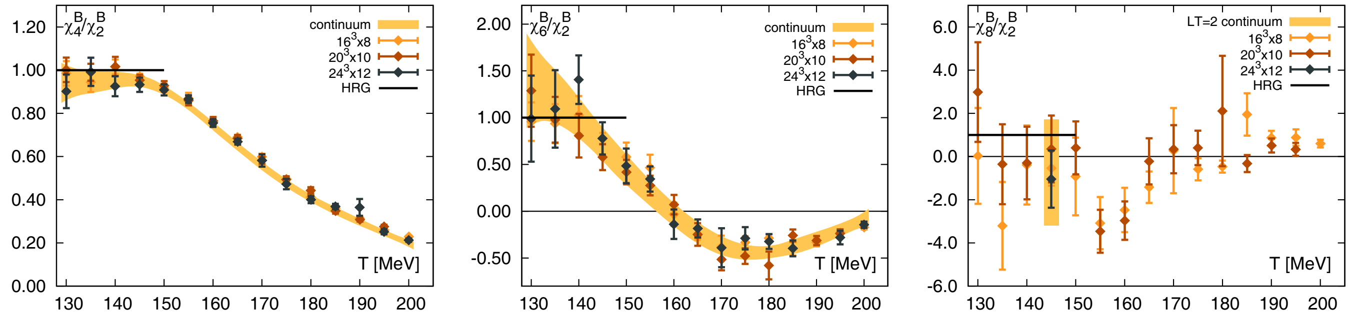

FIG. 1. Our lattice results for the ratios χ_4^B/χ_2^B (left), χ_6^B/χ_2^B (center), and χ_8^B/χ_2^B (right). For the first two, the continuum extrapolation is shown as a yellow band. HRG model predictions are shown as solid black lines in all cases.

$$p_n \equiv \left(\frac{\partial^n (p/T^4)}{\partial(\mu_B/T)^n}\right)_{n_S=0}. \tag{2}$$

Our results for the Taylor coefficient ratios p_4/p_2, p_6/p_2 and p_8/p_2 we show together with the HRG predictions in Fig. 2. We observe mild cutoff effects.

Comparisons with the literature. Our results on the sixth- and eighth-order fluctuations being the first ever continuum extrapolated, we proceed to compare them to previous results from the literature, with an aspect ratio $LT = 4$. In the top panel of Fig. 3, we show the continuum χ_6^B (yellow band) alongside previous results by the Wuppertal-Budapest Collaboration obtained with the imaginary chemical potential method using 12 time slices of 4stout improved staggered fermions [45] (black points) and results by the HotQCD Collaboration obtained with the direct method and eight time slices of HISQ fermions [6] (green band). The latter are not direct data but rather come from a spline interpolation of the direct data. The comparison is fair, since we also use a spline interpolation on our data, to allow for systematic error estimation on the continuum limit. The role of the spline interpolation in thermodynamics studies is to (i) reduce the random noise on the direct data, by utilizing continuity in T, and (ii) allow one to take temperature derivatives, which are needed for the calculation of certain thermodynamic quantities, such as the speed of sound. The HotQCD Collaboration has also used the splined version of their results on high-order fluctuations in determining phenomenological quantities (see, e.g., Ref. [6]). Looking at the three results in comparison, a very simple interpretation emerges. First, at temperatures below 145 MeV, our results at $N_\tau = 12$ agree with our new continuum-extrapolated results, even though the volume is different in the two simulations. On the other hand, the $N_\tau = 8$ HotQCD result does not agree with our old $N_\tau = 12$ results, even though the physical volumes are the same. Unless there is an accidental cancellation between cutoff, volume and methodical effects this means that, at low temperatures, finite volume effects are small in comparison to the present statistical errors. It appears that the HISQ $N_\tau = 8$ lattices are too coarse for phenomenological applications. The $N_\tau = 8$ results show very significant deviations from the hadron resonance gas. For example, it is noteworthy that the sign of $d\chi_6^B/dT$ is opposite to the HRG model prediction at all these low temperatures. Such deviations turned out to be cutoff effects, since the continuum-extrapolated results show good quantitative agreement with the HRG. Finally, note that while we have presented a comparison of splined results, a comparison of the direct data points—without interpolation—would lead to the same conclusion: The $N_\tau = 8$ HISQ results systematically appear roughly 1σ below our continuum-extrapolated results. Since the temperatures are statistically independent, having many points 1σ away in the same direction has a negligible probability to arise due to statistical fluctuations.

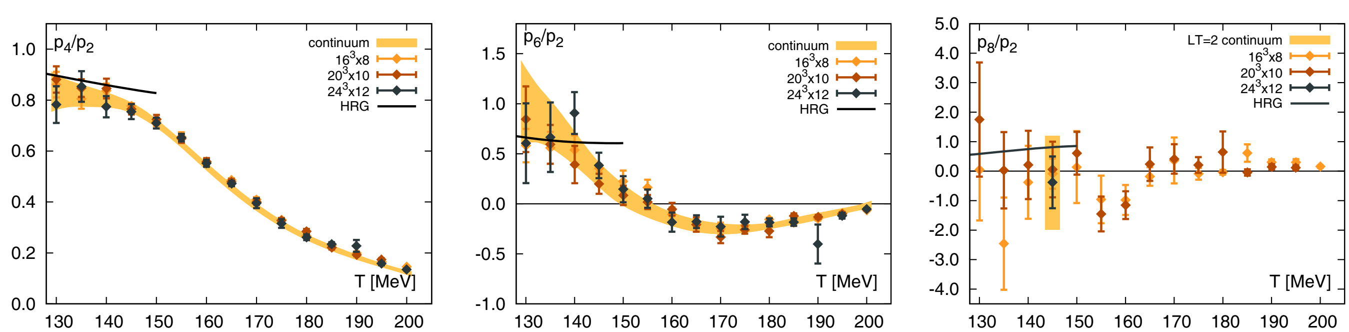

FIG. 2. Our lattice results for the rations of the strangeness neutral ratios expansion coefficients p_4/p_2 (left), p_6/p_2 (center), and p_8/p_2 (right). The continuum extrapolation is shown as a yellow band. HRG model predictions are shown as solid black lines.

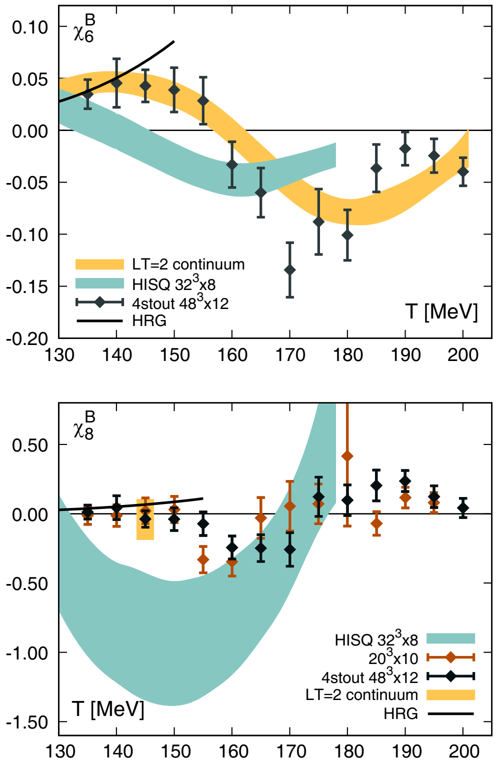

FIG. 3. Our results for sixth- (top) and eighth-order (bottom) baryon number susceptibilities. The HISQ (splined) results are shown as light blue bands, and the 4stout results are shown are black points. Our new results are shown as a yellow band for the continuum extrapolation of χ_6^B and the continuum extrapolation of χ_8^B (at $T = 145$ MeV) and as brown points for χ_8^B on the $20^3 \times 10$ lattice. HRG model predictions are shown as solid black lines.

Actually, one way to present the global significance of this point-by-point disagreement is to look at the spline interpolations presented here.

A similar scenario appears in the bottom panel of Fig. 3, where we compare our new results on $20^3 \times 10$ lattices with results from the same $LT = 4$ simulations—Wuppertal-Budapest N_τ=12 [45] (black points) and HotQCD N_τ=8 [6] (green band)—as shown in the case of χ_6^B. We also include our new continuum extrapolation at $T = 145$ MeV. Besides the markedly smaller errors, our results are in good agreement with each other, showing small volume dependence especially at lower temperature. Moreover, quantitative agreement with HRG model predictions is evident up to $T = 145$ MeV. Our continuum result at $T = 145$ MeV confirms these findings. As in the previous case, it appears that cutoff effects for $T \leq 145$ MeV are too large to allow for a safe use of results on coarse lattices for phenomenological applications. Finally, we note that for $T > 145$ MeV, our old $N_\tau = 12$ large volume and new $N_\tau = 10$ small volume results do not agree. In particular, the local minimum of χ_8^B is shifted to lower temperatures. This is likely a finite volume effect, due to the crossover transition moving to slightly lower T in a smaller volume.

Discussion. In this paper, we have reported the first continuum-extrapolated results for high-order baryon number fluctuations available in the literature. By means of a novel discretization of the QCD action, we were able to carry out a continuum extrapolation using lattices with 8, 10 and 12 time slices. We used an aspect ratio of $LT = 2$. We calculated sixth-order fluctuations in the continuum in a temperature range between $T = 130$ and 200 MeV. We also calculated the eighth-order fluctuations in the continuum at a single temperature $T = 145$ MeV. A comparison of our results with existing results at finite lattice spacing and larger physical volumes showed that, in the temperature regime relevant for the critical point search, volume effects are well under control already for the smaller volume used in our study. In contrast, cutoff effects in previous results in the literature were not always under control, especially at the lower temperatures relevant for constraining the position of the critical end point. Thus, phenomenological conclusions based on erroneous coefficients ought to be reexamined in the near future. These include estimates of the radius of convergence and poles of Padé approximants, used to constrain the location of the critical end point and the convergence of the Taylor expansion for the equation of state, used as input for hydrodynamic simulations as well as estimates of fluctuation observables at $\mu_B > 0$ used to study chemical freeze-out. We plan to revisit all of these points quantitatively in future publications. However, based on the better agreement with the HRG (which can be used as a noncritical baseline for the CEP search) we anticipate that estimates or constraints on the critical end point location should fall to lower temperatures and higher chemical potentials, compared to previous estimates based on the $N_\tau = 8$ HISQ data.

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