Taylor expansions and Padé approximants for cumulants of conserved charge fluctuations at non-vanishing chemical potentials

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Using high statistics datasets generated in (2+1)-flavor QCD calculations at finite temperature we present results for low order cumulants of net baryon-number fluctuations at non-zero values of the baryon chemical potential. We calculate Taylor expansions for the pressure (zeroth order cumulant), net baryon-number density (first order cumulant) and the variance of the distribution on net-baryon number fluctuations (second order cumulant). We obtain series expansions from an eighth order expansion of the pressure and compare these to diagonal Padé approximants. This allows us to estimate the range of values for the baryon chemical potential in which these expansions are reliable. We find $\mu_B/T \leq 2.5$, 2.0 and 1.5 for the zeroth, first and second order cumulants, respectively. We furthermore, construct estimators for the radius of convergence of the Taylor series of the pressure. In the vicinity of the pseudo-critical temperature, $T_{pc} \approx 156.5$ MeV, we find $\mu_B/T \gtrsim 2.9$ at vanishing strangeness chemical potential and somewhat larger values for strangeness neutral matter. These estimates are temperature dependent and range from $\mu_B/T \gtrsim 2.2$ at $T = 135$ MeV to $\mu_B/T \gtrsim 3.2$ at $T = 165$ MeV. The estimated radius of convergences is the same for any higher order cumulant.

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I. INTRODUCTION

While we gained a lot of information on the thermodynamics of strong interaction matter through numerical calculations in the framework of lattice regularized Quantum Chromodynamics (QCD) at finite temperature, the extension to non-vanishing values of conserved charge densities, i.e. net baryon-number ($B$), electric charge ($Q$) and strangeness ($S$), is difficult due to the lack of appropriate numerical techniques. The currently most actively pursued approaches to QCD at non-zero temperature and non-zero conserved charge densities are based on the application of Taylor series expansions in terms of conserved charge chemical potentials, $\vec{\mu} = (\mu_B, \mu_Q, \mu_S)$ [1, 2], or direct simulations at non-zero imaginary chemical potentials [3, 4] (for recent reviews see e.g. [5–7]).

While the former approach has to deal with the range of validity of series expansions arising from a finite radius of convergence of such expansions and truncation errors arising from the limited knowledge on the number of expansion parameters [8], the latter requires analytic continuation to physical, real values of the chemical potential and thus is limited by the ansatz used for analytic continuation of thermodynamic observables [9, 10], which in practice also is limited by the statistical accuracy with which parameters of such an analytic continuation can be constrained.

Recently much effort has been put into a better understanding of the analytic structure of the QCD partition function as function of complex valued chemical potentials. This is important for our ability to generate suitable ansätze for the analytic continuation of calculations performed with imaginary values of the chemical potentials as well as for choosing appropriate resummation schemes that allow to extend results obtained in Taylor series beyond the radius of convergence of such expansions. Poles of the logarithm of the QCD partition function in the complex chemical potential plane might be of simple thermal origin, arising e.g. from the analytic structure of Fermi or Bose distribution functions [11], or stem from universal critical behavior, known as Lee-Yang and Lee-Yang edge singularities [12–15]. Studies of Lee-Yang zeros/singularities have a long history in QCD, recent studies include e.g., [16–18]. The scaling of the Lee-Yang edge singularities and its influence on the QCD phase transition was considered only recently [14, 19–22].

We will focus here on the analysis of the Taylor series expansion of the partition function of (2+1)-flavor QCD and discuss the resummation of such series using Padé approximants. The range of validity of Taylor expansions using cumulants calculated at physical values of the quark masses is limited by singularities of the logarithm of the QCD partition function, i.e. the pressure, that occur for complex valued $\vec{\mu}$. These singularities may either occur for real values of $\vec{\mu}$ or in the complex plane, e.g. where $\text{Im}(\mu_B) \neq 0$. Only poles on the real $\vec{\mu}$-axis correspond to phase transitions in QCD. As recent studies of (2+1)-flavor QCD with lighter than physical quark masses have shown that the chiral phase transition temperature is at $T_c = 132^{+3}_{-6}$ MeV [23] and as this is expected to set an upper bound on the location of a possible critical point at non-zero values of the baryon chemical potential [24], we expect to find only complex poles for the analytically continued pressure in (2+1)-flavor QCD at temperatures above $T \simeq 135$ MeV. Such singularities
will limit the radius of convergence for the Taylor series, which has been estimated ever since the first applications of the Taylor expansion approach in lattice QCD calculations [1, 2, 17].

The singularities in QCD partition functions in the complex $\mu_B$-plane also have impact on the range of applicability of series expansions performed at real values of the chemical potentials. Limitations for the determination of the searched for critical point in QCD, arising from a finite radius of convergence of Taylor expansions, can however be circumvented by using appropriate resummation schemes for the Taylor series [11, 18, 25–29]. Using Padé approximants is one way to gain information on the analytic structure of the QCD partition function. They allow to explore e.g. the pressure of QCD beyond the limit set by a finite radius of convergence of Taylor series [8, 21, 22, 26, 30].

Results for Taylor expansion coefficients, i.e. the cumulants $\chi^{BQS}_{ijk}$, in (2+1)-flavor QCD up to 8th order, i.e. for all $0 < (i + j + k) \leq 8$, get improved steadily by the HotQCD Collaboration [31–33] in calculations with the Highly Improved Staggered Quark (HISQ) action [34]. These expansion coefficients have been used for a determination of the line of pseudo-critical temperatures $T_{pc}(\mu_B)$ [31] and in an analysis of high order cumulants at non-vanishing values of the chemical potentials [32]. The datasets used in these calculations have been extended by adding calculations at a lower temperature, $T \simeq 125$ MeV, for lattices with temporal extent $N_T = 8$, and more statistics has been added on lattices with temporal extent $N_T = 12$ and 16. Based on these updated datasets we presented in Ref. [33] an analysis of first and second order cumulants at vanishing values of the chemical potentials. Using in addition the results for higher order cumulants we present here an analysis of the low order cumulants of conserved charge fluctuations, derived from Taylor expansions for strangeness neutral, isospin symmetric systems and (C) some details on poles of the diagonal $[4,4]$ Padé for the pressure in (2+1)-flavor QCD.

II. TAYLOR EXPANSIONS OF LOW ORDER CUMULANTS AND THE EQUATION OF STATE

A. Computational set-up for Taylor expansion in (2+1)-flavor QCD

The framework for our calculations with the HISQ [34] discretization scheme for (2+1)-flavor QCD with a physical strange quark mass and two degenerate, physical light quark masses is well established and has been used by us in several studies of higher order cumulants of conserved charge fluctuations and correlations. The specific set-up used in our current study has been described in [32]. The framework for Taylor series expansions for strangeness neutral systems with fixed ratio of net electric charge to net baryon-number has been given up to 6th order in Ref. [35]. It has been extended in Ref. [32] by providing the necessary expansion coefficients for calculations involving up to 8th order cumulants. In that publication the 8th order expansion coefficient of the pressure in strangeness neutral systems was not included. In this work, we present an explicit expression for it in Appendix A.

B. Taylor expansion coefficients up to and including $O(\mu_B^n)$

We consider thermodynamic quantities, in particular low order cumulants of conserved charge fluctuations, derived from Taylor expansions for the pressure of (2+1)-flavor QCD,

$$\frac{P}{T^4} = \frac{1}{VT^3} \ln Z(T, V, \vec{\mu}) = \sum_{i,j,k=0}^{\infty} \frac{\chi_{ijk}^{BQS}}{i!j!k!} \hat{\mu}_B^{i} \hat{\mu}_Q^{j} \hat{\mu}_S^{k} ,$$

(1)
with $\hat{\mu}_X \equiv \mu_X / T$ and arbitrary natural numbers $i, j, k$.

The expansion coefficients, $\chi_{ijk}^{BQS}$, are derivatives of $P / T^4$ with respect to the associated chemical potentials, $\hat{\mu} = (\mu_B, \mu_Q, \mu_S)$, evaluated at $\hat{\mu} = 0$,

$$\chi_{ijk}^{BQS} = \frac{1}{VT^3} \left. \frac{\partial \ln Z(T, V, \hat{\mu})}{\partial \hat{\mu}_B \partial \hat{\mu}_Q \partial \hat{\mu}_S} \right|_{\hat{\mu}=0} , \quad i + j + k \text{ even} . \quad (2)$$

Aside from the Taylor expansion of the pressure we will focus here on the analysis of Taylor series for the ratio that enforce strangeness neutrality ($\chi^{B}_{S}$) and isospin symmetric medium, which is realized for $\mu_Q = 0$, $\mu_S = 0$.

$$\frac{\chi^{B}_{S}}{\chi^{B}_{Q}}$$

Explicit expression for $\chi^{B}_{S}$ are given in Appendix A of [32] for $k \leq 7$. For $k = 8$ we give the expansion coefficient $\chi^{B}_{S}$ here in Appendix A. We also note that in the case $\mu_B = \mu_S = 0$ as well as in the isospin symmetric case, $r = 1/2$, the expansion coefficients for the pressure and number density series are closely related,

$$N^{B}_{2k-1}(T) = 2kP_{2k}(T) . \quad (11)$$

For convenience we use here $\chi^{B}_{S}$ rather than $\chi^{B}_{n}$ as this emphasizes the close relation of the constraint expansion coefficients to the standard cumulants of net baryon-number fluctuations $\chi_{n}^{B}$ which equal $\chi^{B}_{n}$ in the case $\mu_B = \mu_S = 0$. Explicit expression for $\chi^{B}_{n}$ are given in Appendix A of [32] for $k \leq 7$. For $k = 8$ we give the expansion coefficient $\chi^{B}_{S}$ here in Appendix A. We also note that in the case $\mu_B = \mu_S = 0$ as well as in the isospin symmetric case, $r = 1/2$, the expansion coefficients for the pressure and number density series are closely related,

$$N^{B}_{2k-1}(T) = 2kP_{2k}(T) . \quad (11)$$

In fact, in the case $\mu_B = \mu_S = 0$ the expansion coefficients of all higher order cumulants are simply related to those of the pressure series, $\chi^{B}_{n}(k) = \frac{(k + n)!}{k!} \chi^{B}_{0}(k+n)$. The expansion coefficients shown in Fig. 1 thus are sufficient to construct the expansions for $P / T^4$ ($n = 0$), $n_B / T^3$ ($n = 1$) and $\chi^{B}_{2}$ ($n = 2$). In the strangeness neutral case, $\mu_B = 0$, $\mu_S = 0$, the above relation only holds for $n = 1$. We thus still need to give results for the expansion coefficients of $\chi^{B}_{2}$ with $k = 2, 4, 6$. We show these expansion coefficients in Appendix B. As expected, the qualitative features of the temperature dependence of $\chi^{B}_{2}$ in the $n_S = 0$ and $\mu_S = 0$ cases are similar, i.e. they behave like $\chi^{B}_{2}$.

In Fig. 1 we show results for $\chi^{B}_{2}$ for the two different cases considered throughout this paper, i.e. we work in the isospin symmetric case, corresponding to $\mu_Q = 0$, and consider for the strangeness sector (i) the case $\mu_S = 0$ (left) and (ii) the strangeness neutral case $n_S = 0$ (right), respectively. Continuum extrapolated result for the leading order expansion coefficient of the pressure series, $\chi^{B}_{0}$, are shown in the two panels on the top of Fig. 1. They are based on datasets generated on lattices with temporal extent $N_t = 6, 8, 12$ and 16. Results for the case $\mu_Q = \mu_S = 0$ at $T > 135$ MeV have been shown already in Ref. [33] we added here our results at $T = 125$ MeV obtained on lattices with temporal extent $N_t = 8$, which have not been used in the continuum extrapolations. The insets given in these figures for $\chi^{B}_{2}$ (left) as well as $\chi^{B}_{2}$ (right) show comparisons with the same cumulants calculated in a hadron resonance gas (HRG) model describing the thermodynamics of non-interacting, point-like hadrons\footnote{Throughout this work we use a model based on non-interacting, point-like hadrons listed in the QMHRG2020 list [33] as HRG model reference system. Such models have been improved by incorporating interactions as described by the S-matrix [36] or more phenomenological through the use of finite volume for baryons [37].}. This calculation uses the hadron spectrum compiled in the QMHRG2020 list [33].

For the $O(\hat{\mu}_B^2)$ expansion coefficients we show in Fig. 1 continuum extrapolations based on $N_t = 6, 8$ and 12

$$N^{B}_{2k-1}(T) = 2kP_{2k}(T) . \quad (11)$$

$$\chi^{B}_{n}(k) = \frac{(k + n)!}{k!} \chi^{B}_{0}(k+n) . \quad (11)$$
datasets. For the higher order expansion coefficients we only use results from our high statistics calculations on lattices with temporal extent $N_T = 8$, where more than 1.5 million gauge field configurations$^2$ have been generated at each temperature value. Results for larger $N_T$ are consistent with these results but have significantly larger statistical errors. However, as can be seen from the lower order expansion coefficients, cut-off effects are generally small for expansion coefficients at non-zero values of $\mu_B$. The interpolating curves for the $O(\mu_B^6)$ and

$^2$ These datasets have been generated using a Rational Hybrid Monte Carlo Algorithm (RHMC) [38, 39]. They contain gauge field configurations that have been stored after 10 subsequent RHMC time units. The actual code package used for our calculations is described in [40].
\[ \mathcal{O}(\mu_B^8) \] expansion coefficients shown in Fig. 1 are cubic spline interpolations.

C. Cumulants and the EoS at non-zero \( \mu_B \)

From the temperature dependence of the \( \mathcal{O}(\mu_B^2) \) expansion coefficient of the pressure shown in Fig. 1 it is apparent that deviations from the thermodynamics of a non-interacting HRG reach about 20\% at the pseudocritical temperature of (2+1)-flavor QCD, \( T_{pc}(0) = 156.5(1.5) \text{ MeV} \) [31] and rapidly become larger at higher temperatures. Below \( T_{pc} \) the leading order expansion coefficient agrees quite well with HRG model calculations [33]. As can be seen also in Fig. 1, already the \( \mathcal{O}(\mu_B^4) \) Taylor coefficient deviates from HRG model results more strongly than the \( \mathcal{O}(\mu_B^2) \) expansion coefficient. For all temperatures in the range 135 MeV \( \leq T \leq 165 \text{ MeV} \) the sixth and eighth order expansion coefficients are negative, in contrast to the non-interacting HRG expansion coefficients, which are all positive. Even at low temperatures we thus expect to find that deviations from HRG model calculations increase with increasing values of the baryon chemical potential.

Compared to our earlier analysis of the QCD equation of state, presented in [35], the new results for the expansion coefficients shown in Fig. 1 are based on 10 times higher statistics for \( N_e = 8 \) and 12 and include also data on lattices with temporal extent \( N_r = 16 \). This allows to determine also the contribution from 8th order expansion coefficients to Taylor series of various thermodynamic observables. The highly improved statistics results in a huge improvement of the current calculation over that published previously [35]. We update in Fig. 2 our results for the pressure and the net baryon-number density calculated in sixth and fifth order of the Taylor expansion, respectively. Results are shown as function of temperature for the case \( \mu_Q = \mu_S = 0 \) using the continuum extrapolated data for \( \chi_B^2 \) and \( \chi_S^2 \), as well as the spline interpolated data for \( \chi_Q^2 \), obtained on lattices with temporal extent \( N_r = 8 \). Obviously, the “wiggly” structure seen in the old calculations for \( \mathcal{O}(\mu_B^6) \) expansions at \( \mu_B = 2.5 \) [35] is smoothed out in our new high statistics analysis and the \( \mathcal{O}(\mu_B^6) \) results agree well with \( \mathcal{O}(\mu_B^2) \) expansions in the entire temperature range.

On the basis of a sixth order Taylor expansion we thus have no indications for a radius of convergence being
smaller than $\hat{\mu}_B = 2.5$ nor do we have indications for a poor convergence of the Taylor expansions of $P/T^4$ and $n_B/T^3$, respectively. This will change when discussing the eighth order contribution to the Taylor series. We stress, however, already here that we need to distinguish between the radius of convergence of the Taylor series, which is the same for all observables determined as derivatives of $P/T^4$ with respect to $\mu_B$, and the rate of convergence of expansions for theses observables to their asymptotic values, which will be slower with increasing order of the derivatives.

Taking also into account the contribution from eighth order Taylor expansion coefficients of the pressure we show in Fig. 3 results for the $\hat{\mu}_B$-dependence of the pressure, net baryon-number density and the second order cumulant of net baryon-number fluctuations. Shown are results obtained by using different orders of the Taylor expansion at a fixed value of the temperature in the vicinity of $T_m$, i.e. $T = 155$ MeV, for the case $\mu_Q = \mu_S = 0$. As can be seen deviations from QMHRG2020 increase with increasing $\hat{\mu}_B$ and these deviations are larger for higher order cumulants. It also is apparent from this figure, that the rate of convergence of the expansions for higher order cumulants slows down. Being limited to a certain order in the expansion thus allows to give reliable results for higher order cumulants only in a smaller $\hat{\mu}_B$ range, although the expansions for all cumulants have the same radius of convergence. We will give a more quantitative discussion of the $\hat{\mu}_B$-range, in which the current Taylor expansions for different cumulants are expected to give reliable results, in Section IV.

In Fig 4 we show the $\hat{\mu}_B$-dependent contribution to the pressure as function of temperature for some values of $\hat{\mu}_s$, i.e. for $\hat{\mu}_B = 1.0, 1.5, 2.0$ and $2.5$, and for the net baryon-number density for $\hat{\mu}_B = 1.0, 1.5, 2.0$. In all cases we show results obtained in different orders of the Taylor series expansion. For these values of the baryon chemical potential the $O(\hat{\mu}_B^3)$ Taylor series for the pressure agrees well with the lower order results. For $n_B/T^3$ we do not show results from an $O(\hat{\mu}_B^3)$ at $\hat{\mu}_B = 2.5$ as it is apparent from Fig. 3 that higher order expansion coefficients will be needed to obtain reliable results for the pressure at that large value of $\hat{\mu}_B$.

In the entire temperature range analyzed by us the Taylor series for pressure converges well for $0 \leq \hat{\mu}_B \leq 2.5$. For the number density this can be stated at present only for the range $0 \leq \hat{\mu}_B \leq 2.0$. Although that may turn out to be somewhat larger once the statistical accuracy in calculations of eighth order expansion coefficients is increased. Nonetheless, based on the analysis of 8th order Taylor expansions of the pressure we have no hint for a radius of convergence smaller than $\hat{\mu}_B \sim 2.5$ that would limit the applicability of Taylor expansions at temperatures $T \gtrsim 125$ MeV.

III. RADIUS OF CONVERGENCE AND PADÉ APPROXIMATIONS

In general the radius of convergence of the Taylor series for a function

$$f(x) = \sum_{n=0}^{\infty} c_n x^n$$

(12)

given by the location of a singularity of $f$ in the complex $x$-plane that is closest to the origin. Of course, rigorous statements on the radius of convergence of a Taylor series can only be made by analyzing the asymptotic behavior of the expansion coefficients in the limit $n \to \infty$. Having at hand only a few expansion coefficients of the Taylor series for the pressure in QCD we naturally can only obtain estimators for the radius of convergence and extract some information on the analytic structure of thermodynamic functions in the plane of complex chemical potentials.

We are dealing with Taylor series in terms of $\hat{\mu}_B$ for which only every second expansion coefficient is non-zero, e.g. the pressure series which has non-vanishing expansion coefficients $\tilde{\chi}_0^{B,0}$ only for even $n$. The simplest estimator, $r_{c,n}$, for the radius of convergence, $r_c = \lim_{n \to \infty} r_{c,n}$, is obtained from subsequent, non-vanishing expansion coefficients. We define $r_{c,n} = n_{\mu_B = 12\hat{\mu}_B}$, with

$$A_n = \frac{c_n}{c_{n+2}} , \ n \text{ even}.$$  
(13)

Another frequently used estimator, with improved convergence properties, has been introduced by Mercer and Roberts [41], $r_{c,n}^{MR} = |A_n^{MR}|^{1/4}$, with

$$A_n^{MR} = \frac{c_{n+2} c_{n-2} - c_n^2}{c_{n+4} c_{n-2} - c_{n+2}^2} , \ n \text{ even}.$$  
(14)

The estimators based on the ratios $A_n$ and $A_n^{MR}$ are related to poles of $[n,2]$ and $[n,4]$ Padé approximants for the series expansion of $f(x)$. We thus will consider the structure of such Padé approximants in the following.

When constructing Padé approximants for the pressure series of $(2+1)$-flavor QCD we take advantage of the fact that the two leading expansion coefficients of the pressure, $P_{2k} = \tilde{\chi}_0^{B,2k}/(2k)!$, $k = 1, 2$, are strictly positive. We thus rescale the pressure by a factor $P_4/P_2^2$ and redefine the expansion parameter as

$$\bar{x} = \sqrt{\frac{P_4}{P_2^2}} \hat{\mu}_B \equiv \sqrt{\frac{\tilde{\chi}_0^{B,4}}{12\tilde{\chi}_0^{B,2}}} \hat{\mu}_B.$$  
(15)

This allows us to re-write the expansion of the pressure in terms of expansion coefficients

$$c_{2k,2} = \frac{P_{2k}}{P_2} \left(\frac{P_2}{P_4}\right)^{k-1} ,$$  
(16)
which gives $c_{2,2} = c_{4,2} = 1$. Therefore, for $\mu_Q = \mu_S = 0$ as well as for the strangeness neutral case, the analytic structure of the QCD pressure, that one can deduce from an eighth order Taylor series in QCD, entirely depends on two expansion parameters, 

$$
c_{6,2} = \frac{P_0 P_2}{P_4^2} = \frac{2}{5} \frac{\chi_6 \chi_2^B}{(\chi_4^B)^2},
$$

$$
c_{8,2} = \frac{P_8 P_2}{P_4^3} = \frac{3}{35} \frac{\chi_8 (\chi_2^B)^2}{(\chi_4^B)^3}.
$$

With this we obtain

$$
\frac{(\Delta P(T, \mu_B)/T^4) P_4}{P_2^2} = \sum_{k=1}^{\infty} c_{2k,2} \bar{x}^{2k},
$$

with $\Delta P(T, \mu_B) = P(T, \mu_B) - P(T, 0)$.

The two diagonal Padé approximants, that can be constructed from our eighth order series for the pressure are given by,

$$
P[2, 2] = \frac{\bar{x}^2}{1 - \bar{x}^2},
$$

$$
P[4, 4] = \frac{(1 - c_{6,2}) \bar{x}^2 + (1 - 2c_{6,2} + c_{8,2}) \bar{x}^4}{(1 - c_{6,2}) + (c_{8,2} - c_{6,2}) \bar{x}^2 + (c_{8,2} - c_{6,2}) \bar{x}^4}.
$$

The [2,2] Padé has a pole on the real axis for $\bar{x}^2 = 1$, i.e. for $\mu_B, c \equiv \tau_{c,2} = \sqrt{12 \chi_2^B / \chi_4^B}$ which is the standard ratio estimator for the radius of convergence. The [4,4] Padé has four poles which come in two pairs, corresponding to zeroes of the polynomial in the denominator of Eq. 21 which is quadratic in $z \equiv \bar{x}^2$. The two zeroes in $z$ are given by

$$
z_{\pm} = \frac{c_{8,2} - c_{6,2} \pm \sqrt{(c_{8,2} - c_{4,2})(c_{8,2} - c_{8,2})}}{2(c_{8,2} - c_{6,2})},
$$

with

$$
c_{8,2}^\pm = -2 + 3c_{6,2} \pm 2(1 - c_{6,2})^{3/2}.
$$

It is easy to see that the argument of the square root appearing in Eq. 22 is positive for $c_{6,2} > 1$. Complex zeroes with Re($\mu_B$) $\neq 0$ thus exist only for

(i) $c_{6,2} < 1$ and $c_{8,2} < c_{8,2} < c_{8,2}^+$.

(ii) $c_{6,2} < 0$ and $c_{8,2}^+ < c_{6,2} < c_{6,2}^2$.

Outside this region the zeroes $z_{\pm}$ are real and thus correspond to pairs of real poles in terms of $\mu_B$ if $z_{\pm} > 0$ and purely imaginary poles if $z_{\pm} < 0$. In fact, as we show in Appendix C, there is a small region in parameter space $(c_{6,2}, c_{8,2})$, close to $c_{8,2}^+$, in which $z_{+} < 0$ and $z_{-} < 0$,
In order to get further information on the poles of the [4,4] Padé approximant for the pressure and, in particular, deduce conditions for the occurrence of real poles we show in Fig. 5 results for $c_{8,2}$ versus $c_{6,2}$ obtained in the temperature range $125 \text{ MeV} < T < 175 \text{ MeV}$ from the spline interpolated $N_r = 8$ expansion coefficients $\hat{x}_0^{B,2}$, $\hat{x}_0^{B,8}$, and the continuum extrapolations for $\chi_0^{B,2}$, $\chi_0^{B,4}$ shown in Fig. 1. Also shown in this figure are the boundaries for the triangular shaped region, bounded by $c_{8,2}$ and $c_{8,2}^-$, inside which only complex poles exist for the [4,4] Padé of the eighth order Taylor series of the pressure. We show results for the case $\mu_Q = \mu_S = 0$ (left) and $\mu_Q = 0$, $\mu_S = 0$ (right), respectively.

As can be seen in Fig. 5, despite the currently large errors on the location of the poles, it is well established that the poles occur in the complex $\mu_B$-plane for all temperatures $135 \text{ MeV} < T < 165 \text{ MeV}$. Within our current statistical errors we cannot rule out that pairs of real and/or purely imaginary poles will occur at temperatures below $T = 135 \text{ MeV}$ as well as for temperatures above $T = 165 \text{ MeV}$. In fact, this is expected to be the case at low enough temperatures, where one can see in Fig. 1 that $\chi_0^{B,6}$ and $\chi_0^{B,8}$ become positive at $T \approx 125 \text{ MeV}$, and also at high temperature where Fig. 1 shows that $\chi_0^{B,6} < 0$ while $\chi_0^{B,8} > 0$ at $T \approx 175 \text{ MeV}$.

At low temperatures the complex valued poles leave the area bounded by $c_{8,2}^+$ in a region of parameter space where $c_{6,2} > 0$ or correspondingly $\chi_0^{B,6} > 0$. As discussed and also indicated in the figure shown in Appendix C for $c_{6,2} > 0$ there is a small region in parameter space above the boundary defined by $c_{8,2}^+$ where all poles are strictly real, before entering the region where a pair of real and imaginary poles exists. One can check that for all $0 < c_{6,2} < 1$ the real pole actually is closer to the origin as long as $c_{6,2}^2 < c_{8,2} < c_{6,2}$. Our results on the temperature dependence of $c_{6,2}^2$ and $c_{8,2}^2$ thus suggest that with decreasing temperature a pair of complex poles moves towards the real axis and gives rise to two real poles. With decreasing temperature one of these real poles moves towards infinity and comes back as an imaginary pole with large magnitude.

In the region where the conditions given in Eq. 24 hold one has four zeroes in terms of $\tilde{x}$ corresponding to the positive and negative roots of $z^{\pm}$. They yield four poles of the [4,4] Padé in the complex $\mu_B$-plane with non-vanishing imaginary part of $\tilde{\mu}_B$. We represent these poles in polar coordinates,

$$
\tilde{\mu}_{B,e}^\pm = \pm r_{c,4} e^{\pm i \theta_{c,4}} .
$$

For temperatures $135 \text{ MeV} < T < 165 \text{ MeV}$ the zeroes $z^{\pm}$ are complex conjugate to each other. In the $\tilde{x}$-plane the absolute value of the distance of the poles from the origin is then given by,

$$
|z^{+} z^{-}|^{1/4} = \left| \frac{1 - c_{6,2}}{c_{6,2}^2 - c_{8,2}} \right|^{1/4} ,
$$

which is the Mercer-Roberts estimator, introduced in Eq. 14, for a series in the rescaled expansion parameter $\tilde{x}$. We note that this relation between the Mercer-Roberts estimator and the magnitude of $|z^{\pm}|$ does not hold for the case of purely real or purely imaginary poles of the [4,4] Padé (see discussion in Appendix C). In these cases the distances to the origin $|z^{+}|$ and $|z^{-}|$ differ from each other.

Using Eqs. 26 and 27 we obtain for $c_{6,2} < 1$ the location of the poles in the complex $\mu_B$-plane

$$
r_{c,4} = r_{c,2} \left| z^{+} z^{-}\right|^{1/4} = \sqrt{\frac{12 \hat{x}_0^{B,2}}{\chi_0^{B,4}} \frac{1 - c_{6,2}}{c_{6,2}^2 - c_{8,2}}}^{1/4} .
$$

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We do not show results for $T = 175 \text{ MeV}$ as errors are even larger than those shown for $T = 170 \text{ MeV}$.
...neutral, isospin symmetric media, respectively. For 135 MeV ≤ T ≤ 165 MeV we find that the poles of the [4,4] Padé appear at a distance from the origin corresponding to |μ_B|≥2.5 at T ≃ 135 MeV and rises to values larger than |μ_B|≥3 for T> T_p. This also are the best estimates for a temperature dependent bound on the radius of convergence of the Taylor series for the pressure, based on the Mercer-Roberts estimator. The information extracted from the [4,4] Padé approximants on the location of poles in the analytic function representing the pressure as function of a complex valued chemical potential μ_B thus seems to be consistent with the good convergence properties of the Taylor series itself.

FIG. 6. Location of poles nearest to the origin obtained from the [4,4] Padé approximants in the complex μ_B-plane. Only poles with Re(μ_B) > 0 are shown. Shown are results the case μ_Q = μ_S = 0 (left) and the strangeness neutral, isospin symmetric case (right).

FIG. 7. Magnitude of poles nearest to the origin obtained from the [2,2] (squares and circles) and [4,4] (bands) Padé approximants for Taylor expansions at μ_Q = μ_S = 0 and for strangeness neutral, isospin symmetric media, respectively.

\[ \Theta_{c,4} = \arccos\left( \frac{c_{6,2} - c_{8,2}}{2\sqrt{(1 - c_{6,2})(c_{6,2}^2 - c_{8,2}^2)}} \right) \]

Expressing the relation given in Eq. 28 in terms of the cumulants \( \tilde{\chi}_0^{B,n} \) entering the Taylor series for the pressure, Eq. 7, we have in the region of complex poles,

\[ r_{c,4} = \left( \frac{8}{4} \right)^{1/4} \left| \frac{30(\tilde{\chi}_0^{B,4})^2 - 12\tilde{\chi}_0^{B,6}\tilde{\chi}_0^{B,2}}{56(\tilde{\chi}_0^{B,6})^2 - 30\tilde{\chi}_0^{B,8}\tilde{\chi}_0^{B,4}} \right|^{1/4} \]
FIG. 8. Comparison of the [n,4] Padé approximants for the pressure (n = 4), the net baryon-number density (n = 3) and the second order cumulant of net baryon-number fluctuations (n = 2) with corresponding Taylor expansions. Shown are results for T = 135 MeV (left), 155 MeV (middle) and 165 MeV (right) versus µB for the case µQ = µS = 0. Also shown are derivatives of the [4,4] Padé approximants with respect to µB (green bands).

IV. COMPARISON OF PADÉ APPROXIMANTS AND TAYLOR SERIES

In Fig. 8 we compare the [n,4] Padé approximants for the pressure (n = 4), the net baryon-number density (n = 3) and the second order cumulant of net baryon-number fluctuations (n = 2) with corresponding Taylor expansions that use expansion coefficients 3k−n with k ≤ 8. We show results obtained at three temperatures in the interval in which our results clearly yield complex valued poles only, i.e., T = 135, 155, and 165 MeV, respectively. As error bands quickly become large for large µB we show errors only up to the point where relative errors are less then 15%. In this range of µB values also the Padé approximants and the straightforward Taylor expansions agree quite well.

In the entire temperature interval 135 MeV ≤ T ≤ 165 MeV the expansion coefficient 3k−n is negative for µQ = µS = 0 as well as for µQ = 0, µS = 0. It will dominate the expansion at large µB and thus forces the Taylor expansion of P/T4 to have a maximum at some value of µB max. As the net baryon-number density is the derivative of P/T3 with respect to µB it has a maximum below µB max and vanishes at µB max. Similarly, the second order cumulant reaches a maximum at an even smaller value of µB. As can be seen in Fig. 8 the [n,4] Padé approximants (blue bands), the direct µB-derivative of the [4,4] Padé (green bands) and the Taylor expansions (red bands) agree quite well up to values of the chemical potentials close to the respective value of µB max and this maximum arises at larger µB as the temperature increases. This is in accordance with the increase of the estimator μB^{N}(T) for the magnitude of the Padé poles given in Fig. 7.

Starting with a Taylor series limited to 8th order obviously the expansions possible for higher order derivatives becomes shorter. Correspondingly, the order of a [n,4] Padé used by us becomes smaller. If, however, the Padé approximant used for the original pressure series, i.e. in our case the [4,4] Padé approximant, provides a good approximation for the pressure in the complex µB-plane, taking directly subsequent derivatives with respect to µB will give good resummed approximants for e.g. the net baryon-number density and higher order cumulants. In Fig. 8 we thus also show approximations for nB/T3 and 3/2 obtained by taking the first and second derivative of the [4,4] Padé approximant of P/T4 (green bands). By construction the poles of these approximants are identical to those of the [4,4] Padé approximant of P/T4. As can
be seen these derivatives agree with the corresponding \([n,4]\) approximants up to values of \(\hat{\mu}_B\) similar to those where the latter start to differ from the corresponding Taylor series.

Although the radius of convergence for the Taylor series of all higher order cumulants is determined by that of the pressure series, the currently available \(8^{\text{th}}\) order Taylor series for the pressure clearly does provide a reliable approximation for higher order cumulants only in a smaller interval of \(\hat{\mu}_B\) values. We consider the range of \(\mu_B\) values indicated by the range of error bars given in Fig. 8 as the region where current results on the pressure, net baryon-number density and the second order cumulant of net baryon-number fluctuations are reliable. As can be seen in that figure this range of baryon chemical potentials is somewhat larger at higher temperatures than at lower temperatures.

In Fig. 9 we compare results obtained for these observables using Taylor expansions as well as Padé approximants for several values of \(\hat{\mu}_B\). We show results in the entire temperature range \(135 \text{ MeV} \leq T \leq 175 \text{ MeV}\) using values of the chemical potential up to the largest value indicated by the bands given in Fig. 8. As can be seen for the pressure we find excellent agreement up to values of the chemical potential \(\hat{\mu}_B \simeq 2.5\). The corresponding largest values of \(\hat{\mu}_B\) for \(n_B/T^3\) and \(\chi_B^2\) are \(\hat{\mu}_B = 2\) and 1.5, respectively. This choice of \(\hat{\mu}_B\) values is enforced by demanding good agreement between Taylor series results and Padé approximants at the lowest temperature. At higher temperatures Figs. 7 and Fig. 8 suggest that in the vicinity of \(T_{pc}\) the range of \(\hat{\mu}_B\) values, in which \(8^{\text{th}}\) order Taylor series can provide reliable results is larger, e.g. \(\hat{\mu}_B \lesssim 3\) for \(P/T^4\).
V. CONCLUSIONS

We have presented results for eighth order Taylor series expansions of the pressure in (2+1)-flavor QCD for isospin symmetric matter corresponding to vanishing electric charge chemical potentials. From this Taylor series we derived the first two cumulants of net baryon-number fluctuations, corresponding to the mean and variance of the net baryon-number distribution. We used Padé approximants to resum these Taylor series.

We have shown that the $[4,4]$ Padé approximant, which reproduces the eighth order Taylor series of the pressure series has only complex poles in the entire temperature interval $135 \text{ MeV} \leq T \leq 165 \text{ MeV}$, which gives further support to the observation that a possible critical point in the QCD phase diagram may only be found at temperatures below 135 MeV. From the location of the poles in the complex plane we estimate the radius of the convergence for these Taylor series expansions to be slightly temperature dependent, increasing from $\mu_{B,c} \simeq 2.2$ at $T = 135 \text{ MeV}$ to $\mu_{B,c} \simeq 3.2$ at $T = 165 \text{ MeV}$. In the vicinity of the pseudo-critical temperature, $T_{pc} \simeq 156.5 \text{ MeV}$, we find $\mu_B/T \gtrsim 2.9$ at vanishing strangeness chemical potential and somewhat larger values for strangeness neutral matter. If poles of $[n,n]$ Padé approximants continue to lie in the complex $\mu_B$-plane an efficient resummation of the Taylor series of the QCD pressure to even larger values of $\mu_B$ will be possible in this temperature range.

A comparison of Taylor series and Padé approximants for the Taylor series of the pressure and the first two cumulants of net baryon-number fluctuations allows us to estimate the range of $\mu_B$ values in which current series expansions give reliable results. For the pressure and the first two cumulants in (2+1)-flavor QCD we deduce that the current eighth order series for the pressure and its derivatives agree well with the resummed $[4,4]$ Padé approximants and its derivatives for $\mu_B \leq 2.5$ (pressure), 2.0 (net number-density) and 1.5 (second order cumulant). All data presented in the figures of this paper can be found in [42].

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Appendix A: Taylor expansion coefficients for strangeness neutral, isospin symmetric QCD matter

We give here the general form of the eighth order expansion coefficients $\chi_n^{B,k}$ for $n$th order cumulants of net baryon-number fluctuations. In the context of this work it only is needed for the pressure series ($n = 0$) in the case $\mu_Q = 0$, which corresponds to setting $q_n = 0$ in the following expression. Expansion coefficients of all other cumulants, $\chi_n^{B,k}$ that involve only cumulants $\chi_n^{B,Q}$ with $i + j + k \leq 8$ are given in Appendix A of [32].

$$\chi_{n,8}^{B,S} = 40320\chi_{n,02}^{B,Q}s_1s_7 + 40320\chi_{n,02}^{B,Q}s_3s_5 + 6720\chi_{n,04}^{B,Q}s_1s_5 + 10080\chi_{n,04}^{B,Q}s_1^2s_3 + 336\chi_{n,06}^{B,Q}s_1^3s_3$$

The remaining coefficients are given in Table A of Appendix A.
Appendix B: Taylor expansion coefficients for the \( \chi_2^B \) in the case \( \mu_Q = 0, n_s = 0 \)

In Fig. 10 we show the expansion coefficients, \( \chi_2^{B,k} \), for the Taylor series of the second order cumulant of net baryon-number fluctuations in (2+1)-flavor QCD defined in Eq. 9.

Appendix C: Location of real and imaginary poles in the parameter space \( (c_{6,2}, c_{8,2}) \)

We discuss here the occurrence of complex and real poles in the plane of the two real expansion parameters appearing in the Taylor series for the pressure, \( (c_{6,2}, c_{8,2}) \), and characterize the location of [4,4] Padé approximants constructed from the 8th order Taylor series of the pressure in (2+1)-flavor QCD.

As discussed in Section III there is a triangular shaped region in this parameter space, bounded by lines \( c_{8,2}^\pm \) given in Eq. 23, in which all four poles of the [4,4] Padé are complex with non-vanishing real and imaginary parts. Outside this region poles of the [4,4] Padé are either real or purely imaginary. For \( z^+ > 0 \) there exists a pair of real poles in terms of \( \mu_B \), for \( z^- < 0 \) one has a pair of purely imaginary poles. In the parameter space \( (c_{6,2}, c_{8,2}) \) one can have two pairs of purely imaginary poles \( (ii) \), two pairs of real poles \( (rr) \), or a pair of each of these types, \( (ir) \) or \( (ri) \). In the latter case we use the convention that the first letter corresponds to that pair of poles that is closest to the origin. The parameters \( (c_{6,2}, c_{8,2}) \) for which these different types of poles appear are shown in Fig. 11.

In the following we give some further details on the boundaries for the different regions in parameter space: We re-write Eq. 22 as

\[
z^\pm = \frac{c_{8,2} - c_{6,2}}{2(c_{8,2} - c_{6,2})^2} \pm \frac{(c_{8,2} - c_{6,2})^2 + 4(c_{8,2} - c_{6,2})(1 - c_{6,2})}{2(c_{8,2} - c_{6,2})^2}. \tag{C1}\]

The zeroes \( z^+ \) and \( z^- \) are related to each other through

\[
z^+ z^- = \frac{1 - c_{6,2}}{c_{8,2} - c_{6,2}}. \tag{C2}\]

Outside the region bounded by \( c_{8,2}^\pm \) both zeroes have the same sign, if \( z^+ z^- > 0 \), i.e. if numerator and denominator in Eq. C2 have the same sign, which is the case for

either \( c_{6,2} > 1 \) and \( c_{8,2} > c_{6,2}^2 \), \tag{C3}

or \( c_{6,2} < 1 \) and \( c_{8,2} < c_{6,2}^2 \). \tag{C4}

In the first case it is obvious that \( c_{8,2} > c_{6,2}^2 > c_{6,2} \) holds. It thus is evident from Eq. C1 that \( z^+ > 0 \) and the region defined in Eq. C3 corresponds to a region with two real poles in the complex \( \mu_B \)-plane. For all other regions with \( c_{6,2} > 1 \) a pair of real and a pair of purely imaginary poles exists. However, only for \( c_{8,2} < c_{6,2} \) it is the imaginary pair of poles that is closest to the origin.
In the second case, Eq. C4, we obtain from Eq. 23,

\[ c^2_{6,2} - c^+_{8,2} = (1 - c_{6,2}) (2 - c_{6,2} - 2\sqrt{1 - c_{6,2}}) > 0. \]  

(C5)

It thus is evident from Eq. C1 that \( z^+ < 0 \) for \( c_{6,2} < 0 \). In the range \( c^+_{8,2} < c_{8,2} < c^+_{6,2} \) one thus finds two pairs of purely imaginary poles in the complex \( \mu_B \)-plane. On the other hand, for \( 0 < c_{6,2} < 1 \) one finds in the same \( c_{8,2} \) interval that \( z^- > 0 \). In this case one thus has two pairs of real poles in the complex \( \mu_B \)-plane. Finally there is a second region for purely real poles, which is allowed by Eq. C4. This is the case of \( c_{8,2} < c^+_{6,2} \), as also in this case one finds \( z^+ > 0 \). In all other case one finds a pair of real and a pair of complex poles. These different parameter regions in the \( (c_{6,2}, c_{8,2}) \) plane are shown in Fig. 11.

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