Searching for the QCD critical point along the pseudo-critical/freeze-out line using Padé-resummed Taylor expansions of cumulants of conserved charge fluctuations

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Using high-statistics datasets generated in (2+1)-flavor QCD calculations at finite temperature we construct estimators for the radius of convergence from an eighth order series expansion of the pressure as well as the number density. We show that the estimator for pressure and number density will be identical in the asymptotic limit. In the vicinity of the pseudo-critical temperature, $T_{pc} \approx 156.5$ MeV, we find the estimator of the radius of convergence to be $\mu_B/T \gtrsim 3$ for strangeness-neutral matter. We also present results for the pole structure of the Padé approximants for the pressure at non-zero values of the baryon chemical potential and show that the pole structure of the [4,4] Padé is consistent with not having a critical point at temperatures larger than 135 MeV and a baryon chemical potential smaller than $\mu_B/T \approx 2.5$.

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1. Introduction

Taylor expansion and analytic continuation are the two most commonly used techniques to understand the properties of strongly interacting matter at non-zero values of the chemical potentials. Although both methods

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provide reliable estimates for thermodynamic observables at small chemical potentials, they suffer from systematic effects (truncation effects, limitation of analytic continuation ansatz etc.) at moderate to large chemical potentials as only few expansion coefficients are known \[1\]. Hence, recently, there is a lot of effort going on in the lattice QCD community aiming at an efficient resummation of the standard series expansions \[2, 3, 4, 5\] to get reliable estimates also at large chemical potentials. Here we will focus on the use of Padé approximations to resum the Taylor series to estimate the radius of convergence of Taylor series of pressure in (2+1)-flavor QCD at finite chemical potentials. A comparison of Taylor expansions and Padé resummation has been presented recently by the HotQCD collaboration in \[6\].

One of the central goals in QCD at large chemical potential is to find evidence for the existence of the so-called critical end point (CEP) in the QCD phase diagram. Phase transitions (critical points) are related to the singularities of the free energy on the real chemical potential axis, which one could estimate by analyzing the behavior of the expansion coefficients of Taylor series or by determining the poles of Padé approximants for thermodynamic observables obtained as derivatives of the partition function with respect to \(T\) or the chemical potentials \[7\]. In the following we will elaborate on these ideas in the context of QCD at finite temperature and densities. Being forced to work with a finite number of Taylor coefficients Padé approximants are good choice as one can easily distinguish real and complex poles. Lattice QCD calculations at smaller-than-physical quark masses, combined with our model-based understanding of the QCD phase diagram, suggest that this critical point, if it exists, needs to be searched for at temperatures below/around the QCD chiral critical temperature(\(\sim 135\) MeV) \[8, 9, 10\]. Thus we extend our calculations down to temperatures of 125 MeV and use the high statistics results for conserved charge cumulants up to 8th order, obtained by the HotQCD collaboration, to resum the Taylor expansions of the logarithm of the QCD partition function.

In the following sections, we will show that the poles one obtains from the diagonal \([4,4]\) Padé-approximants for 8th order Taylor series of pressure in terms of baryonic chemical potential are complex at least for \(T\geq140\) MeV, i.e. the singularity closest to the origin, which will control the radius of convergence of Taylor series, is in the complex plane. Of course, one has to confirm in the future, that this will be the case also for higher order diagonal Padé-approximants. This is consistent with the fact that the CEP does not exist for \(T\geq140\) MeV.
2. Taylor expansion and Padé approximants of isospin symmetric matter in (2+1)-flavor QCD

The Taylor expansions for the pressure of (2 + 1)-flavor QCD is given by,

\[
P(T^4) = \frac{1}{VT^3} \ln Z(T, V, \bar{\mu}) = \sum_{i,j,k=0}^{\infty} \chi_{ijk}^{BQS} \frac{\partial}{\partial \mu_i^B} \frac{\partial}{\partial \mu_j^Q} \frac{\partial}{\partial \mu_k^S},
\]

with \(\bar{\mu}_X \equiv \mu_X/T\). Here, \(\chi_{ijk}^{BQS}\) are derivatives of \(P/T^4\) with respect to the corresponding chemical potentials, \(\bar{\mu} = (\mu_B, \mu_Q, \mu_S)\), evaluated at \(\bar{\mu} = 0\).

\[
\chi_{ijk}^{BQS} = \frac{1}{VT^3} \left. \frac{\partial \ln Z(T, V, \bar{\mu})}{\partial \mu_i^B \partial \mu_j^Q \partial \mu_k^S} \right|_{\bar{\mu}=0}, \quad i + j + k \text{ even}. \quad (2)
\]

To study strangeness neutral \((n_S = 0)\) isospin-symmetric \((n_Q/n_B = 0.5 \leftrightarrow \mu_Q = 0)\) matter, we introduce constraints on the strangeness chemical potentials,

\[
\mu_S(T, \mu_B) = s_1(T)\mu_B + s_3(T)\mu_B^3 + s_5(T)\mu_B^5 + .. \quad (3)
\]

The expansion coefficients \(s_i\) with \(i = 1, 3, 5, 7\) are given in [11, 12]. Substituting \(\mu_S\) by using Eq. 3 with \(\mu_Q = 0\) and using Eq.(1) we obtained

\[
\frac{P(T, \mu_B) - P(T, 0)}{T^4} = \sum_{k=1}^{\infty} P_{2k}(T)\mu_B^{2k} : \frac{n_B(T, \mu_B)}{T^3} = \sum_{k=1}^{\infty} N_{2k-1}^{B}(T)\mu_B^{2k-1} \quad (4)
\]

where, \(N_{2k-1}^{B} = \frac{\chi_{2k-1}^{B}}{2k-1!} \) and \(P_{2k} = 2kN_{2k-1} = \frac{\chi_{2k}^{B}}{2k!} \).

The simplest estimator, \(r_{c,n}\), for the radius of convergence, \(r_c = \lim_{n \to \infty} r_{c,n}\), is obtained from the ratio of the subsequent, non-vanishing expansion coefficients. We define for pressure and number density respectively,

\[
r_{c,2k}^P = |P_{2k-2}/P_{2k}|^{1/2} \quad \text{and} \quad r_{c,2k}^{n_B} = |N_{2k-3}/N_{2k-1}|^{1/2} \quad (5)
\]

\[
r_{c,2k}/r_{c,2k}^{n_B} = \sqrt{[2k/(2k-2)]} = 1 + 1/k + O(k^2) \quad (6)
\]

\[
r_c = \lim_{k \to \infty} r_{c,2k}^P = \lim_{k \to \infty} r_{c,2k}^{n_B} \quad (7)
\]

In Fig. [11] we show the two highest order subsequent expansion coefficients. For these two expansion coefficients we only used the spline interpolation of the datasets on \(N_\tau = 8\) lattice data for which we have about 1.5 million configurations for each temperature value.
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3. Searching for CEP using [4,4] Padé approximants

Since the first two expansion coefficients in Eq. (4) are strictly positive in the temperature range $T \in [135 - 175]$ MeV, we rescale the expansion coefficients in the Taylor series, $c_{2k,2} = \frac{P_{2k}}{P_2^2} \left( \frac{P_4}{P_2^4} \right)^{k-1}$, $\bar{x} = \sqrt{\frac{P_4}{P_2^2}}$, to obtain,

$$\chi_B^0(T, \hat{\mu}_B) \frac{P_4}{P_2^2} = \sum_{k=1}^{\infty} c_{2k,2} \bar{x}^{2k} = \bar{x}^2 + c_{6,2} \bar{x}^6 + c_{8,2} \bar{x}^8$$

The [2,2] and [4,4] Padé can then be written as

$$P[2,2] = \frac{\bar{x}^2}{1 - \bar{x}^2}, \quad P[4,4] = \frac{(1 - c_{6,2}) \bar{x}^2 + (1 - 2c_{6,2} + c_{8,2}) \bar{x}^4}{(1 - c_{6,2}) + (c_{8,2} - c_{6,2}) \bar{x}^2 + (c_{8,2}^2 - c_{8,2}) \bar{x}^4}. \quad (9)$$

The poles of the Padés can be obtained by determining the roots of the denominators of Eq.(9) as function of $\bar{x}$. For, the case of the [2,2] Padé one gets $\bar{x}^2 = 1$, i.e. for $\mu_{B,c} \equiv r_{c,2} = \sqrt{12 \chi_0^{B,2} / \chi_0^{B,4}}$, which is the standard ratio estimator for the radius of convergence. In the case of the [4,4] Padé there are four possibilities. Depending on the values of $c_{8,2}$ and $c_{6,2}$ one will either find 4 complex, or 2 real plus 2 imaginary, or 4 real, or 4 imaginary poles. Inside the triangular shaped regions bounded by black lines, shown in Fig. 2 (left), the poles are complex. We show in Fig. 2 (left), $c_{8,2}$ and $c_{6,2}$ obtained in (2+1)-flavor QCD. From that it can be established that one obtains 4 complex poles in the temperature range $135$ MeV $\leq T \leq 165$ MeV. In Fig. 1 our two highest expansion coefficients $\bar{x}_0^{B,6}$ and $\bar{x}_0^{B,8}$ become positive at $T \approx 125$ MeV, although errors still are large at lower temperatures. Hence, within our current statistical errors we cannot rule out a pair of real and/or purely imaginary poles at temperatures below $T = 135$ MeV. The
Fig. 2. $c_{8,2}$ vs $c_{6,2}$ on $N_f = 8$ lattice in the temperature range $125 \text{ MeV} < T < 175 \text{ MeV}$ (left). Magnitude of poles nearest to the origin obtained from the [2,2] (squares) and [4,4] (bands) Padé approximants (middle). Location of poles with $\text{Re}(\mu_B) > 0$ nearest to the origin obtained from the [4,4] Padé approximants in the complex $\mu_B$-plane (right).

estimator for the radius of convergence for the complex poles can be written as,

$$r_{c,4} = \sqrt[4]{\frac{12\chi_0 B_2}{\chi_0 B_4} \left| \frac{1}{c_{6,2}} - \frac{c_{8,2}}{c_{6,2}} \right|} \ ,$$

which can be identify as the Mercer-Roberts estimator \cite{14} as long as the poles are complex. As seen from Fig. (2) (middle) estimates for the radius of convergence, obtained from diagonal Padé approximants lead to larger values with increasing temperature. We find $\mu_B/T > 3$ in the temperature range $T \sim [135 - 165] \text{ MeV}$. We estimate $\mu_B/T > 3$ close to the pseudo-critical temperature $T_{pc} \sim 156.5 \text{ MeV}$. In Fig. (2) (right) we also show the location of complex poles with a positive real part obtained in a temperature range between $T = [135 : 165] \text{ MeV}$. They clearly show a tendency to move towards the real axis as the temperature decreases. As mentioned earlier, our current statistical errors do not allow us to draw any conclusion about the nature of the poles at temperature lower than $T \leq 135 \text{ MeV}$.

4. Conclusions

Using diagonal Padé approximants of an eighth order Taylor series of (2+1)-flavor QCD we estimate a radius of convergence of $\mu_B/T > 3$ close to the $T_{pc}$. We also show that the poles of the Padé approximants in the temperature range $T = [135 : 165] \text{ MeV}$ are all complex, disfavoring the existence of a critical point at temperature larger than $T \sim 135 \text{ MeV}$. Furthermore, we also argued that for $T < 130 \text{ MeV}$ the [4,4] Padé-approximants can have real poles, which could signal the occurrence of a phase transition,
at lower temperatures. As the decrease of the QCD pseudo-critical temperature with increasing baryon chemical potentials is small, such low temperatures can only be reached for high baryon densities $\mu_B/T \gtrsim 2.5$ MeV, i.e. at beam energies below the lowest beam energy used at RHIC in collider mode, $\sqrt{s} \lesssim 7.7$ GeV.

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