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Hadronic fluctuations and correlations at nonzero chemical potential

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We present a lattice study of fluctuations and correlations among the conserved charges baryon number and strangeness in (2+1)-flavor QCD. The lattice calculations are based on a Taylor expansion of the pressure. Results are presented at zero and nonzero density on lattices with four and six time slices, corresponding to a lattice spaceing of $a \approx 0.25$ fm and $a \approx 0.16$ fm, respectively. The quark masses are almost physical, i.e. the light quark mass has been choosen to one tenth of the physical strange quark mass while the strange quark mass has been set to its physical value. We find that all analysed fluctuations and correlations develop a peak at nonzero density, when they are treated in an expansion up to sixth order. Especially below the critical temperature (T_c) fluctutations and correlations increase drastically, whereas above T_c they are rather unaffected.

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1. Introduction

Fluctuations of conserved charges, like baryon number, electric charge and strangeness are generally considered to be sensitive indicators for the structure of the thermal medium that is produced in heavy ion collisions [1]. In fact, if at non-vanishing baryon number a critical point exists in the QCD phase diagram, this will be signaled by divergent fluctuations of e.g. the baryon number density [2].

We present here results from lattice calculations of baryon number and strangeness fluctuations in QCD with dynamical light and strange quark degrees of freedom. The results are based on calculations with an improved staggered fermion action (p4-action) that strongly reduces lattice cut-off effects in bulk thermodynamics at high temperature. The values of the quark masses used in this calculation are almost physical; the strange quark mass, m_s, is fixed to its physical value while the light up and down quark masses are taken to be degenerate and equal to $m_s/10$. This is about twice as large as the average up and down quark masses realized in nature. We obtained results from calculations performed with two different values of the lattice cut-off, corresponding to lattices with temporal extent $N_\tau = 4$ and 6. This allows us to judge the magnitude of systematic effects arising from discretization errors in our improved action calculations. The spatial volume has been chosen to be $V^{1/3}T = 4$, which insures that finite volume effects are small.

At the QCD critical endpoint (CEP) the correlation length of the chiral critical mode σ will diverge. Correspondingly, all kinds of fluctuations of conserved charges, which couple to the σ-field, become large in the vicinity of, and diverge at the CEP. It has been argued in [2, 3] that quadratic variances of event-by-event observables such as particle abundances, particle ratios or mean transverse momenta will reflect these divergent fluctuations and are thus good experimental observables for the determination of the CEP. It will thus be very interesting to study baryon number and strangeness fluctuations as well as baryon number-strangeness correlations at nonzero density as they are related to the event-by-event fluctuations of the proton, the kaon and their ratio. The latter has been recently measured by the NA49 collaboration for central Pb-Pb collisions at five different SPS energies [4].

2. The Taylor expansion method

Direct lattice calculations at nonzero baryon density are not possible by means of standard Monte Carlo methods. We follow here the Taylor expansion approach to finite density QCD on the lattice, as described in detail in [5, 6]. Starting from an expansion of the logarithm of the QCD partition function, *i.e.* the pressure, one obtains

$$\frac{p}{T^4} \equiv \frac{1}{VT^3} \ln Z(V,T,\mu_B,\mu_S) = \sum_{i,j} c_{i,j}^{B,S} \left(\frac{\mu_B}{T}\right)^i \left(\frac{\mu_S}{T}\right)^j , \tag{2.1}$$

where

$$c_{i,j}^{B,S}(T) = \frac{1}{i!\,j!} \frac{\partial^i}{\partial \mu_B^i} \frac{\partial^j}{\partial \mu_S^j} \frac{\ln Z(V,T,\mu_B,\mu_S)}{VT^3} \bigg|_{\mu_B=\mu_S=0} . \tag{2.2}$$

Here μ_B and μ_S are the baryon and strangeness chemical potentials, respectively, which can be obtained as appropriate linear combinations of the quark chemical potentials. Note that we treat

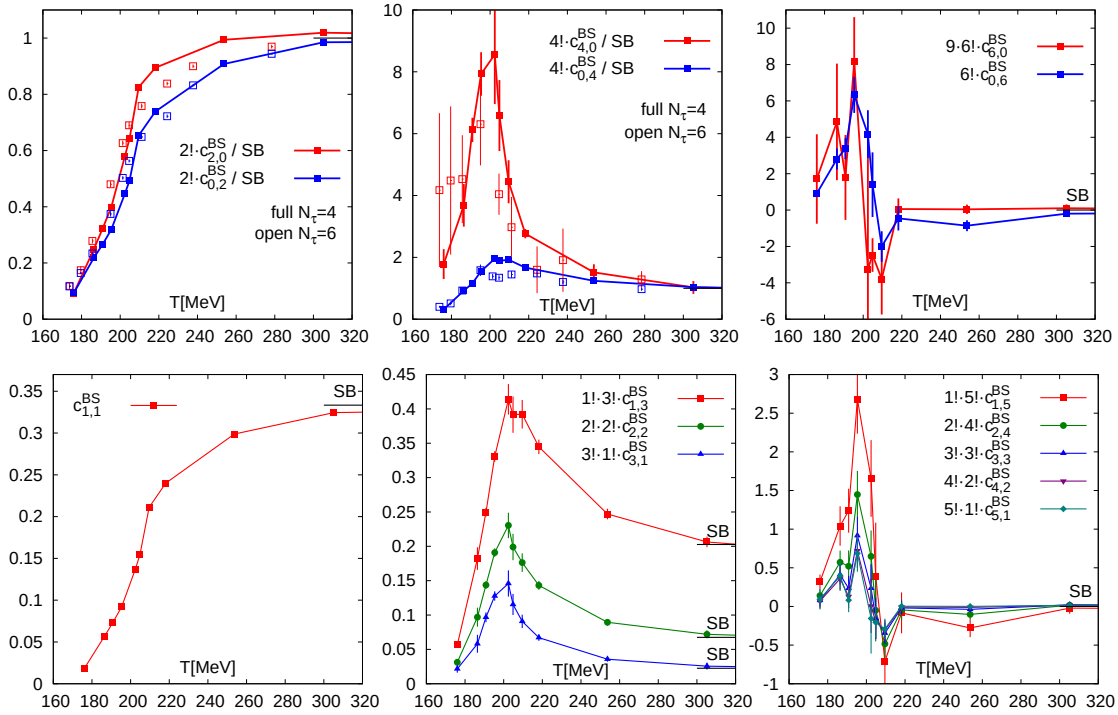

Figure 1: Diagonal (upper row) and off-diagonal (lower row) expansion coefficients of the pressure of 2nd (left column), 4th (middle column) and 6th (right column) order. For diagonal coefficients up to the 4th order we compare results from two different lattice spacings ($N_\tau = 4$ and $N_\tau = 6$ lattices). Here we have normalized the data by its corresponding SB-values.

the up and down quarks as degenerated, both in mass as well as net quark number density. Accordingly, isospin and electric charge chemical potential vanish. Due to charge conjugation symmetry only coefficients with $i + j$ even are nonzero. In Fig. 1 we show the diagonal and off-diagonal coefficients of this expansion up to 6th order. For diagonal coefficients up to 4th order we show results that have been obtained for different lattice spacings, i.e. on $N_\tau = 4$ and $N_\tau = 6$ lattices. We note that results obtained on lattices with temporal extent $N_\tau = 6$ are in good agreement with those obtained on the coarser $N_\tau = 4$ lattice. The slight shift towards smaller temperatures, visible for the $N_\tau = 6$ data relative to the $N_\tau = 4$ data, is consistent with findings for the equation of state, e.g. the trace anomaly $(\varepsilon - 3p)/T^4$, and also reflects the shift in the transition temperature observed when comparing the locations of the cusp in the chiral susceptibility [7].

The general pattern of the coefficients can be understood from the structure of the singular part of the free energy. In the chiral limit of our (2+1)-flavor simulations, *i.e.* with vanishing light quark masses, but finite and physical strange quark mass, we expect the QCD transition to be of second order [8]. The relevant scaling field which contains the baryon chemical potential will be the reduced temperature, for which we make the ansatz

$$t = \frac{T - T_c}{T_c} + \kappa \left(\frac{\mu_B}{T}\right)^2 . \tag{2.3}$$

Accordingly two derivatives of the free energy with respect to μ_B (at $\mu_B = 0$) are similar to one

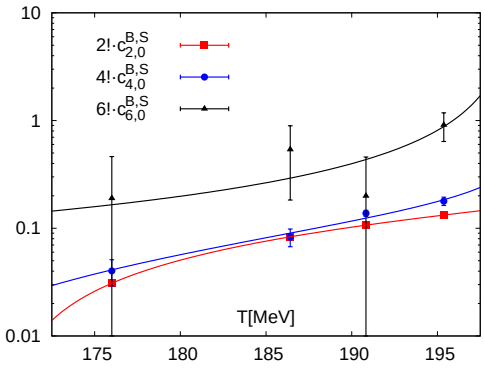

Figure 2: A fit to the expansion coefficients of the pressure below T_c, inspired by the critical behavior of the free energy. At this lattice size and quark mass ($N_\tau = 4$, $m_q = 0.1m_s$) we have $T_c \approx 202$ MeV.

derivative with respect to the temperature. Therefore we obtain the following formulas, which can be used to fit the critical behavior of the Taylor expansion coefficients

$$2! \cdot c_{B,S}^{2,0} \sim \mp 2A_\pm(2-\alpha)\kappa|t|^{1-\alpha} + b_2 t + c_2 \,; \tag{2.4}$$

$$4! \cdot c_{B,S}^{4,0} \sim -12A_\pm(2-\alpha)(1-\alpha)\kappa^2|t|^{-\alpha} + b_4 t + c_4 \,; \tag{2.5}$$

$$6! \cdot c_{B,S}^{6,0} \sim \pm 120A_\pm(2-\alpha)(1-\alpha)(-\alpha)\kappa^3|t|^{-1-\alpha} \,. \tag{2.6}$$

Here uppers signs are valid for $t > 0$, whereas lower signs are for $t < 0$. We see that the critical behavior is governed by the critical exponent α, which is small and negative for the universality classes of interest. For staggered fermions at finite lattice spacing, were the chiral symmetry is broken down to a $U(1)$ subgroup, we expect the relevant universality class to be that of the 3d-$O(2)$ symmetric model, where we have $\alpha \sim -0.015$. We thus expect $c_{B,S}^{4,0}$ to develop a cusp, while $c_{B,S}^{6,0}$ will diverge in the chiral limit. $c_{B,S}^{2,0}$ will be dominated by the regular part of the free energy. Hence, we took into account the leading order regular terms, indicated by the coefficients b_2, b_4, c_2, and c_4 in Eq. 2.4 and Eq. 2.5. For $T < T_c$ we show the fit results in Fig. 2. Although the ansatz is strictly valid only in the chiral limit, the fit works quite well. It has already been observed previously that at this quark mass ($m_q = 0.1m_s$) the QCD thermodynamics enters the scaling regime of the critical behavior [8]. Currently the coefficient κ, which determines the slope of the critical line as function of μ_B is, however, not very well constrained.

3. Baryon number and strangeness fluctuations

We now construct baryon number and strangeness susceptibilities which measure fluctuations at nonzero chemical potentials. The corresponding expansions can be expressed in terms of the pressure coefficients from Eq. 2.1. We obtain for the baryon number fluctuations

$$\chi_B \equiv \frac{\langle N_B^2\rangle - \langle N_B\rangle^2}{VT^3} = \sum_{i=1}^{\infty}(2i)(2i-1)c_{B,S}^{2i,0}\left(\frac{\mu_B}{T}\right)^{2i-2} \,, \tag{3.1}$$

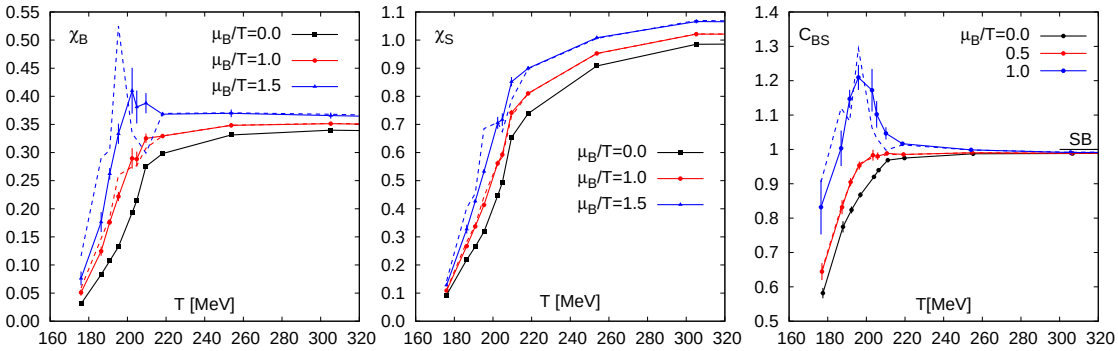

Figure 3: Baryon number fluctuations (left), strangeness fluctuations (middle) and baryon number strangeness correlation coefficient (right) at nonzero baryon chemical potential. Data points are obtained by a truncated Taylor series up to the 4th order in μ_B/T, while dashed lines indicate the 6th order results.

and for the strangeness fluctuations

$$\chi_S \equiv \frac{\langle N_S^2 \rangle - \langle N_S \rangle^2}{VT^3} = \sum_{i=0}^{\infty} 2c_{B,S}^{2i,2} \left(\frac{\mu_B}{T}\right)^{2i} . \tag{3.2}$$

Here $\langle \cdot \rangle$ indicates the expectation value evaluated in the grand canonical ensemble in lattice simulations. N_B and N_S are the net number of baryons and strange particles, respectively. In Fig. 3 (left and middle) we show results for the baryon number and strangeness fluctuations at zero and nonzero μ_B/T, obtained by truncating the series (3.1 and 3.2) after the 4th order. We have also indicated the 6th order results by dashed lines in order to give a feeling for the truncation errors. At $\mu_B/T = 0$, the generic form of the temperature dependence is a smooth crossover, while the leading order term in $(\mu_B/T)^2$ has a peak at T_c. It is thus clear that at sufficiently large values of μ_B/T the fluctuations will develop a peak. However, it is important to stay within the radius of convergence of the series, in order to keep the truncation errors small. We will discuss the radius of convergence in Sec. 5 in more detail; here we find that for $\mu_B/T \leq 1.5$ the truncation error is small. For this value of the chemical potential the baryon number fluctuations show already a small peak, whereas the strangeness fluctuations are only slightly enhanced.

We note, that all fluctuations of modes that couple to the relevant chiral critical mode at the QCD critical point (the sigma-field) will diverge at the QCD critical endpoint (CEP). As light quarks carry also a baryon number, the baryon number fluctuations are expected to diverge at the CEP.

4. The baryon number – strangeness correlation

The baryon number-strangeness coefficient was introduced as a diagnostic tool for the effective degrees of freedom in the quark gluon plasma [9]. It is defined as

$$C_{BS} \equiv -3 \frac{\langle N_B N_S \rangle - \langle N_B \rangle \langle N_S \rangle}{\langle N_S^2 \rangle - \langle N_S \rangle^2} . \tag{4.1}$$

Lattice calculations of this quantity in the (partially) quenched approximation [10] and $2+1$-flavor QCD [5] indicate that this quantity reaches unity for temperatures larger than $1.5T_c$, whereas it is significantly smaller for $T < T_c$. *I.e.*, the quark flavors are uncorrelated above T_c as in the ideal Quark Gluon Plasma (QGP). This behavior indicates the transition from hadronic degrees of freedom to that of a QGP.

Similar to the expansion of baryon number fluctuations (Eq. 3.1) and strangeness fluctuations (Eq. 3.2) we can also expand the baryon number- strangeness coefficient. Again we express its expansion coefficients in terms of the expansion coefficients of the pressure (Eq. 2.1) and obtain

$$C_{BS}(\mu_B/T) = C_{BS}^{(0)} + C_{BS}^{(2)} \left(\frac{\mu_B}{T}\right)^2 + C_{BS}^{(4)} \left(\frac{\mu_B}{T}\right)^4 + \mathscr{O}\left[\left(\frac{\mu_B}{T}\right)^6\right] , \tag{4.2}$$

with

$$C_{BS}^{(0)} = -\frac{3c_{1,1}^{B,S}}{2c_{0,2}^{B,S}} ; \quad C_{BS}^{(2)} = \frac{3c_{1,1}^{B,S}c_{2,2}^{B,S} - 9c_{0,2}^{B,s}c_{3,1}^{B,S}}{2\left(c_{0,2}^{B,S}\right)^2} ; \tag{4.3}$$

and

$$C_{BS}^{(4)} = \frac{-3c_{1,1}^{B,S}\left(c_{2,2}^{B,S}\right)^2 + 9c_{0,2}^{B,S}c_{2,2}^{B,S}c_{3,1}^{B,S} + 3c_{0,2}^{B,S}c_{1,1}^{B,S}c_{4,2}^{B,S} - 15\left(c_{0,2}^{B,S}\right)^2 c_{5,1}^{B,S}}{2\left(c_{0,2}^{B,S}\right)^3} . \tag{4.4}$$

In Fig. 3 (right) we show the correlation C_{BS} at zero and nonzero density. We find that at nonzero baryon number density a peak is developing already at small values of μ_B/T where the truncation errors are small (data points are the 4th order results, while the dashed lines indicate the 6th order results). At $\mu_B/T = 1.0$, the correlations at T_c increase by almost 50%, and rise to a value which is about 20% larger than the Stefan-Boltzmann value. It will be interesting to see whether the increase in the baryon number strangeness coefficient will give rise to a peak in proton over kaon fluctuations obtained in Heavy Ion Collisions and whether these fluctuations can be used as an experimental signal for locating the critical point. Also below T_c the correlations increase drastically with increasing μ_B, whereas above T_c the correlation coefficient C_{BS} remains rather unaffected by the increasing baryon density.

5. The radius of convergence

It is known that in the temperature region close to T_c the convergence properties of the Taylor expansion of the pressure (Eq. 2.1) and therefore also of the expansions of the baryon number and strangeness fluctuations (Eq. 3.1) and (Eq. 3.2) are poor. Here the expansion coefficients wildly fluctuate in sign and magnitude. Only for temperatures below the CEP, this might be better as in this case all expansion coefficients are positive. It has been argued that the radius of convergence can be used to determine the location of the CEP [12]. One way to define the radius of convergence of the pressure series in μ_B/T (Eq. 2.1) is

$$\rho = \lim_{n\to\infty} \rho_n \quad \text{with} \quad \rho_n = \mu_B^{(n)}/T^{(n)} = \sqrt{c_{n,0}^{B,S}/c_{n+2,0}^{B,S}} . \tag{5.1}$$

The convergence radius can be estimated in a similar manner by the coefficients in the series of the baryon number fluctuations (Eq. 3.1). Each order ρ_n will, however, differ by a constant factor

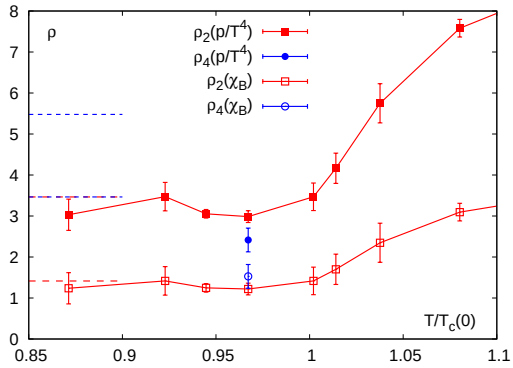

Figure 4: Two estimates of the radius of convergence of the pressure series (full symbols) and the series of baryon number fluctuations (open symbols) as a function of temperature. ρ_4 indicates our best estimate for the location of the critical endpoint. Dashed lines show the resonance gas limit of the different estimators.

which goes to one in the limit $n \to \infty$. We define a second estimator of the convergence radius, based on the χ_B-series as

$$\rho_n[\chi_B] = \sqrt{\frac{n(n-1)}{(n+1)(n+2)}}\,\rho_n[p/T^4]\,. \tag{5.2}$$

The method to estimate the location of the CEP by the radius of convergence works in two steps:

1. Find the largest temperature where all (available) expansion coefficients are positive. Only if all expansion coefficients are positive, the corresponding singularity which is limiting the convergence radius lies on the real axis and can be associated with the physical phase transition.

2. Estimate the radius of convergence at this temperature by using Eq. 5.1 or Eq. 5.2.

It is clear, that in practice we can not perform the limit $n \to \infty$ but have to stop at some finite n. Eventually at this point different estimators of the radius of convergence will agree within errors.

In Fig. 4 we have summarized current results on the radius of convergence. The first non trivial approximation which does not explicitly include contributions from the gluon sector (contributes to $c^{B,S}_{0,0}$), is given by ρ_2, shown by the square data points. Here both contributing expansion coefficients ($c^{B,S}_{2,0}$ and $c^{B,S}_{4,0}$) are positive for all values of the temperature, hence an approximation for the temperature ($T^{(2)}$) of the CEP can not be deduced. At this order the estimates from the pressure series (full symbols) and from the series of the baryon number fluctuations differ quite dramatically. The next higher approximation ρ_4 of the CEP, which is currently our best approximation, is shown by the circle data point. We obtain for the temperature $T^{(4)} \approx 0.96 T_c(\mu_B = 0)$. Here the difference between the two estimators becomes less severe. For the convergence radius they span the range of $\rho \approx (1.5 - 2.4)$. It is interesting to note that the two different estimators of the convergence radius seem to approach the $n \to \infty$ limit from different sites. However, the χ_B-estimator seems to be the more stable one. Also shown are the resonance gas limits of the two approximations, indicated by the dashed lines.

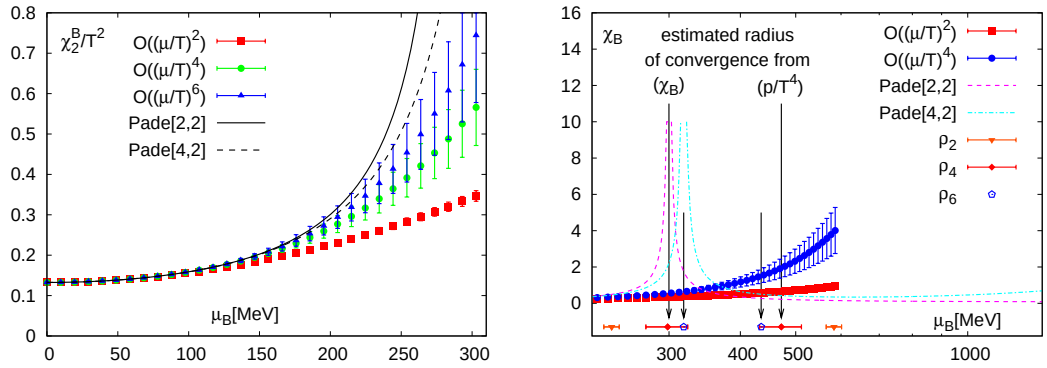

Figure 5: Baryon number fluctuations at $T = 0.96T_c \approx T^{\rm CEP}$ as a function of the baryon chemical potential (left). We compare different order of the truncated Taylor series vs two Padé approximants. The right panel shows the same but on a much larger scale.

6. Taylor expansion vs. Padé approximation

So far our analysis of observables at nonzero baryon density has been based on the Taylor expansion of the pressure (Eq. 2.1) around $\mu_B/T = 0$. Now we want to discuss the Padé approximation, which is usually considered to be a better approximation of the true function, even beyond the radius of convergence [11]. One can construct different Padé approximants from the Taylor expansion coefficients. Padé approximants are rational functions which differ by the order of the polynomials in the numerator and denominator. For the baryon number fluctuations we obtain e.g.

$$\mathrm{Pade}[2,2]\left(\chi_B\right) = \frac{4c_{B,S}^{2,0}c_{B,S}^{4,0} + 2\left(12\left(c_{B,S}^{4,0}\right)^2 - 5c_{B,S}^{2,0}c_{B,S}^{6,0}\right)\left(\frac{\mu_B}{T}\right)^2}{2c_{B,S}^{4,0} - 5c_{B,S}^{6,0}\left(\frac{\mu_B}{T}\right)^2} \tag{6.1}$$

In Fig. 5(left) we compare different orders of the truncated Taylor series (Eq. 3.1) with the Padé approximations [2,2] and [4,2], where the latter one has a fourth order polynomial in the numerator. We show the baryon number fluctuations at fixed, but varying baryon chemical potential. $T \approx 0.96T_c$ is currently our best approximation for the temperature of the critical endpoint ($T^{\rm CEP}$) as it was estimated by the radius of convergence method. The most prominent feature of the Padé approximations is the appearance of a pole. The location of the poles are given by the roots of the denominator. From Eq. 6.1 it is obvious that the pole in the [2,2] approximation exactly coincides with the $\rho_4[\chi_B]$ estimate of the convergence radius.

Note that for the Taylor series of χ_B which was truncated after the 6th order, as well as for the [4,2] Padé approximant we need the coefficient $c_{B,S}^{8,0}$. In the following analysis we set the so far unknown coefficient to $c_{B,S}^{8,0} \equiv c_{B,S}^{6,0}/x$.

Given the coefficients $c_{B,S}^{2,0} - c_{B,S}^{6,0}$ at $T \approx 0.96T_c$, we vary the strength of $c_{B,S}^{8,0}$ by the parameter x. We have fixed the parameter x by assuming that the asymptotic behavior of the [4,2] Padé approximant for large μ_B should be governed by the free gas result which is given by

$$\lim_{\mu_B\to\infty}\chi_B \approx \frac{1}{3} + \frac{1}{9\pi^2}\left(\frac{\mu_B}{T}\right)^2 . \tag{6.2}$$

Using this property, we obtain $x \approx 4.95$ and the next approximation for the convergence radius ($\rho_6 = \sqrt{x}$), which we also shown in Fig. 5(right). Again we find that the Pole in the [4,2] Padé approximant for χ_B coincides exactly with the corresponding estimator for the convergence radius $\rho_6[\chi_B]$.

7. Summary and conclusions

We have performed a comprehensive study of the Taylor expansion coefficients of the baryon number fluctuation, strangeness fluctuation as well as their correlations, based on the Taylor expansion coefficients of the pressure. We found that all these quantities will develop a peak at $T \approx T_c$ for nonzero baryon chemical potential, which is the dominant effect from the leading order coefficient in μ_B. The sub-leading coefficient will in general lead to a shift of the peak, i.e. a μ_B-dependence of the peak position. Our current analysis takes into account the coefficients up to 6th order. On the highest order the errors are barely under control. As most observales at nonzero chemical potential crucially depend on the relative strengh of the coefficients, a more refined analysis which also takes into account the 8th order coefficents is highly desired. This will also help to confirm the structure of the Taylor expansion coefficients which can be understood in terms of an appropriate scaling ansatz of the free energy in the chiral limit. With a combined fit of all Taylor expansion coefficients it will in principle be possible to determine the μ_B-dependent curvature of the critical temperature in the chiral limit.

When comparing different orders of the truncated Taylor series we find small truncation errors below $\mu_B/T \lesssim (1-1.5)$, while for $\mu_B/T \approx (1.5-2.5)$ consecutive orders become compatible. The latter fact can be used to estimate the radius of convergence of the Taylor series, which will be connected with a physical singularity in the QCD phase diagram (critical endpoint) when all expansion coefficients are positive. The temperaure of the cirical endpoint we currently approximate to $T^{\rm CEP} \approx 0.96 T_c$.

We also constructed Padé approximants from the Taylor coefficients. Again we find good agreement between different approximants as well as the truncated Taylor series below $\mu_B/T \lesssim (1-1.5) T_c$.

Acknowledgments

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