PROCEEDINGS OF SCIENCE

New results for QCD at non-vanishing chemical potentials from Taylor expansion

Edwin Laermann[*†]
Universität Bielefeld
E-mail: edwin@physik.uni-bielefeld.de

Recent results of the BNL-CCNU-Bielefeld collaboration on the Taylor expansion of the pressure up to sixth order in the baryon, strangeness and electric charge chemical potentials are presented, with the focus on the QCD equation of state. The calculations have been performed with the Highly Improved Staggered Quark action on lattices with aspect ratio 4 and temporal extents ranging from 6 to 16, i.e. at four different values of the lattice spacing. The strange quark mass has been tuned to its physical value, and two ratios of the light to the strange mass, $m_l/m_s = 1/20$ and $1/27$ have been investigated. The comparison of sixth order Taylor expansion in the chemical potentials with fourth order ones shows that the truncation errors are small at least up to baryon chemical potential of $\mu_B/T \simeq 2$.

34th annual International Symposium on Lattice Field Theory
24-30 July 2016
University of Southampton, UK

[*]Speaker.
[†]For the BNL-CCNU-Bielefeld collaboration

PoS(LATTICE2016)079

1. Introduction

The temperature and density dependence of bulk thermodynamic quantities, commonly summarized as the equation of state (EoS), provide the most basic characterization of equilibrium properties of strong-interaction matter. Quite recently, continuum extrapolated results for the EoS of QCD with physical light and strange quark masses have been obtained at vanishing chemical potentials [1, 2]. Bulk thermodynamic observables such as pressure (P), energy density (ε) and entropy density (s) and other quantities have been calculated. In accordance with the analysis of the chiral transition temperature, $T_c \simeq (154 \pm 9)$ MeV [3], these observables change smoothly in the transition region. At low temperature they are found to be in quite good agreement with hadron resonance gas (HRG) model calculations, although some systematic deviations have been observed, which may be attributed to the existence of additional resonances which are not taken into account in HRG model calculations based on well established resonances listed in the particle data tables [4, 5].

While the EoS at vanishing chemical potentials provides important input to the modelling of the hydrodynamic evolution of the matter created in heavy ion collisions at the LHC and the highest RHIC beam energies, knowledge of the EoS at non-vanishing baryon (μ_B), strangeness (μ_S) and electric charge (μ_Q) chemical potentials is indispensable at the conditions met in the beam energy scan (BES) at RHIC. Due to the well-known sign problem for lattice QCD formulations at non-zero chemical potential a direct calculation of the EoS at non-zero μ_B, μ_Q or μ_S is unfortunately not yet possible. At least for small values of the chemical potentials this can be circumvented by using a Taylor expansion of the thermodynamic potential [6, 7]. Yet, if one wants to cover the range of chemical potentials, $0 \le \mu_B/T \lesssim 3$ that is expected to be explored with the BES at RHIC by varying the beam energies in the range 7.7 GeV $\le \sqrt{s_{NN}} \le$ 200 GeV results for higher than second order expansion coefficients are clearly needed. In this work we want to present our results for (and only for) the EoS at non-vanishing chemical potentials in Taylor expansions up to sixth order. A full account including more results and a comprehensive set of references is given in [8].

2. Outline of the Calculation

Our goal is the calculation of Taylor expansion coefficients for basic bulk thermodynamic observables of strong-interaction matter in terms of chemical potentials μ_X for conserved charges ($X = B, Q, S$). We start with the expansion of the pressure, P, in terms of the dimensionless ratios $\hat{\mu}_X \equiv \mu_X/T$,

$$\frac{P}{T^4} = \frac{1}{VT^3} \ln \mathscr{Z}(T,V,\hat{\mu}_u,\hat{\mu}_d,\hat{\mu}_s) = \sum_{i,j,k=0}^{\infty} \frac{\chi_{ijk}^{BQS}}{i!\,j!\,k!} \hat{\mu}_B^i \hat{\mu}_Q^j \hat{\mu}_S^k \, , \tag{2.1}$$

with $\chi_{000}^{BQS} \equiv P(T,0)/T^4$ and the chemical potentials for the conserved charges of course being related to the quark chemical potentials, $\mu_u = 1/3\mu_B + 2/3\mu_Q$, $\mu_d = 1/3\mu_B - 1/3\mu_Q$, and $\mu_s = 1/3\mu_B - 1/3\mu_Q - \mu_S$. The expansion coefficients χ_{ijk}^{BQS}, i.e. the so-called generalized susceptibilities, can be calculated at vanishing chemical potential[1],

$$\chi_{ijk}^{BQS} \equiv \chi_{ijk}^{BQS}(T) = \left. \frac{\partial P(T,\hat{\mu})/T^4}{\partial \hat{\mu}_B^i \partial \hat{\mu}_Q^j \partial \hat{\mu}_S^k} \right|_{\hat{\mu}=0} . \tag{2.2}$$

While it is straightforward to obtain the Taylor series for the number densities from Eq. 2.1 ,

$$\frac{n_X}{T^3} = \frac{\partial P/T^4}{\partial \hat{\mu}_X} , \; X = B,\; Q,\; S . \tag{2.3}$$

energy (ε) and entropy (s) densities require derivatives of the generalized susceptibilities with respect to temperature. These are the expansion coefficients of the trace anomaly,

$$\Delta(T,\hat{\mu}_B,\hat{\mu}_Q,\hat{\mu}_S) \equiv \frac{\varepsilon - 3P}{T^4} = T\frac{\partial P/T^4}{\partial T} = \sum_{i,j,k=0}^{\infty} \frac{\Xi_{ijk}^{BQS}}{i!j!k!} \hat{\mu}_B^i \hat{\mu}_Q^j \hat{\mu}_S^k , \tag{2.4}$$

with $i+j+k$ even and

$$\Xi_{ijk}^{BQS}(T) = T\frac{\mathrm{d}\chi_{ijk}^{BQS}(T)}{\mathrm{d}T} . \tag{2.5}$$

With this one finds for the Taylor expansions of e.g. the energy density,

$$\frac{\varepsilon}{T^4} = \sum_{i,j,k=0}^{\infty} \frac{\Xi_{ijk}^{BQS} + 3\chi_{ijk}^{BQS}}{i!\,j!\,k!} \hat{\mu}_B^i \hat{\mu}_Q^j \hat{\mu}_S^k. \tag{2.6}$$

In a heavy ion collision, electric charge and strangeness chemical potentials are fixed by additional constraints and become functions of the baryon chemical potential and temperature. More generally, we consider here constraints that can be fulfilled order by order in the Taylor series expansion. Thus, for the construction of the 6^{th} order Taylor series of the pressure in terms of $\hat{\mu}_B$ we need to know the expansion of $\hat{\mu}_Q(T,\mu_B)$ and $\hat{\mu}_S(T,\mu_B)$ up to fifth order in $\hat{\mu}_B$,

$$\begin{aligned} \hat{\mu}_Q(T,\mu_B) &= q_1(T)\hat{\mu}_B + q_3(T)\hat{\mu}_B^3 + q_5(T)\hat{\mu}_B^5 + \dots , \\ \hat{\mu}_S(T,\mu_B) &= s_1(T)\hat{\mu}_B + s_3(T)\hat{\mu}_B^3 + s_5(T)\hat{\mu}_B^5 + \dots . \end{aligned} \tag{2.7}$$

The above parametrization includes the cases of vanishing electric charge and strangeness chemical potentials, $\mu_Q = \mu_S = 0$, as well as the strangeness neutral case with fixed electric charge to baryon-number ratio.

Implementing the constraints specified in Eq. 2.7 in the Taylor series for e.g. the pressure one obtains a series in terms of the baryon chemical potential only,

$$\frac{P(T,\mu_B)}{T^4} - \frac{P(T,0)}{T^4} = \sum_{k=1}^{\infty} P_{2k}(T)\hat{\mu}_B^{2k} , \tag{2.8}$$

where the P_{2k} are somewhat more complicated expressions involving q_i and s_i. These and other formulae for number density as well as energy density and entropy are given in full detail in [8].

[1] We often suppress the argument (T) of the generalized susceptibilities. We also suppress superscripts and subscripts of χ_{ijk}^{BQS} whenever one of the subscripts vanishes, e.g. $\chi_{i0k}^{BQS} \equiv \chi_{ik}^{BS}$.

PoS(LATTICE2016)079

The generalized susceptibilities χ_{ijk}^{BQS} have been calculated on gauge field configurations generated for (2+1)-flavor QCD using the Highly Improved Staggered Quark (HISQ) action [9] and the tree-level improved Symanzik gauge action. All calculations are performed using a strange quark mass m_s tuned to its physical value. We performed calculations with two different light to strange quark mass ratios, $m_l/m_s = 1/27$ and $1/20$. The former corresponds to a pseudo-scalar Goldstone mass, which in the continuum limit yields a pion mass $m_\pi \simeq 140$ MeV, the latter leads to a pion mass $m_\pi \simeq 160$ MeV. These parameters are fixed using the line of constant physics determined by HotQCD from the f_K scale. More details on the scale determination are given in [3].

All calculations have been performed on lattices of size $N_\sigma^3 N_\tau$ with an aspect ratio $N_\sigma/N_\tau = 4$. We perform calculations in the temperature interval $T \in [135\text{ MeV}, 330\text{ MeV}]$. At temperatures $T \leq 175$ MeV all calculations have been performed with the lighter, physical quark mass ratio $m_l/m_s = 1/27$. In the high temperature region quark mass effects are small and we based our calculations on existing data sets for $m_l/m_s = 1/20$, which have previously been generated by the HotQCD collaboration and used for the calculation of second order susceptibilities [10]. These data sets have been extended for the calculation of higher order susceptibilities. Gauge field configurations are stored after every 10^{th} molecular dynamics trajectory of unit length.

On lattices with temporal extent $N_\tau = 6$ and 8 all 4^{th} and 6^{th} order expansion coefficients have been calculated. In these cases we gathered a large amount of statistics. At low temperatures we have generated up to 1.2 million trajectories for $N_\tau = 6$ and up to 1.8 million trajectories for $N_\tau = 8$. At high temperature less than a tenth of this statistics turned out to be sufficient. The 2^{nd} order expansion coefficients have been calculated on lattices with temporal extents $N_\tau = 6,\ 8,\ 12,\ 16$. At fixed temperature this corresponds to four different values of the lattice cut-off, which we used to extract continuum extrapolated results for the second order expansion coefficients. We also extrapolated results for the higher order expansion coefficients to the continuum limit. However, having at hand results from only two lattice spacings for these expansion coefficients we consider these extrapolations as estimates of the results in the continuum limit.

The traces of all operators needed have been calculated stochastically. For the calculation of 2^{nd} and 4^{th} order coefficients we follow the standard approach of introducing a chemical potential as an exponential prefactor for time-like gauge field variables [11], which insures that all observables calculated are free of ultra-violet divergences. For the calculation of the 6^{th} order coefficients we use the so-called linear-μ approach [12, 13] as no ultra-violet divergences appear in 6^{th} order cumulants and above. In the linear-μ formulation the number of operators that contribute to cumulants is drastically reduced. The final error on the traces depends on the noise due to the use of stochastic estimators for the inversion of the fermion matrices M_f, $f = l, s$, as well as on the gauge noise. Among all the operators calculated, $D_1 = \mathrm{tr} M_f^{-1} dM_f/d\mu_f$ is the one most sensitive to stochastic noise. This operator has therefore been measured using 2000 random noise vectors. For the calculation of traces of all other operators we used 500 random noise vectors. This suffices to reduce the stochastic noise well below the gauge noise.

All fits and continuum extrapolations shown in the following are based on spline interpolations with coefficients that are allowed to depend quadratically on the inverse temporal lattice size. Our fitting ansatz and the strategy followed to arrive at continuum extrapolated results are described in detail in Ref. [2]. For the current analysis we found it sufficient to use spline interpolations with quartic polynomials and 3 knots whose location is allowed to vary in the fit range.

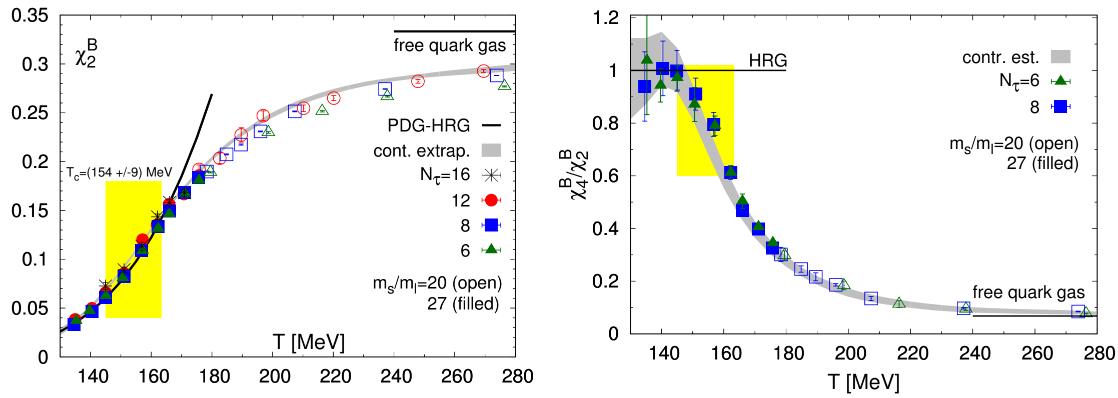

Figure 1: Left: The leading order ($\mathcal{O}(\mu_B^2)$) correction to the pressure calculated at zero baryon chemical potential versus temperature. Right:The ratio of fourth and second order cumulants of net-baryon number fluctuations (χ_4^B/χ_2^B) versus temperature. The yellow boxes indicate the transition region, $T_c = (154 \pm 9)$ MeV, grey bands show continuum extrapolation and estimate resp.. The black lines denote the Hadron Resonance Gas (HRG) model calculation and the free quark gas limit.

3. Results

First we will show the results for the baryon cumulants. In Fig.1 (left) the second order coefficient χ_2^B is shown over a wide range of temperatures. From the lattices with temporal extent up to 16 is it seen that the lattice artefacts are quite small and allow for a safe extrapolation to the continuum limit. At temperatures below the transition regime, indicated by the yellow box, the agreement with a Hadron Resonance Gas (HRG) model calculation based on the states as given by the Particle Data Group (PDG) is also good. However, at closer look, see [8], the existence of more hadron states is prefered by the lattice data. On the right the next order coefficient χ_4^B is shown normalized to χ_2^B. Here the deviation from the HRG starts at the lower end of the transition range and becomes as large as about 60 % already at a temperature of 165 MeV.

We first discuss the case of vanishing potentials for strangeness and electric charge $\mu_S = \mu_Q = 0$. In this case the lowest order terms for the contributions from non-vanishing baryon potential are easily obtained as

$$\frac{P(T,\mu_B)-P(T,0)}{T^4} = \frac{\chi_2^B}{2}\left(\frac{\mu_B}{T}\right)^2\left[1+\frac{1}{12}\frac{\chi_4^B}{\chi_2^B}\left(\frac{\mu_B}{T}\right)^2\right] \tag{3.1}$$

indicating already the suppression of higher orders for moderate values of the baryon potential. This is corroborated in Fig.2 where total pressure and total energy density are shown for various values of μ_B/T from the Taylor expansion up to and including sixth order. Note that the size of the contribution from non-vanishing μ_B is quite small in absolute numbers relative to the result at $\mu_B = 0$, and also the error is dominated by the one in this limit.

Secondly, we will briefly discuss the situation as it is met in heavy-ion collisions. Here the thermal system is supposed to be strangeness neutral, i.e. the strangeness density n_S is zero, and the ratio between electric charge and baryon density is fixed, in most cases to $n_Q/n_B = 0.4$. These are two constraints which lead to elimination of the electric charge and the strangeness chemical potential, in favor of the baryon one, i.e. to relations Eq.2.7 with fixed (and case dependent)

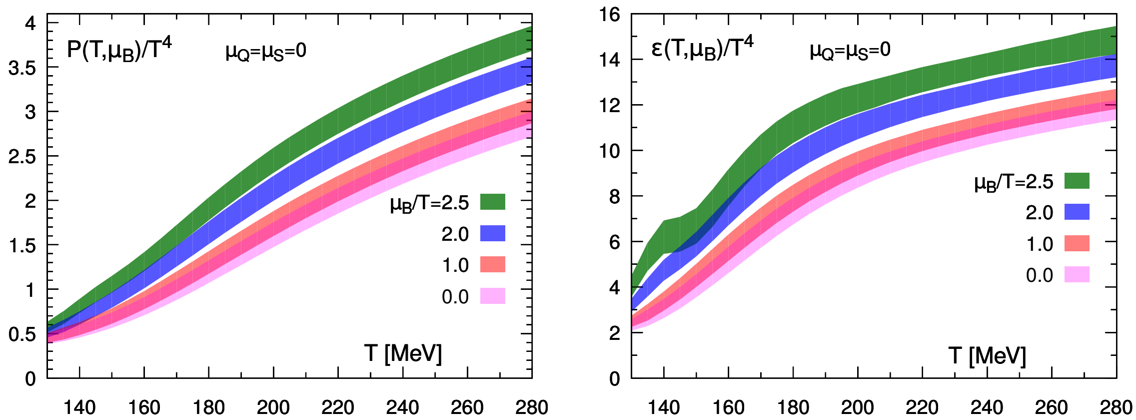

Figure 2: Left: The total pressure in (2+1)-flavor QCD in $\mathcal{O}(\hat{\mu}_B^6)$ for several values of μ_B/T. Right: The total energy density in (2+1)-flavor QCD in $\mathcal{O}(\hat{\mu}_B^6)$ for several values of μ_B/T. The results for $\hat{\mu}_B = 0$ are taken from Ref. [2].

coefficients q_i, s_i. In Fig.3 (left) we show the μ_B dependent contributions to the pressure as a function of temperature for different values of μ_B/T in dependence of what order in the Taylor expansion has been taken into account. As can be seen, for $\mu_B/T = 1$ the higher than lowest orders don't contribute visibly. This changes slightly with larger values of μ_B/T but even at $\mu_B/T = 2$ the fourth order calculation seems to be sufficient. Finally, in Fig.3 (right) we show total energy and total pressure at two values of μ_B. As above also here current errors on the total pressure and energy density are dominated by errors on these observables at $\mu_B = 0$. In the figure we also show the results coming from analytically continued results obtained within the stout discretization at imaginary potential [14]. The total pressure agrees quite well, although the results obtained from the analytic continuation within the stout scheme tend to stay systematically below the central values obtained from the analysis of Taylor series expansions in the HISQ discretization.

4. Conclusion

We have presented results on the QCD equation of state obtained from a sixth order Taylor-expansion of the pressure of (2+1)-flavor QCD with physical light and strange quark masses. We considered expansions at vanishing strangeness and electric charge chemical potential $\mu_S = \mu_Q = 0$ as well as for strangeness neutral systems $n_S = 0$ with a fixed electric charge to net baryon-number ratio, $n_Q/n_B = 0.4$, which is appropriate for situations met in heavy ion collisions. The results, however, can easily be extended to arbitrary ratios of n_Q/n_B. All results discussed here indicate that the present order of expansion works reliably up to $\mu_B \leq 2T$.

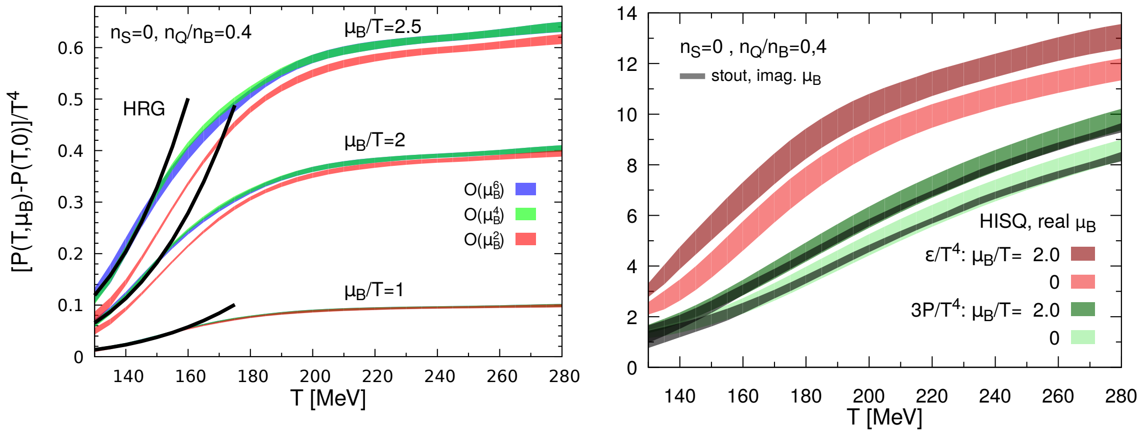

Figure 3: Left: The μ_B dependent contribution to the pressure for several values of the baryon chemical potential in units of temperature. Right:The total energy density (upper two curves) of (2+1)-flavor QCD for $\mu_B/T = 0$ and 2, respectively. The lower two curves show corresponding results for three times the pressure. The dark lines show the results obtained with the stout action from analytic continuation with sixth order polynomials in $\hat{\mu}_B$ [14].

References

[1] S. Borsanyi, Z. Fodor, C. Hoelbling, S. D. Katz, S. Krieg and K. K. Szabo, Phys. Lett. B **730** 99 (2014) [arXiv:1309.5258 [hep-lat]].

[2] A. Bazavov *et al.* [HotQCD Collaboration], Phys. Rev. D **90**, 094503 (2014) [arXiv:1407.6387 [hep-lat]].

[3] A. Bazavov, T. Bhattacharya, M. Cheng, C. DeTar, H. T. Ding, S. Gottlieb, R. Gupta and P. Hegde *et al.*, Phys. Rev. D **85** 054503 (2012) [arXiv:1111.1710 [hep-lat]].

[4] A. Majumder and B. Muller, Phys. Rev. Lett. **105**, 252002 (2010) [arXiv:1008.1747 [hep-ph]].

[5] A. Bazavov, H.-T. Ding, P. Hegde, O. Kaczmarek, F. Karsch, E. Laermann, Y. Maezawa and S. Mukherjee *et al.*, Phys. Rev. Lett. **113**, 072001 (2014) [arXiv:1404.6511 [hep-lat]].

[6] R. V. Gavai and S. Gupta, Phys. Rev. D **64** 074506 (2001) [hep-lat/0103013].

[7] C. R. Allton, S. Ejiri, S. J. Hands, O. Kaczmarek, F. Karsch, E. Laermann, C. Schmidt and L. Scorzato, Phys. Rev. D **66** 074507 (2002) [hep-lat/0204010].

[8] A. Bazavov *et al.*, [arXiv:1701.04325].

[9] E. Follana *et al.* [HPQCD and UKQCD Collaborations], Phys. Rev. D **75** 054502 (2007) [hep-lat/0610092].

[10] A. Bazavov *et al.* [HotQCD Collaboration], Phys. Rev. D **86** 034509 (2012) [arXiv:1203.0784 [hep-lat]].

[11] P. Hasenfratz and F. Karsch, Phys. Lett. **125B**, 308 (1983).

[12] R. V. Gavai and S. Sharma, Phys. Rev. D **85**, 054508 (2012) [arXiv:1112.5428 [hep-lat]].

[13] R. V. Gavai and S. Sharma, Phys. Lett. B **749**, 8 (2015) [arXiv:1406.0474 [hep-lat]].

[14] J. Gunther, R. Bellwied, S. Borsanyi, Z. Fodor, S. D. Katz, A. Pasztor and C. Ratti, [arXiv:1607.02493].