Thermodynamic Properties of Strongly Interacting Matter at Non-zero Baryon Number Density

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Abstract. We present recent lattice results on QCD thermodynamics at non-vanishing baryon number density obtained from a 6th order Taylor expansion in the chemical potential. Results for bulk thermodynamic observables, in particular for fluctuations in the baryon number density, are found to be well described by a hadron resonance gas model at low temperature and an ideal quark gluon gas at high temperature. We also analyze the radius of convergence of the Taylor series and discuss the information it provides on the occurrence of a second order phase transition point in the QCD phase diagram.

1. Introduction

Two quite different aspects of the studies of QCD thermodynamics on the lattice gained most attention in the heavy ion community during recent years – studies of the QCD phase diagram at non-zero baryon chemical potential and the analysis of the influence of a thermal heat bath on basic properties of hadrons, e.g. their masses and widths. Here we will concentrate on the former. For a recent discussion of in-medium properties of hadrons we refer to the proceedings of this years Quark Matter [1] and Lattice [2] conferences.

Lattice calculations at vanishing baryon chemical potential, \( \mu_B \), suggest that for physical values of the quark masses the transition to the high temperature phase of QCD is just a rapid crossover rather than a phase transition which would be signaled by singularities in bulk thermodynamic observables. On the other hand many QCD motivated model calculations suggest that for \( \mu_B > 0 \) and small values of the temperature the transition indeed is a first order phase transition. This suggests that somewhere in the interior of the phase diagram there exists a second order phase transition point (chiral critical point) as an end point of a line of first order transitions.

For vanishing light quark masses this point would be a tri-critical point \( \mathbf{3} \) which, with increasing value of the strange quark mass, is expected to move towards lower values of \( \mu_B \) and eventually could reach the \( \mu_B = 0 \) axis.

The expected generic phase diagram for physical values of the quark masses is shown in Fig. 1. Its exploration for large temperatures and small values of the baryon chemical potential became accessible to lattice calculations through the application of different techniques such as Ferrenberg-Swendsen reweighting [4], Taylor series expansions [5, 6] as well as through simulations with an imaginary chemical potential [7, 8]. This led to a first analysis of the baryonic contribution to bulk thermodynamic observables like the pressure, baryon number density and various susceptibilities.
Figure 1. Generic phase diagram of QCD with physically realized quark mass values (left). The occurrence of a second order endpoint in the interior of the phase diagram is expected to be a consequence of the existence of a regime of first order transitions in 3-flavor QCD at vanishing $\mu_B$ and for small values of the up, down and strange quark masses. The chiral critical point then lies on a hyper-surface of second order transition points emerging from the $\mu_B = 0$ plane (right).

Moreover, it provided first estimates for the location of the chiral critical point at which the transition to the high temperature phase of QCD turns from a rapid crossover into a first order phase transition; recent calculations suggest a critical value $\mu_{B}^{\text{crit}} \sim 400$ MeV. We will discuss these results in more detail in section 3. However, before turning to this it seems appropriate to briefly review results on the QCD transition at vanishing baryon chemical potential where we try to emphasize the role of the strange quark in QCD thermodynamics. We will do so in section 2. Section 4 is devoted to a comparison of lattice results on thermodynamics in the low temperature hadronic phase at $\mu_B > 0$ with a phenomenological approach in terms of a hadron resonance gas model. This has been discussed in more detail at this conference by K. Redlich.

2. The thermal QCD transition at vanishing baryon chemical potential

For $\mu_B = 0$ the transition from the low temperature hadronic phase to the high temperature phase has been analyzed in many numerical calculations. In particular, it has been found that for the case of QCD with three degenerate light quarks the transition is first order. In fact, the use of improved discretization schemes for the fermionic part of the QCD Lagrangian has shifted this regime to rather small values of the quark masses which correspond to a pion mass even below its physically realized value. This strongly suggests that the transition is continuous for the physically realized spectrum of two light ($u$, $d$)-quarks and a heavier $s$-quark. A second order phase transition can then only show up at non-vanishing chemical potential if the hyper-surface of 2\textsuperscript{nd}-order phase transition, in which also the line of 2\textsuperscript{nd}-order transitions found at $\mu_B = 0$ in the $(ud, s)$-plane lies, bends over the physical point. This situation is illustrated in Fig. (right). The left hand part of this figure shows the resulting phase diagram of QCD with the physically realized mass spectrum.
The light quark chiral condensate in QCD with 2 light up, down and a
heavier strange quark mass (open symbols) and in 3-flavor QCD with degenerate
quark masses (full symbols) \[17\]. The right hand part of the figure shows the
pressure calculated in QCD with different number of flavors as well as in a pure
gauge theory \[18\]. Note that (2+1)-flavor QCD here refers to QCD with two light
quarks and a heavier (strange) quark with a mass proportional to the temperature,
\(m_s \sim T\).

This suggests that at least at \(\mu_B = 0\) the strange quark has little influence
on the dynamics of the transition. The calculations performed with improved actions
\[17\] indicate that for the physically realized quark mass spectrum the transition
to the high temperature phase is signaled by a rapid but continuous change in bulk
thermodynamic observables. The transition temperature of (2+1)-flavor QCD found
in a recent analysis with the Naik action \[17\]^

\[1\]


\[T_c = (172 \pm 11 \pm 7) \text{ MeV}, \]

is consistent with earlier findings for 2-flavor QCD based on simulations with the
p4-action, \(T_c = (173 \pm 8 \pm \text{ sys. err.}) \text{ MeV} \[18\].

\[\parallel\] In the calculation of the pressure in (2+1)-flavor QCD shown in Fig.2 the strange quark mass has
been taken to be proportional to the temperature, i.e. \(m_s / T = \text{const}\). If one keeps instead \(m_s\) fixed
to its physical value the pressure will gradually approach the high temperature limit of 3-flavor QCD.
This can be inferred, for instance, from the calculation performed in \[22\].

\[\parallel\parallel\] Here we have averaged over the two fits performed in \[17\] to extrapolate to the chiral limit and
included systematic uncertainties arising from these different fits in the systematic error.
3. Taylor expansion of the pressure at non-zero baryon chemical potential

As mentioned in the introduction different approaches have been followed to study the phase structure of QCD at non-vanishing baryon chemical potential and to determine basic thermodynamic observables. All these approaches are currently limited to the regime of large temperatures and $\mu_q/T \lesssim 1$, where $\mu_q = \mu_B/3$ is the quark chemical potential. We will concentrate here on a discussion of Taylor expansions of the partition function of 2-flavor QCD around $\mu_B = 0$.

At fixed temperature and small values of the chemical potential the pressure may be expanded in a Taylor series around $\mu_q = 0$,

$$\frac{p}{T^4} = \frac{1}{VT^3} \ln Z = \sum_{n=0}^{\infty} c_n(T) \left( \frac{\mu_q}{T} \right)^n,$$

where the expansion coefficients are given in terms of derivatives of $\ln Z(V, T, \mu_q)$, i.e. $c_n(T) = \frac{1}{n!} \partial^n \ln Z \left( \frac{\mu_q}{T} \right)^n$. The series is even in $(\mu_q/T)$ which reflects the invariance of $Z(V, T, \mu_q)$ under exchange of particles and anti-particles. The first coefficient, $c_0$, simply gives the pressure at $\mu_q = 0$ shown in Fig. 2(right). The next non-zero coefficient, $c_2$, is proportional to the quark number susceptibility at $\mu_q = 0$ [21],

$$\chi_q T^2 = \left( \frac{\partial^2 p}{\partial (\mu_q/T)^2} \right) = 2c_2 + 12c_4 \left( \frac{\mu_q}{T} \right)^2 + \mathcal{O} \left( (\mu_q/T)^4 \right).$$

Its rise with temperature has been attributed to changes in the interaction among quarks and anti-quarks in the vector channel [22]. Further Taylor expansion coefficients entering the calculation of the pressure have been analyzed now up to $\mathcal{O}(\mu_q^6)$ [10, 23, 24]. The coefficients for $n = 2, 4$ and 6 are shown in Fig. 3.

In the high temperature, ideal gas limit, only the first three expansion coefficients are non-zero, $c_0(T = \infty) = 7n_f \pi^2/60$, $c_2(T = \infty) = n_f/2$ and $c_4(T = \infty) = n_f/4\pi^2$. As can be seen in Fig. 3 at $T \approx 2T_0$ all coefficients reach their corresponding ideal gas values within $\sim 20\%$.

The next-to-leading order coefficient, $c_4$, is strictly positive and develops a pronounced peak at the $\mu_q = 0$ transition temperature, $T_0$, which in turn, also leads to a large peak in the quark number susceptibility once $\mu_q/T \gtrsim 0.5$ [10] (see
Fig. 5(right)). This has been interpreted as an indication for an approach to the chiral critical point at which $\chi_q$ is expected to diverge$^+$. A new feature shows up in the expansion coefficients at $O(\mu^6)$. The coefficient $c_6$ is positive only below $T_0$ and changes sign in its vicinity. This has important consequences for the analytic structure of the QCD partition function and gives first hints at the convergence properties of the Taylor series: If there exists a 2nd order phase transition point in the QCD phase diagram this would be related to a Lee-Yang zero of the QCD partition function for some real and positive value of $(\mu_q/T)^2$. This critical value will be directly related to the radius of convergence, $\rho(T)$, of the Taylor expansion, if the partition function has no further zeroes in the complex $(\mu_q/T)$-plane closer to the origin. A sufficient condition for the radius of convergence to be due to a zero on the real $(\mu_q/T)$-axis is that all expansion coefficients in the Taylor series are positive. This apparently is the case for all $c_n(T)$ analyzed so far at $T < \sim 0.95 T_0$.

Ratios of subsequent expansion coefficients provide an estimate for the radius of convergence of the Taylor series,

$$\rho(T) = \lim_{n \to \infty} \rho_n \equiv \lim_{n \to \infty} \sqrt{\frac{c_n}{c_{n+2}}} .$$

These ratios are shown in Fig. 4(left). While the first ratio, $c_4/c_2$ is well determine in current lattice calculations the ratio $c_6/c_4$ still has large errors. It is, however, apparent that these ratios change drastically across $T_0$ and seem to be approximately temperature independent in the low temperature phase. As we will discuss in the next section this is expected to be the case also for a non-interacting resonance gas which has an infinite radius of convergence. At present, however, the large errors on $\rho_n(T)$ prohibit to draw a firm conclusion on the asymptotic behavior of $\rho(T)$.

Similar caution is requested when interpreting the large fluctuations in the quark number densities signaled by the rapid rise of the quark number susceptibility (see Fig. 5). As mentioned above we expect $\chi_q$ to diverge at a 2nd order transition point. The rapid increase of $\chi_q$ is, however, partly due to the rapid rise of $n_q$ itself as well as due to the rapid increase in the pressure for $T \sim T_0$. A quantity reflecting the relative magnitude of fluctuations is given by the ratio,

$$\frac{\Delta p}{T^2\chi_q} = \frac{1}{2} \left( \frac{\mu_q}{T} \right)^2 \frac{1 + \frac{c_4}{c_2} \left( \frac{\mu_q}{T} \right)^2 + \frac{c_6}{c_2} \left( \frac{\mu_q}{T} \right)^4}{1 + 6 \frac{c_4}{c_2} \left( \frac{\mu_q}{T} \right)^2 + 15 \frac{c_6}{c_2} \left( \frac{\mu_q}{T} \right)^4} .$$

This quantity only depends on ratios of Taylor expansion coefficients, and should vanish at a 2nd order phase transition point. Its temperature dependence is shown in Fig. 4(right). As can be seen the ratio rises rapidly across $T_0$ and approaches the ideal gas value. It, however, does not show any sign for a drop in the vicinity of $T_0$ that could be taken as evidence for the existence of a second order transition.

4. Resonance gas versus lattice results

Aside from the obviously rapid change of bulk thermodynamic observables at temperatures close to $T_0$ it is a striking feature of the Taylor expansion that ratios of the expansion coefficients are, to a first approximation, temperature independent$^+$. Fluctuations in the net quark number density are related to the isothermal compressibility,

$$\kappa_T = -V^{-1} \left( \frac{\partial V}{\partial \rho} \right)_{T,N_q} = -N_q^{-1} \left( \frac{\partial V}{\partial \rho_q} \right)_{T,N_q} = \chi_q/n_q^2 ,$$

which diverges at a 2nd order transition point.
below $T_0$ and distinctively different from the ratios above $T_0$. While for $T > T_0$ the ratios rapidly approach the corresponding ideal gas values their low temperature behavior can be understood in terms of the properties of a hadronic resonance gas. For $T \lesssim T_0$ the baryonic contribution to the pressure arises entirely from hadrons, which have masses significantly larger than the relevant temperatures, i.e. $m_{\text{baryon}} \geq m_P \gtrsim 5T_0$. Their contribution may be approximated by a non-interacting resonance gas obeying Boltzmann statistics. The pressure is then given by,

$$\left(\frac{\Delta p}{T^4}\right)_{\text{res. gas}} \equiv f_B(T) (\cosh(\mu_B/T) - 1) ,$$

where $f_B(T)$ contains all the information on the resonance mass spectrum. Within this approximation the ratio of Taylor expansion coefficients is given by $(c_{n+2}/c_n)_{\text{res. gas}} = 9/((n + 2)(n + 1))$ and thus is indeed temperature independent. Moreover, the ratios are not affected by details of the hadronic mass spectrum and, in particular, are not affected by the quark mass dependence of the hadron spectrum. A straightforward comparison with lattice calculations which generally are performed at unphysically large quark mass values thus is justified. Similarly, the ratio $\Delta p/T^2\chi_q = (1 - 1/\cosh(3\mu_q/T))/9$ is independent of the resonance spectrum $f_B(T)$ and does not vary with temperature for fixed $\mu_B/T$. These estimates are shown as straight lines in Fig. 4 for temperatures below $T_0$. Of course, the simple form of the $\mu_B$-dependence in the resonance gas, Eq. does not lead to any critical behavior in its own. At all temperatures the quark number susceptibility will rise with increasing $\mu_q/T$ and for fixed $\mu_q/T$ it rapidly rises with temperature. Moreover, as in the resonance gas model the dependence of e.g. the pressure on $\mu_q/T$ only appears through the factor $\cosh(3\mu_q/T)$ the radius of convergence of a Taylor expansion, of course, is infinite. i.e. $\lim_{n \to \infty} (c_{n+2}/c_n)_{\text{res. gas}} = 0$. Any unambiguous evidence for the existence of a chiral critical point in the QCD phase diagram thus should also show up as clear deviation from resonance gas behavior.

A direct comparison of resonance gas model calculations for thermodynamic observables like the pressure or susceptibility with lattice calculations is somewhat less...
Figure 5. Comparison of the resonance gas model prediction for the temperature dependence of the coefficient $c_2(T)$ with lattice results (left) and the resulting dependence of $\chi_q/T^2$ on temperature (right) for various values of the chemical potential. Shown are results from Ref. [25] where the resonance gas is compared to lattice calculations up to $O(\mu^4)$ only. The different curves shown in the left hand figure correspond to $A = 0.9, 1.0, 1.1$ and 1.2 (top to bottom).

stringent as it is necessary to adjust the resonance spectrum to the still unphysical conditions that, at present, could be realized on the lattice. The Taylor series discussed in section 3 is based on lattice calculations performed with quark masses that correspond to a pseudo-scalar (pion) mass of about 770 MeV. In this case the mass of the lightest baryonic state is about twice as large as the experimental value for the nucleon mass. This quark mass dependence of the baryon spectrum, $m_H(m_{PS})$, has been modeled using the ansatz $m_H(m_{PS})/m_H = 1 + A(m_{PS}/m_H)^2$ [25], where $m_H$ is the experimental value of baryon resonances and $m_{PS}$ is the pseudo-scalar meson mass used in the lattice calculations. A comparison with the first expansion coefficient which only depends on the baryonic part of the spectrum*, $c_2(T) = 9f_B(T)/2$, shows that the temperature dependence for $T \lesssim T_0$ is well reproduced with $A \approx 1$. With this also the temperature dependence of the quark number susceptibility is well described by the resonance gas in the low temperature phase (see Fig. 5). This comparison can be extended to the meson sector contributing to $p/T^4$ at $\mu_B = 0$ or to other quantum number channels controlled by other combinations of the quark chemical potentials, for instance the iso-vector channel with $\mu_I \equiv \mu_u - \mu_d$. Also in these cases lattice results for thermodynamic observables at low temperature are well described by a hadronic resonance gas model [15].

5. Conclusions

We have shown that the thermodynamics of QCD at small values of the baryon chemical potential can well be studied in terms of a Taylor expansion of the logarithm of the QCD partition function. In fact, a 6th order expansion seems to

* The leading term, $c_0(T)$, receives contributions from the mesonic as well as the baryonic part of the spectrum.
be quite sufficient for a reliable determination of the change in pressure as well as a
determination of the temperature dependence of the net baryon number density for
\( \mu_B \lesssim 3T \). The good agreement between lattice results in the low temperature hadronic
phase and resonance gas models is on the one hand conceptually appealing as the
resonance gas model has also been so successful in the description of experimental
data on observed particle ratios in heavy ion collisions. On the other hand it
shows that higher order calculations with high accuracy and/or calculations at smaller
quark masses are needed in order to find deviations from resonance gas behavior and to
deduce evidence for the existence of a chiral critical point in the QCD phase diagram.

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