Thermodynamics of 2 and 3 flavour QCD

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Abstract. We will discuss recent results on the thermodynamics of QCD in the presence of light dynamical quark degrees of freedom. In particular, we will concentrate on an analysis of the flavour and quark mass dependence of the QCD phase diagram, the equation of state and the transition temperature. Moreover, we present recent results on the heavy quark free energy.

INTRODUCTION

Lattice calculations have provided a rather detailed picture of the thermodynamics of gluonic matter. We know that a phase transition exists, which separates a confining low temperature phase (glueball gas) from a deconfined gluon gas phase at high temperature. The transition between these two phases is first order, as originally predicted by Svetitsky and Yaffe [1]. Although the low temperature phase only consists of rather heavy glueballs, the lightest of which has a mass of about 1.8 GeV [2], the phase transition temperature turns out to be rather small, $T_c \approx 0.637(5) \sqrt{\sigma} \simeq 270$ MeV. This suggests that $T_c$ does not sensitively depend on the mass of the lightest excitations in the confining phase. In fact, it agrees quite well with values extracted from resonance gas models based on the excitation spectrum of a gluonic string [3]. Bulk thermodynamic observables like the energy density and pressure change rapidly at $T_c$ and asymptotically approach the ideal gas limit. Their rapid rise signals the liberation of many new light degrees of freedom at $T_c$. However, even at temperatures a few times $T_c$ one still observes significant deviations from the asymptotic ideal gas behaviour. This suggests that also in the high temperature phase non-perturbative effects play an important role, which give rise to large screening masses and quasi-particle excitations.

Gluonic matter is described by an $SU(3)$ gauge theory, which is obtained as the infinite quark mass limit of QCD. In this limit the entire fermionic sector of QCD decouples and does not contribute to the thermodynamics; quarks only serve as static sources (quenched QCD). This allows, for instance, a study of thermal modifications (screening) of the forces between external charges, which shows that the linear confining potential weakens with increasing temperature; the string tension decreases and vanishes at $T_c$.

Some of these basic aspects of gluonic thermodynamics clearly will change drastically in the presence of light dynamical quark degrees of freedom. The asymptotic high temperature limit for bulk thermodynamic observables like the energy density or pressure rises with increasing number of light degrees of freedom. Absolute confinement is lost in the presence of quarks with finite mass already at low temperatures; the heavy quark free energy will no longer diverge when one tries to separate a static quark anti-quark pair. Moreover, the order of the QCD phase transition and even its very existence
will crucially depend on the number of light degrees of freedom and their masses.

During recent years these basic qualitative changes in the thermodynamics of QCD, which result from the presence of light quark degrees of freedom, have been observed in lattice calculations [4, 5]. We will discuss here the current status of their quantitative analysis. This will make clear that unlike in the quenched sector of QCD we did not yet reach a similarly detailed quantitative understanding of the relevant parameters that control the critical behaviour of QCD with a realistic spectrum of quark masses. However, thermodynamic calculations on the lattice steadily improve. This partly is due to the rapid development of computer technology. However equally important has been and still is the development of improved discretization schemes, i.e. improved actions. This is of particular relevance for thermodynamic calculations which are not only sensitive to the long distance physics at the phase transition but also probe properties at short distances in calculations of e.g. the energy density or the heavy quark potential [6].

In the following we will discuss some recent results on the flavour and quark mass dependence of QCD thermodynamics. We will not go into any details on the lattice formulation of QCD at finite temperature, which have been discussed elsewhere [7].

**THE QCD PHASE DIAGRAM**

The quark mass and flavour dependence of the QCD phase transition at finite temperature and vanishing baryon number density has been studied extensively in lattice calculations. The basic qualitative and quantitative features expected from universality arguments [1, 8] on the one hand and phenomenological considerations on the other hand have been reproduced by these calculations. The transition is found to be first order in the limit of infinitely heavy quarks as well as in the chiral limit of 3-flavour QCD. In the case of 2-flavour QCD the transition is found to be continuous. The current status of the analysis of universal properties in the chiral limit, however, is not really satisfying [9]. The demonstration that for 2-flavour QCD the transition belongs to the universality class of 3-d, O(4) symmetric spin models still is ambiguous.

The regions of first order transitions are separated from a broad crossover region by lines of second order phase transitions. These lines are expected to belong to the universality class of the 3-d Ising model [10], which is quite remarkable as the global $Z(2)$ symmetry which gets restored at these transitions is not a symmetry of the QCD Lagrangian. This makes it obvious that the bare couplings appearing in the QCD Lagrangian cannot be the relevant scaling fields that control the critical behaviour at these lines of second order transitions. It therefore also is not obvious a priori what is the correct order parameter for these transitions. The energy-like and magnetization-like operators of the effective Hamiltonian that controls the critical behaviour at this critical point will be linear combinations of the basic fields appearing in the QCD Lagrangian and the relevant temperature-like and ordering-field like couplings will be linear combinations of the bare parameters of the QCD Lagrangian, i.e. the gauge coupling $\beta \equiv 6/g^2$ and the quark masses $m_q$.

Understanding the critical behaviour and the relevant scaling fields in the vicinity of the chiral critical line at small values of the quark masses is, of course, interesting
in its own rights. However, it eventually will also be of importance for a discussion of the physics in the vicinity of the critical endpoint which is expected to exist in the temperature-density phase diagram [11]. In an extended phase diagram, which also includes the dependence on the chemical potential, these critical points lie in the same critical surface of second order transitions.

The critical point separating the first order from the crossover region has recently been studied in some detail for the case of three degenerate quark mass flavours [12]. Through an analysis of cumulants of the chiral condensate, \( \langle \bar{\psi} \psi \rangle \), as well as joint probability distributions for the chiral condensate and the gluonic part of the QCD action it could be shown that the transition indeed belongs to the universality class of the 3-d Ising model and that the corresponding order parameter can be constructed as a linear combination of the chiral condensate and the gluonic action. In Figure 1 we show the result of a calculation of the fourth cumulant of the chiral condensate (Binder cumulant),

\[
B_4 = \frac{\langle (\bar{\psi} \psi)^4 \rangle}{\langle (\bar{\psi} \psi)^2 \rangle^2}.
\]  

The cumulant has been calculated for different values of the quark mass at the pseudo-critical couplings. Up to finite volume corrections the cumulants obtained on different size lattices will cross at the critical quark mass corresponding to the second order phase transition point. The value of \( B_4 \) at this point is universal and unambiguously identifies the transition as an Ising-like transition.

In order to judge whether QCD with a realistic spectrum of light u,d quarks and a heavier strange quark lies in the first order or crossover region of the phase diagram it is necessary to determine the location of the critical line quantitatively. The calculations performed so far with 3 degenerate quark masses and different fermion actions [12] show that the critical mass parameter, e.g. the value of the pseudo-scalar meson mass at the
chiral critical point, is rather sensitive to cut-off effects. While the calculation performed with the standard staggered fermion action led to a critical value \( m_{ps} \approx 300 \text{ MeV} \), calculations with an improved staggered fermion action gave \( m_{ps} \approx 200 \text{ MeV} \). These calculations thus need further confirmation through studies closer to the continuum limit. Nonetheless, the current estimates consistently yield rather small values for the pseudo-scalar meson mass at the critical endpoint in 3-flavour QCD, which makes it quite unlikely that the physical point in the phase diagram, corresponding to a realistic quark mass spectrum with two light u,d, and a heavier strange quark, would lie in the first order region. This would also be in agreement with an earlier estimate of the Columbia group [13].

Our current understanding of the QCD phase diagram of 3-flavour QCD at vanishing baryon number density is summarized in Figure 2.

**3-flavour phase diagram**

\[ T_{\chi}^m \sim 175 \text{ MeV} \quad \text{N}_f = 2 \quad \text{Pure} \]

\[ T_{d} \sim 270 \text{ MeV} \]

\[ m_{PS}^{\text{crit}} \approx 2.5 \text{ GeV} \]

\[ T_{\chi}^m = 3 \sim 155 \text{ MeV} \]

\[ m_{u, d}, m_{s} \]

**FIGURE 2.** The QCD phase diagram of 3-flavour QCD with degenerate (u,d)-quark masses and a strange quark mass \( m_{s} \).

### THE TRANSITION TEMPERATURE

It should be clear from the previous discussion of the phase diagram that for a large range of quark masses the transition to the high temperature plasma phase is not a phase transition, i.e. the transition does not correspond to singularities in the QCD partition function. Nonetheless, also for these quark masses the transition occurs in a narrow temperature interval and thus is well localized. This transition region is characterized by peaks in susceptibilities, e.g. the chiral susceptibility \( \chi_m \) or the Polyakov-loop susceptibility \( \chi_L \),

\[
\chi_m = \frac{\partial}{\partial m_q} \langle \bar{\psi} \psi \rangle \quad , \quad \chi_L = N_{f}^{3} \left( \langle L^2 \rangle - \langle L \rangle^2 \right) \quad .
\]  

(2)
Here

\[ L = \frac{1}{N^3_\sigma} \sum_{\vec{x}} \text{Tr} \, L_{\vec{x}} \]  

(3)

denotes the spatial average over Polyakov-loops\(^1\), \(L_{\vec{x}}\), defined at the spatial sites \(\vec{x}\) of a lattice of size \(N^3_\sigma \times N_\tau\). A calculation of the pseudo-critical temperature, \(T_c = 1/N_\tau \, a(\beta_{pc})\) still requires the determination of the lattice spacing \(a(\beta_{pc})\) at the pseudo-critical couplings \(\beta_{pc}\) which in turn are defined through the location of the susceptibility peaks. The lattice spacing can be determined through the calculation of an independent physical observable. In order to quote \(T_c\) in physical units, i.e. MeV, we need a physical observable which does not crucially depend on the values of the quark masses. For physical values of the quark masses it would, of course, be most appropriate to use a hadron mass, e.g. the rho-meson mass, to set the physical scale for \(T_c\). The hadron masses, however, are themselves strongly dependent on the quark mass values; their masses diverge in the infinite quark mass limit. Nonetheless, we can assign a physical value to the transition temperature in this limit. In quenched QCD the natural scale for \(T_c\) is the square root of the string tension, \(\sqrt{\sigma}\). In fact, the string tension as well as quenched hadron masses\(^2\) seem to describe the experimentally known QCD spectrum reasonably well already in the infinite quark mass limit. These quantities thus seem to have a weak quark mass dependence and are suitable to set the scale for \(T_c\) at arbitrary values of \(m_q\). This situation is illustrated in Figure 3.

On the left hand side of Figure 3 we show the transition temperature in units of the vector meson mass \(m_V\) versus the ratio \(m_{ps}/m_V\), which in the chiral limit is proportional to the square root of the quark mass. Here the drop in \(T_c/m_V\) observed with increasing quark mass mainly is due to the quark mass dependence of \(m_V\) and does not reflect the quark mass dependence of \(T_c\). This figure shows, however, that calculations based on different discretization schemes for the gauge and fermion actions do yield consistent results for \(T_c\) and its dependence on \(m_q\). In the chiral limit one finds for the critical temperature in 2 and 3-flavour QCD

\[
\begin{align*}
\text{2-flavour QCD} : & \quad T_c = \begin{cases} 
(171 \pm 4) \text{ MeV}, & \text{clover-improved Wilson fermions [14]} \\
(173 \pm 8) \text{ MeV}, & \text{improved staggered fermions [15]}
\end{cases} \\
\text{3-flavour QCD} : & \quad T_c = (154 \pm 8) \text{ MeV}, \text{ improved staggered fermions [15]}
\end{align*}
\]

Here \(m_\rho\) has been used to set the scale for \(T_c\). We note that all the results presented in Figure 3 have been obtained on lattices with a rather small temporal extent \((N_\tau = 4)\). The lattice spacing is therefore still quite large in the vicinity of \(T_c\), i.e. \(a \simeq 0.3 \text{ fm}\). Moreover,

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\(^1\) The Polyakov-loop is a purely time-like Wilson loop which is closed due to the periodicity of the lattice in temporal direction. Its definition as well as further details on the lattice formulation of QCD thermodynamics may, for instance, be found in [7].

\(^2\) In the calculation of quenched hadron masses the contribution of dynamical light sea quarks is suppressed. Only the valence quark contributions and interactions with the gluonic vacuum are taken into account.
FIGURE 3. Transition temperatures in units of $m_V$ (left) and in units of $\sqrt{\sigma}$ (right). The left hand figure shows results for 2-flavour QCD obtained with different gauge and fermion actions. The right hand figure shows the transition temperature in 2 (filled squares) and 3 (circles) flavour QCD obtained with improved staggered fermions (p4-action). Also shown are results for 2-flavour QCD obtained with the standard staggered fermion action (triangles). The dashed band indicates the uncertainty on $T_c/\sqrt{\sigma}$ in the quenched limit. The straight line is the fit given in Eq. 4. The vertical lines correspond to physical values of the hadron masses and a string tension of 425 MeV.

there are uncertainties involved in the ansatz used to extrapolate to the chiral limit. We estimate that the systematic error on the value of $T_c/m_\rho$ still is of similar magnitude as the purely statistical error quoted above. The critical temperature thus is at present only known with an error of about 10%.

On the right hand side of Figure 3 we give $T_c$ in units of $\sqrt{\sigma}$. This reflects the expected behaviour; with increasing values of the quark mass the hadrons become heavier and it becomes more difficult to create a dense hadronic system that could undergo a transition to a quark-gluon plasma phase; the transition temperature thus increases. It is, however, striking that the quark mass dependence of $T_c$ is so weak. The straight line shown in Figure 3 is a fit to the 3-flavour data, which gave

$$(T_c/\sqrt{\sigma})_x = (T_c/\sqrt{\sigma})_0 + 0.04(1) \, x \quad \text{with} \quad x = m_{ps}/\sqrt{\sigma}$$

This suggests that also heavier resonances, which are little affected by changes of the quark mass, play an important role for building up the critical density needed to trigger the QCD phase transition. Moreover, we note that for pseudo-scalar masses larger than about $6\sqrt{\sigma} \simeq 2.5$ GeV the transition temperature agrees with the value found in the pure gauge theory, $T_c \simeq 0.637\sqrt{\sigma} \simeq 270$ MeV. In this heavy quark mass regime all the hadronic states are heavier than typical glueball masses and thus decouple from the thermodynamics, which only is controlled by gluonic degrees of freedom. In this heavy mass regime the transition also changes again from a crossover to a first order phase transition.
THE QCD EQUATION OF STATE

The temperature dependence of bulk thermodynamic observables like the energy density ($\varepsilon$) and pressure ($p$) has been analyzed in detail in the pure gauge sector. These calculations show that $\varepsilon/T^4$ as well as $p/T^4$ rapidly increase above $T_c$. However, even at $T \simeq 4 T_c$ the Stefan-Boltzmann limit is not yet reached [16]. Deviations stay at the level of 15%, which is too much to be understood in terms of perturbative corrections [17]. Even at these high temperatures non-perturbative effects seem to play an important role for the thermodynamics. This finds further support from studies of the heavy quark free energy [18], the spatial string tension [19] as well as the gluon propagator in fixed gauges [20]. The analysis of the temperature dependence of these observables also suggests that the temperature dependent running coupling constant remains large in the plasma phase and electric and magnetic screening masses differ significantly from perturbative results even at temperatures which are several orders of magnitude larger than $T_c$ [21]. In view of this it may even be surprising that models with weakly interacting quasi-particles [22] as well as calculations based on self-consistent resummation schemes [23] do provide a quite satisfactory description of bulk thermodynamics down to temperatures a few times $T_c$.

At least at high temperature, where the energy density and pressure are expected to approach the free gas limit, the QCD equation of state will strongly depend on the number of light partonic degrees of freedom. Already for two massless quark flavours the Stefan-Boltzmann constant increases by more than a factor two relative to the pure gauge theory. For $n_f$-flavour QCD one has,

$$\frac{\varepsilon_{SB}}{T^4} = \frac{3p_{SB}}{T^4} = \left(16 + \frac{21}{2} n_f\right) \frac{\pi^2}{30} .$$

As the influence of non-zero quark masses on bulk thermodynamic observables will be exponentially suppressed at high temperature, Eq. 5 also gives the dominant high temperature behaviour for massive quark even when the masses are of the order of the (critical) temperature. In fact, this has been observed in lattice calculations with fairly large quark masses [24].

The overall pattern of the temperature dependence of bulk thermodynamic observables in QCD with 2 and 3 light quark flavours is very similar to the case of the pure gauge theory. With increasing number of light degrees of freedom the critical temperature shifts to smaller values and the asymptotic high temperature limit for $p/T^4$ becomes larger. This is seen in the left hand part of Figure 4. However, after rescaling the thermodynamic observables with the corresponding Stefan-Boltzmann constants they look quite alike in units of $T/T_c$. Of course, they still differ in details. In particular, it is apparent from the right hand part of Figure 4 that at $T_c$ the rescaled pressure of QCD with light quarks is significantly larger than in the pure gauge theory. This also is the case for the energy density which is found to be $\varepsilon_c/T^4_c \simeq 6$ in QCD with light quarks [24, 25], while it is only $\varepsilon_c/T^4_c \simeq 1$ in the SU(3) gauge theory$^3$. Much of this factor 6 difference in $\varepsilon_c/T^4_c$ is due to the pressure, while the energy density is discontinuous in the case of the pure gauge theory. The latent heat is found to be $\Delta \varepsilon / T^4_c = 1.40(9)$ [26] with $\varepsilon / T^4_c \simeq 2$ in the high temperature phase.

$^3$ The energy density is discontinuous in the case of the pure gauge theory. The latent heat is found to be $\Delta \varepsilon / T^4_c = 1.40(9)$ [26] with $\varepsilon / T^4_c \simeq 2$ in the high temperature phase.
\( \varepsilon_c / T_c^4 \), however, seems to arise from the difference in \( T_c \) between QCD with light quarks and the purely gluonic theory. The critical energy densities turn out to be quite similar. Unfortunately, the current error on \( T_c \), which is about 10\%, amplifies in the calculation of the energy density, which makes \( \varepsilon_c \) still badly determined in lattice calculations,

\[ \varepsilon_c = (0.3 - 1.3) \text{ GeV/fm}^3. \tag{6} \]

**THE HEAVY QUARK FREE ENERGY**

The confining properties of the thermal heat bath generated by quarks and gluons can be probed by analyzing the response of the medium to the insertion of static sources. Static quark sources are described by the Polyakov-loop \( L_\vec{x} \). In the pure gauge limit the expectation value of its spatial average, \( \langle L \rangle \) (Eq. 3), is an order parameter for the deconfinement transition,

\[ \langle L \rangle \begin{cases} = 0, & T < T_c \\ > 0, & T > T_c \end{cases}. \tag{7} \]

This reflects the long distance behaviour of the correlation function for static quark anti-quark sources,

\[ e^{-F(r,T)/T} = \langle \text{Tr}L_0 \text{Tr}L_\vec{x}^\dagger \rangle, \quad r \equiv |\vec{x}|, \tag{8} \]

which approaches the cluster value \( |\langle L \rangle|^2 \) in the limit of infinite separation between the quark anti-quark pair. In the confined phase this correlation function vanishes for \( r \to \infty \) which signals that the free energy needed to separate the two sources is infinite. This is no longer the case if dynamical quarks with a finite mass are contributing to the thermal heat bath. The static sources can then be screened by quarks and anti-quarks present in the heat bath and even in the zero temperature limit this becomes possible through the generation of \( q\bar{q} \)-pairs from the vacuum. The free energy needed to separate the static sources thus will stay finite at all temperatures.
In Figure 5 we show the free energy of a static quark anti-quark pair calculated in 3-flavour QCD at various temperatures and for different separation of the static sources. At low temperatures, \( T \leq 0.7 \, T_c \), the heavy quark free energy coincides with the confining Cornell-type potential, \( V(r) = -\alpha / r + \sigma r \) with \( \alpha = 0.25 \pm 0.05 \), up to distances \( r \approx 1.5/\sqrt{\sigma} \approx 0.7 \) fm. With increasing temperature \( F(r,T) \), however, gets screened earlier and at \( T_c \) it starts to deviate from the zero temperature potential already at distances \( r \approx 0.3 \) fm. Moreover, it becomes much easier to separate the heavy quark sources. As an estimate for the dissociation energy we show in the right hand part of Figure 5 the difference in free energy of a \( q\bar{q} \)-pair at infinite separation and a \( q\bar{q} \)-pair at distance \( r_q = \sqrt{\alpha/\sigma} \),

\[
\Delta F \equiv \lim_{r \to \infty} F(r,T) - F(\sqrt{\alpha/\sigma}) .
\]  

The rapid decrease of \( \Delta F \) close to \( T_c \) clearly will have consequences for the formation and existence of heavy quark bound states not only in the high temperature phase but also in the vicinity of \( T_c \). Already at \( T \approx 0.9 \, T_c \) the free energy difference for a heavy quark pair separated by a distance similar to the \( J/\psi \) radius (\( r_{\psi} \approx 0.2 \) fm) and a \( q\bar{q} \)-pair at infinite separation is only 500 MeV, which is compatible with the average thermal energy of a gluon (\( \sim 3 \, T_c \)). The \( c\bar{c} \)-bound states are thus expected to dissolve already close to \( T_c \), maybe even below \( T_c \) [27].

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