Thermodynamics of Four-Flavour QCD with Improved Staggered Fermions

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ABSTRACT

We have calculated the pressure and energy density in four-flavour QCD using improved fermion and gauge actions. We observe a strong reduction of finite cut-off effects in the high temperature regime, similar to what has been noted before for the SU(3) gauge theory. Calculations have been performed on $16^3 \times 4$ and $16^4$ lattices for two values of the quark mass, $ma = 0.05$ and 0.1. A calculation of the string tension at zero temperature yields a critical temperature $T_c/\sqrt{\sigma} = 0.407 \pm 0.010$ for the smaller quark mass value.
1 Introduction

In the pure gauge sector of QCD improved actions have been shown to lead to a drastic reduction of systematic errors introduced by the non-zero lattice spacing \((\text{finite cut-off effects})\) in the calculation of thermodynamic observables \([1, 2, 3]\). This is particularly evident in the high temperature regime where analytic calculations in the infinite temperature, ideal gas limit show that deviations from the continuum result can be drastically reduced already with tree level improved Symanzik actions \([1]\). However, also close to \(T_c\) and even at \(T_c\) an improvement has been observed already with tree level improved actions \([3]\).

At non-zero temperature the finite cut-off effects become visible as a \(\text{finite size effect}\) because the lattice spacing in units of the temperature is given by the temporal extent, \(N_\tau\), of the lattice, \text{i.e.} \(aT = 1/N_\tau\). In the standard Wilson formulation of lattice QCD with staggered fermions these cut-off effects are known to be \(\mathcal{O}((aT)^2 \equiv 1/N_\tau^2)\). In the high temperature, ideal gas limit one finds, for instance, for the gluonic and fermionic contributions to the energy density of QCD with \(n_f\) massless flavours

\[
\frac{\epsilon^G}{T^4} = \frac{8\pi^2}{15} \left( 1 + \frac{30}{63} \frac{\pi^2}{N_\tau^2} + \mathcal{O}(N_\tau^{-4}) \right), \\
\frac{\epsilon^F}{T^4} = n_f \frac{21\pi^2}{60} \left( 1 + \frac{310}{147} \frac{\pi^2}{N_\tau^2} + \mathcal{O}(N_\tau^{-4}) \right). \tag{1}
\]

On lattices with small temporal extent these \(\mathcal{O}(N_\tau^{-2})\) corrections lead to large distortions of the continuum Stefan-Boltzmann limit \([4]\). In the staggered fermion formulation the deviations from the continuum ideal gas are as large as 77\% on a lattice with temporal extent \(N_\tau = 4\) and are still 20\% for \(N_\tau = 12\).

As the computational effort for calculating thermodynamic observables, which generally have dimension \(a^{-4}\), increases approximately like \(N_\tau^{10}\) it is highly desired to be able to extract continuum physics from results of simulations on lattices with small temporal extent. In addition the improvement of the fermion action rapidly becomes computationally very demanding. In the inversion of the fermion matrix the time per iteration is proportional to the number of non-zero entries in a given row of the fermion matrix, \text{i.e.} the number of neighbours to a given lattice site used to discretize the kinetic part of the Lagrangian. In particular in simulations with dynamical fermions this gives a very serious constraint and does, at present, make it impossible to use, for instance, a complicated fixed point action \([4]\). In this first exploratory study, which aims at an examination of the influence of an improved fermion sector on the behaviour of thermodynamic observables at high temperature, we therefore have chosen a straightforward improvement scheme for the free fermion sector. The minimal extension of the standard staggered fermion
discretization scheme which is capable to remove $O(a^2)$ errors in the free fermion action involves in addition to the standard one-link term an appropriately weighted, straight three-link term. This preserves all the symmetries of the staggered action and doubles the computational effort in the fermion sector.

In the next section we specify the improved action used here and discuss the cut-off dependence of thermodynamic observables in the infinite temperature, ideal gas limit. Section 3 is devoted to a discussion of the equation of state of four-flavour QCD. In section 4 we discuss a calculation of the critical temperature in units of the string tension. Finally we present our conclusions in section 5.

2 Improved actions

When formulating a discretized version of QCD one has a great deal of freedom in choosing a lattice action. Different formulations may differ by subleading powers of the lattice cut-off, which vanish in the continuum limit. This has, for instance, been used to systematically improve lattice regularized $SU(N)$ gauge theories following the Symanzik improvement programme. In addition to the elementary plaquette term appearing in the standard Wilson formulation of lattice QCD larger loops can be added to the action in such a way that the leading $O(a^2)$ deviations are eliminated from the free fermion action. In our previous studies of the pure gauge sector of QCD we have found that already the addition of a planar (1,2) loop to the standard Wilson action eliminates the main systematic errors in the high temperature limit and even at $T_c$ compares well with a non-perturbatively improved (tadpole) action and a fixed point action. We therefore use the tree-level improved (1,2)-Symanzik action for discretizing the pure gauge sector of QCD,

$$S^{(1,2)} = \sum_{x,\nu > \mu} \frac{5}{3} \left( 1 - \frac{1}{N} \text{Re} \ Tr \ \Box_{\mu\nu}(x) \right)$$

$$- \frac{1}{6} \left( 1 - \frac{1}{2N} \text{Re} \ Tr \ \left( \Box_{\mu\nu}(x) + \Box_{\mu\nu}(x) \right) \right).$$

In the fermion sector we use an improved action, $S^F = \bar{\psi} M \psi$, where a higher order difference scheme is used to eliminate the $O(a^2)$ errors in the discretization of the derivatives $\partial_{\mu}$ appearing in the free fermion action. A three-link term is added which preserves all the symmetries of the staggered action. Gauge fields are then introduced on the shortest path connecting the staggered fermion and anti-fermion.
fields. The improved fermion matrix thus reads

$$M[U]_{ij} = m \delta_{i,j} + \eta_i \left( \frac{9}{16} A[U]_{ij} - \frac{1}{48} B[U]_{ij} \right)$$

(3)

with \( \eta_i \) denoting the phase factors for staggered fermions and

$$A[U]_{ij} = \sum_\mu \left( U_{i,\mu} \delta_{i,j-\mu} - U_{i-\mu,\mu} \delta_{i,j+\mu} \right)$$

$$B[U]_{ij} = \sum_\mu \left( U_{i,\mu} U_{i+\mu,\mu} U_{i+2\mu,\mu} \delta_{i,j-3\mu} - U_{i-\mu,\mu} U_{i-2\mu,\mu} U_{i-3\mu,\mu} \delta_{i,j+3\mu} \right).$$

(4)

The entire action is given by

$$S^I[U] = \beta S^{(1,2)} + S^F_3.$$ 

The importance of improved actions for thermodynamic calculations becomes evident from an analysis of the high temperature ideal gas limit on lattices of size \( N_3^2 N_\tau \). One indeed finds a strong reduction of the cut-off dependence relative to the standard Wilson formulation. In order to quantify this we previously had calculated the energy density of a free gluon gas \([1]\) which shows explicitly that corrections to the continuum Stefan-Boltzmann law only start at \( O(N^{-4}_\tau) \). We give here the corresponding results for a free massless fermion gas using the improved fermion action for calculations on spatially infinite lattices with temporal extent \( N_\tau \),

$$\frac{\epsilon^F(N_\tau)}{T^4} = 3n_f N_\tau^4 \int_0^1 d^3\vec{p} \left[ N_\tau^{-1} \sum_{n_0=0}^{N_\tau-1} \frac{f^2((2n_0 + 1)\pi/N_\tau)}{\omega^2(2\pi\vec{p}) + 4f^2((2n_0 + 1)\pi/N_\tau)} \right.
\left. - \int_0^1 dp_0 \frac{f^2(2\pi p_0)}{\omega^2(2\pi\vec{p}) + 4f^2(2\pi p_0)} \right],$$

(5)

where \( n_0 = 0, 1, ..., N_\tau - 1 \) labels the discrete set of Matsubara modes, \( \omega^2(2\pi\vec{p}) = 4 \sum_{\mu=1}^3 f^2(p_\mu) \), and the function \( f(p) \) gives the momentum dependent terms in the free fermion propagator,

$$f(p) = \frac{9}{16} \sin(p) - \frac{1}{48} \sin(3p).$$

(6)

Results for the free gluon and fermion energy densities are given in Table \([1]\). We note that in the gluon sector the deviation from the continuum limit is below 3% already on \( N_\tau = 4 \) lattices while the fermion action still shows about 27% deviations on this size lattice. Still the cut-off dependence is drastically reduced compared to the standard staggered fermion formulation, which is given for comparison in the last column of Table \([1]\).
Table 1: The energy density of a free gluon ($\epsilon^G$) and a free fermion ($\epsilon^F$) gas on spatially infinite lattices with temporal extent $N_\tau$ relative to the corresponding values in the continuum, $\epsilon^G/T^4 = 8\pi^2/15$ and $\epsilon^F/T^4 = 7n_f\pi^2/20$. The last two columns give results for the energy density of four-flavour QCD in the infinite temperature limit relative to the corresponding continuum result, $\epsilon_{SB}/T^4 = (\epsilon^G + \epsilon^F)/T^4$.

| $N_\tau$ | $\epsilon^G(N_\tau)/\epsilon^G$ | $\epsilon^F(N_\tau)/\epsilon^F$ | $\epsilon(N_\tau)/\epsilon_{SB}$ |
|----------|-------------------------------|-------------------------------|-------------------------------|
| 4        | 0.986568                      | 1.269896                      | 1.191737                      |
| 6        | 0.997528                      | 1.005633                      | 1.003397                      |
| 8        | 1.000309                      | 0.963731                      | 0.978222                      |
| 10       | 1.000253                      | 0.986795                      | 0.990507                      |
| 12       | 1.000150                      | 0.996509                      | 0.997513                      |

3 QCD equation of state

We have analyzed the thermodynamics of four-flavour QCD using the improved action defined in Eq. 2. We have performed calculations on $16^3 \times 4$ and $16^4$ lattices with quark masses $m_\alpha = 0.05$ and 0.1 using the hybrid Monte Carlo algorithm. The inclusion of the contributions from the three-link terms to the equations of motion is straightforward. At each value of the gauge coupling, $\beta$, typically 1500 trajectories of length $\Delta t = 0.6$ have been analyzed on the finite temperature lattice and 500 trajectories on the zero temperature lattice.

The basic observables entering the calculation of thermodynamic quantities are the expectation values for the gauge action, $\langle S^{(1,2)} \rangle$, and the chiral condensate, $\langle \bar{\chi}\chi \rangle$, i.e. the derivatives of the partition function $Z = \int dU d\bar{\chi} d\chi \exp (-S^I)$ with respect to the gauge coupling and the quark mass, respectively. In particular we will need the differences between expectation values calculated on the finite temperature lattice ($16^3 \times 4$) and the zero temperature lattice ($16^4$),

$$\langle S^{(1,2)} \rangle = \langle S^{(1,2)} \rangle_0 - \langle S^{(1,2)} \rangle_T$$
$$\langle \bar{\chi}\chi \rangle = \langle \bar{\chi}\chi \rangle_0 - \langle \bar{\chi}\chi \rangle_T,$$

where the normalization of the expectation values in both cases has been defined per lattice site, i.e. $\langle S^{(1,2)} \rangle = -N_\sigma^{-3} N_\tau^{-1} \partial \ln Z/\partial \beta$ and $\langle \bar{\chi}\chi \rangle = N_\sigma^{-3} N_\tau^{-1} \partial \ln Z/\partial m_\alpha$. Our results for these differences are summarized in Figure 3 for both values of the quark mass. The curves shown in the Figure are spline interpolations, which have been used for the subsequent calculation of the pressure ($p$) and energy density ($\epsilon$).
Figure 1: Difference of expectation values of the gluonic action and chiral condensates calculated on $16^3 \times 4$ and $16^4$ lattices at two values of the quark mass, $m_\alpha = 0.05$ and 0.1.

Like in the pure gauge theory the pressure can be obtained from an integration of the difference of gluonic action densities $\langle S^{(1,2)} \rangle$ \[10\]

$$
\frac{p}{T^4} \bigg |_{\beta_0} = N^4_{\tau} \int_{\beta_0}^{\beta} d\beta' \langle S^{(1,2)} \rangle .
$$

The calculation of energy density involves in addition also the differences of the chiral condensates at zero and non-zero temperature. Furthermore one needs to know the cut-off dependence of the two bare couplings, $\beta$ and $m_\alpha$,

$$
\Delta \equiv \frac{\epsilon - 3p}{T^4} = -N^4_{\tau} \left[ R_\beta \langle S^{(1,2)} \rangle - R_m \langle \bar{\chi}\chi \rangle \right]
$$

with

$$
R_\beta = \frac{d\beta}{d \ln a} , \quad R_m = \frac{d m_\alpha}{d \ln a} . \tag{10}
$$
In the chiral limit the derivative $R_m$ vanishes and $(\epsilon - 3p)$ is again proportional only to the $\beta$-function, $R_{\beta}$, as it is the case in the pure gauge sector. The derivatives of the bare couplings $\beta$ and $ma$ with respect to the lattice cut-off can be obtained from the cut-off dependence of two physical observables. In general we may follow Ref. [12] and use two meson masses for this, $m_\pi$ and $m_\rho$. If we parametrize the quark mass dependence of these masses as

$$a^2 m^2_\pi = h(\beta)ma\ ,$$
$$am_\rho = f(\beta) + g(\beta)ma\ ,$$

we find for the derivatives

$$R_{\beta} = \frac{f}{f'} \left( 1 - \frac{ma\frac{h'}{h}}{1 + ma(\frac{2}{g} - \frac{h}{h'})\frac{f}{f'}} \right) = \frac{f}{f'} + \mathcal{O}(ma)\ ,$$
$$R_m = 2ma \left( 1 - \frac{h'}{2h} R_{\beta} \right) .$$

Here the prime denotes derivatives with respect to $\beta$. In the asymptotic scaling regime the ratios $f/f'$ as well as $h/h'$ will be given by the leading term in the QCD renormalization group equation, i.e. $f/f' = h/h' = -25/4\pi^2$. The second derivative thus becomes asymptotically $R_m = ma + \mathcal{O}((ma)^2)$. We find strong deviations from these asymptotic relations in the parameter range studied here. This is immediately evident from the quark mass dependence of the pion mass. To a first approximation the pion slope turns out to be independent of $\beta$. This shows that $R_m \simeq 2ma$. In fact, for both quark mass values and all $\beta$-values studied by us we find this relation to be satisfied within 15%.

Rather than using the rho-meson mass to determine $R_{\beta}$ we have used an approach which turned out to describe quite well the deviations from asymptotic scaling in the pure gauge theory. We define an effective coupling, $\beta_{\text{eff}}$, in terms of the expectation value of the gluonic part of the action,

$$\beta_{\text{eff}} = \frac{12}{\langle S(1,2) \rangle (\beta)} ,$$

and use the dependence of $\beta_{\text{eff}}$ on $\beta$ to calculate the derivative $R_{\beta}$ with the help of the asymptotic two-loop renormalization group equation. This also fixes the temperature scale,

$$\frac{T}{T_c} = \left( \frac{\beta_{\text{eff}}}{\beta_c} \right)^{-77/625} \exp \left( 4\pi^2/25(\beta_{\text{eff}} - \beta_c) \right) ,$$
We use this approximation for $R_\beta$ also in the calculation of $R_m$ and determine in addition the ratio $h'/h$ from the pion slope.

The critical couplings for both quark masses have been determined from the Polyakov-loop susceptibility and the chiral susceptibility. The location of the peaks in both susceptibilities coincide within errors. From this we find

\[
\beta_c = \begin{cases} 
3.57 \ (3) \ , & m a = 0.1 \\
3.49 \ (3) \ , & m a = 0.05 
\end{cases},
\]

which fixes the temperature scale through Eq. 14.

In Figure 2 we show the results of a calculation of the pressure for both values of the quark mass. As can be seen the result is quite insensitive to the value of the quark mass. Moreover, we note that the overall structure of the temperature dependence of the pressure is quite similar to that of the pure gauge sector \[11\]. This also can be seen in Figure 2, where we show the pressure of the $SU(3)$ gauge theory rescaled by an appropriate ratio of the number of degrees of freedom so that the high temperature limit coincides with that of four-flavour QCD.

In Figure 3a we show the difference between the energy density and three times the pressure calculated according to Eq. 9. As discussed above, the second term in this equation, \textit{i.e.} the term being proportional to the chiral condensates, will not contribute in the chiral limit. We therefore show in Figure 3b also the difference ($((\epsilon - 3p)/T^4)_0$ defined only in terms of the gluonic part,

\[
\Delta_0 = -N^4 \tau R_\beta \langle S^{(1,2)} \rangle
\]
Figure 3: The difference $(\epsilon - 3p)/T^4$ calculated according to Eq. 9 ($\Delta$) as well as Eq. 16 ($\Delta_0$). The lines are spline interpolations to the data, with the full line for $m/T = 0.2$, the dotted one for $m/T = 0.4$ and dash-dotted for the quenched results.

We note that in the high temperature regime, $T/T_c \gtrsim 2$, the quark mass dependence, which is visible in $\Delta$ is completely eliminated in $\Delta_0$. This suggests that at least in this temperature regime $\Delta_0$ can be viewed as a reasonable extrapolation of $(\epsilon - 3p)/T^4$ to the chiral limit, $ma \to 0$. Close to $T_c$ this is not that evident. In fact, neither in Figure 3a nor in 3b we see any significant quark mass dependence for $T \lesssim 1.2T_c$. In the case of $(\epsilon - 3p)/T^4$ this is due to the cancellation of two effects in the contribution from the chiral condensate term. On the one hand the derivative factor $R_m$ decreases with decreasing quark mass. On the other hand the difference of chiral condensates, $\langle \bar{\chi}\chi \rangle$, still increases because the critical coupling gets shifted towards smaller values (Eq. 15). As the first effect will ultimately dominate and will force the entire contribution of the condensate term to vanish in the chiral limit we expect that $\Delta_0$ is already a good approximation to the final result in the chiral limit. Of course, this should eventually be checked by performing simulations at smaller quark masses.

Also shown in Figure 3b is the result for the pure gauge theory which again has been rescaled with the appropriate number of degrees of freedom $(29/8)$ as it has been done for the pressure alone. This too gives support to our extrapolation to the chiral limit and suggests that the equation of state in four-flavour QCD indeed shows a temperature dependence which is very similar to that of the pure gauge theory.

We use the results for the pressure and the difference $\epsilon - 3p$ to extract the energy density. This is shown in Figure 4. The energy density does come close to the ideal gas limit immediately above $T_c$. We do observe an overshooting of the ideal gas limit close to $T_c$ for the non-zero quark masses considered here. This is a feature not seen in the pure gauge sector. The overshooting does, however, seem to disappear when we determine the energy density from $\Delta_0$. As discussed above this may be viewed as an extrapolation to the chiral limit (see also [16]).
Figure 4: Energy density of four-flavour QCD on a $16^3 \times 4$ lattice. The lower set of curves shows an extrapolation to the chiral limit which has been obtained by ignoring the second term in Eq. 9, i.e. from Eq. 16 (see text).

4 The critical temperature

In the pure gauge sector it has been found that the critical temperature for the deconfinement transition calculated with the standard Wilson action in units of the square root of the string tension, $\sqrt{\sigma}$, deviates by about 10% from the continuum extrapolation at $aT_c = 1/4$. This cut-off dependence gets strongly reduced already with tree level improved actions [13]. To our knowledge the ratio $T_c/\sqrt{\sigma}$ has previously been determined for the chiral transition in four-flavour QCD only once using the standard staggered formulation with a quark mass $m/T = 0.08$ at $aT_c = 1/8$ [15]. This gave $T_c/\sqrt{\sigma} = 0.39$ (3).

We have analyzed the heavy quark potential on the $16^4$ lattices at the critical couplings given in Eq. [13]. For this purpose we have generated 300 gauge field configurations separated by 10 trajectories for the quark mass $ma = 0.05$ and 200 configurations for the larger mass, $ma = 0.01$. The potential has then been extracted using smeared Wilson loops and following the approach used also in the pure gauge theory [17]. The potentials have been fitted to an ansatz including a linear and a Coulomb term, $V_{qq}(R) = V_0 + \alpha/R + \hat{\sigma}R$. The string tension in units of the cut-off, $\hat{\sigma} \equiv \sigma a^2$ turns out to be significantly larger than in the SU(3) gauge theory at a comparable value of the cut-off, i.e. $aT_c = 1/4$. The potentials have been fitted in the range $3 \leq R \leq 6$. From the fits we obtain

$$T_c/\sqrt{\sigma} = \begin{cases} 0.407 \ (10) & , \ ma = 0.05 \\ 0.430 \ (8) & , \ ma = 0.1 \end{cases}$$

(17)
5 Conclusions

We have analyzed the thermodynamics of four-flavour QCD using an improved fermion action. We find that the $O(a^2)$ improvement of the free fermion action also leads to a strong reduction of the cut-off dependence in the high temperature phase. In the ideal gas limit deviations from the continuum Stefan-Boltzmann law are still about 20%. A further improvement will thus be necessary in order to reduce the cut-off dependence to only a few percent as it is the case in the pure gauge sector. In addition one would also like to achieve a reduction of the flavour symmetry breaking in the staggered action. This does not seem to be the case for the improved action we have used here [17].

For the dependence of the pressure on $T/T_c$ we obtain results which closely follow that of the $SU(3)$ gauge theory when rescaled with the number of degrees of freedom. The same holds for the energy density after an extrapolation to the chiral limit. The critical temperature itself drops to $T_c = 0.407(10)\sqrt{\sigma}$ at a quark mass $m/T = 0.2$.

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