Equation of State for the SU(3) Gauge Theory

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Abstract

Through a detailed investigation of the SU(3) gauge theory at finite temperature on lattices of various size we can control finite lattice cut-off effects in bulk thermodynamic quantities. We calculate the pressure and energy density of the SU(3) gauge theory on lattices with temporal extent $N_t = 4, 6$ and 8 and spatial extent $N_s = 16$ and 32. The results are extrapolated to the continuum limit. We find a deviation from ideal gas behaviour of (15-20)%, depending on the quantity, even at temperatures as high as $T \sim 3T_c$. A calculation of the critical temperature on lattices with temporal extent $N_t = 8$ and 12 and the string tension on $32^4$ lattices at the corresponding critical couplings is performed to fix the temperature scale. An extrapolation to the continuum limit yields $T_c/\sqrt{\sigma} = 0.629(3)$. 
Reaching a quantitative understanding of the equation of state (EOS) of QCD is one of the central goals in finite temperature field theory. The intuitive picture of the high temperature phase of QCD behaving like a gas of weakly interacting quarks and gluons is based on leading order perturbation theory. However, the well-known infrared problems of QCD lead to a poor convergence of the perturbative expansion of the thermodynamic potential even at temperatures very much higher than $T_c$. Non-perturbative studies of the EOS on the lattice have been pursued ever since the first finite temperature Monte Carlo calculations.

Lattice calculations of energy density ($\epsilon$), pressure ($p$) and other thermodynamic variables led to some understanding of the temperature dependence of these quantities in the QCD plasma phase. The energy density, for instance, has been found to rise rapidly at $T_c$ and approach the high temperature ideal gas limit from below. However, except for a very recent calculation for the $SU(2)$ gauge theory, all studies of the QCD EOS have been restricted to lattices with only four sites in the Euclidean time direction ($N_\tau = 4$). This limitation is quite severe as it is well known that the small extent of the lattice in the time direction causes large cut-off effects in thermodynamic quantities. Asymptotically these corrections are $O(N_\tau^{-2})$. For an ideal gluon gas they are given by

$$\epsilon = 3p = (N^2 - 1)\left[\frac{\pi^2}{15} + \frac{2\pi^4}{63} \cdot \frac{1}{N_\tau^2} + O\left(\frac{1}{N_\tau^4}\right)\right].$$

These cut-off effects result from the discretization of the field strength tensor which introduces $O(a^2)$ deviations from its continuum counterpart, i.e. $O((aT)^2 \equiv N_\tau^{-2})$ corrections at finite temperature $T$. In the case of a free gas it is found that the corrections are as large as 50% for $N_\tau = 4$. The leading $O(N_\tau^{-2})$ term yields the dominant contribution to the $N_\tau$-dependence only for $N_\tau \geq 6$. In order to compare lattice calculations of the EOS with continuum perturbation theory or phenomenological models like the bag EOS, it is thus mandatory that the finite cut-off effects on lattices with varying time extent $N_\tau$ are under control. This is the aim of this paper.

Controlling the continuum limit requires a systematic analysis of thermodynamic quantities on lattices with varying $N_\tau$, which then allows an extrapolation of the numerical results to the continuum limit ($N_\tau \to \infty$). There are two basic ingredi-
ents for such an analysis. First, one needs high precision results for the Euclidean action density, calculated on symmetric, zero temperature lattices of size $N^4_\sigma$ and on asymmetric finite temperature lattices of size $N^3_\sigma \times N_\tau$. All basic thermodynamic quantities can then be calculated from the difference of action densities at zero ($S_0$) and finite ($S_T$) temperature \[\Delta S = N^4_\tau (S_0 - S_T)\].

The action densities are proportional to plaquette expectation values, $S_{0(T)} = 6(1 - \frac{1}{3} \text{Tr} U_1 U_2 U_3 U_4)$. Second, one needs control over the variation of the physical temperature with the bare gauge coupling, $T^{-1} = N_\tau a(g^2)$, also in a region where the asymptotic scaling relation, given by the two universal terms of the QCD $\beta$-function, is not yet applicable.

We have addressed both problems in a systematic study of the thermodynamics of the $SU(3)$ gauge theory. We calculate thermodynamic quantities from high precision data for the action densities obtained on lattices of size $16^3 \times 4$ and $32^3 \times N_\tau$ with $N_\tau = 6$ and 8. The temperature scale is determined through calculations of the critical couplings of the deconfinement transition on lattices with $N_\tau = 4, 6, 8$ and $12$ and a calculation of the string tension on $32^4$ lattices at these critical couplings. The results from different size lattices are then used to extrapolate to the continuum limit.

For our simulations we use an overrelaxed heatbath algorithm. Depending on the bare coupling strength we perform 4-9 overrelaxation updates followed by one heatbath update (≡ one iteration). At each value of the coupling we have performed between 20,000 and 30,000 iterations on the finite temperature lattices and about 5,000 to 10,000 iterations on the $32^4$ and $16^4$ lattices. In the following we will first discuss the determination of the temperature scale and then continue with a discussion of the equation of state.

The temperature scale: Asymptotically, for large values of $\beta = 6/g^2$, the temperature $T = 1/N_\tau a(\beta)$ is given by the unique scaling relation $a \Lambda_L = R(\beta)$, with

\[
R(\beta) = \left( \frac{8\pi^2 \beta}{33} \right)^{51/121} \exp[-4\pi^2 \beta/33].
\]
Quite general, the relation between the cut-off, $a$, and $g^2$ is obtained through the calculation of a physical quantity in units of the lattice cut-off, e.g. the string tension, $\sigma a^2$, or the critical temperature, $T_c a$. Different observables will then generally lead to relations $a(g^2)$, which differ from each other by $O(a^2)$ terms. However, nonetheless it seems that such corrections are small for intermediate values of the gauge coupling. In any case, if one chooses a particular relation $a(g^2)$, obtained from one physical observable, all $O(a^2)$ corrections will drop out in the extrapolation to the continuum limit.

Here we will fix the relation between $a$ and $g^2$ through a calculation of the critical temperature on lattices of size $N_\tau = 4, 6, 8$ and 12. The critical couplings have been extracted from the locations of peaks in the Polyakov loop susceptibility using a Ferrenberg-Swendsen interpolation between four couplings selected close to the estimated critical point $[3, 7]$. For the $N_\tau = 4$ and 6 lattices our analysis of the critical couplings is in complete agreement with earlier high statistics calculations $[8]$. For $N_\tau = 8$ and 12 we find, however, significantly larger values than those obtained in previous calculations $[8]$. Our analysis on $32^3 \times 8$ and 12 lattices yields $[7]$

$$\beta_c(N_\tau) = \begin{cases} 
6.0609 \pm 0.0009 & , \ N_\tau = 8 \\
6.3331 \pm 0.0013 & , \ N_\tau = 12 
\end{cases}$$

A comparison with the results of Ref. $[3]$, which have been obtained on smaller spatial lattices, shows, however, that our result is consistent with the expected shift towards larger values due to the larger spatial volume used in our simulation.

The absolute scale will be fixed through a determination of the string tension on $16^4$ and $32^4$ lattices at the critical couplings $\beta_c(N_\tau)$. We have obtained the string tension from an analysis of heavy quark potentials calculated from smeared Wilson loops $[7]$. For $N_\tau = 4$ and 6 the ratio $T_c/\sqrt{\sigma}$ has been evaluated at the critical couplings extrapolated to the infinite volume limit. For $N_\tau = 8$ and 12 we evaluate this ratio at the critical couplings obtained on lattices with finite $N_\sigma/N_\tau$. From the volume dependence of the critical couplings studied in Ref. $[8]$ we expect that the infinite volume critical couplings will be larger by about 0.0017 for $N_\tau = 8$ and 0.0057 for $N_\tau = 12$. We therefore systematically underestimate the ratio $T_c/\sqrt{\sigma}$ in these cases. The expected systematic error due to this effect has been estimated by
assuming an exponential scaling of $\sqrt{\sigma}a$ according to the asymptotic renormalization group equation.

The results for $T_c/\sqrt{\sigma}$ are summarized in Table 1. Although the ratios hardly show any systematic cut-off dependence, we have extrapolated the results for the different $N_T$-values to the continuum limit using a fit of the form $a_0 + a_2/N_T^2$. This yields

$$\frac{T_c}{\sqrt{\sigma}} = 0.625 \pm 0.003 \, (+0.004) \, .$$

The number in brackets indicates the systematic shift we expect from the infinite volume extrapolation of the critical couplings. We note that this estimate of $T_c/\sqrt{\sigma}$ is about 10% larger than earlier estimates [12], which is due to our newly determined critical couplings for the larger lattices. It is only 10% below the corresponding result for the $SU(2)$ gauge theory [12] and string model predictions [13]. Using $\sqrt{\sigma} = 420$ MeV we find a critical temperature of about 260 MeV.

The lattice cut-off, extracted from the location of the critical couplings, shows the well known deviations from the asymptotic scaling relation, Eq. 3. The major part of these deviations can be taken care of through a replacement of the bare coupling by a renormalized coupling [11]. We will adopt here the definition $\beta_{\text{eff}} = 6(N^2 - 1)/S_0$. This relation can be used to determine the cut-off as $a\Lambda_L = R(\beta_{\text{eff}})\lambda_{\text{eff}}$, with $\lambda_{\text{eff}} = 0.4818$. For the parameterization of the remaining discrepancy between

| $N_T$ | $\beta_c$ | $\sqrt{\sigma}a$ | $T_c/\sqrt{\sigma}$ |
|-------|----------|------------------|-------------------|
| 4     | 5.6925 (2) | 0.4179 (24) | 0.5983 (30)         |
| 6     | 5.8941 (5) | 0.2734 (37) | 0.6096 (71)         |
| 8     | 6.0609 (9) | 0.1958 (17) | 0.6383 (55) (+13)   |
| 12    | 6.3331 (13) | 0.1347 (6)  | 0.6187 (28) (+42)   |

Table 1: String tensions calculated at the critical couplings for the deconfinement transition, $\beta_c(N_T)$. For $N_T = 4$ and 6 we evaluate $\sigma a^2$ at the infinite volume critical coupling using an interpolation of values from Ref. 11. For $N_T = 8$ and 12 we have calculated the string tension at the finite volume critical couplings. The systematic errors is also given in these cases. Details are discussed in the text.
this relation and the numerical data we use the ansatz
\[ a \Lambda_L = R(\beta_{\text{eff}}) \cdot \lambda(\beta) \, . \] (6)

The function \( \lambda(\beta) \) was chosen such that the calculated critical temperatures \( T_c^{-1} = N_a g_c^2 \) are reproduced. The quality of this interpolating function is best seen in the \( \Delta \beta \)-function, which describes the change in \( \beta \) needed to change the cut-off by a factor of two. This is shown in Figure 1 together with a determination of \( \Delta \beta \) from a recent MCRG analysis of ratios of Wilson loops [14]. It is obvious, that the determination of \( \lambda(\beta) \) may depend on the observable used to calculate \( \Delta \beta \) only for \( \beta < 6.0 \). In particular for our \( N_f = 8 \) calculation such an ambiguity therefore does not arise. In order to judge the relevance of the choice of parameterization of this function we also use in the following the simple ansatz \( \lambda(\beta) \equiv \lambda_{\text{eff}} \), which also is shown in Figure 1.

Figure 1: Shown is the \( \Delta \beta \)-function, \( \Delta \beta(a) = \beta(a) - \beta(2a) \), which is obtained from MCRG studies [14] (squares) and from our finite temperature calculation (circles). The dashed-dotted and dashed curves show the \( \Delta \beta \)-function obtained from the asymptotic form of the renormalization group equation using the coupling \( \beta \) and the effective coupling \( \beta_{\text{eff}} \), respectively. The solid curve is our interpolation, which fixes \( \lambda(\beta) \).

**Equation of state:** Our calculation of thermodynamic quantities is based on a
direct evaluation of the free energy density in large spatial volumes, i.e. close to the thermodynamic limit. From this other thermodynamic observables can be obtained by taking derivatives with respect to the temperature [5]. The calculation of the free energy density requires a numerical integration of the difference of action densities, Eq. 4.

\[
\frac{p}{T^4}\bigg|_{\beta_i} \equiv \frac{-\widetilde{f}}{T^4}\bigg|_{\beta_0} = N^4 T \int_{\beta_0}^{\beta} d\beta' (S_0 - S_T) .
\]

The above relation gives the pressure (free energy density) difference between two temperatures corresponding to the two couplings \(\beta_0\) and \(\beta\). In practice we will choose the lower temperature corresponding to \(\beta_0\) small enough so that the pressure can be approximated by zero at this point.

Making use of basic thermodynamic relations we can then evaluate the energy density in the thermodynamic limit from

\[
\frac{\epsilon - 3p}{T^4} = T \frac{\partial}{\partial T} \left( \frac{p}{T^4} \right) = -6 N^4 a \frac{\partial g^{-2}}{\partial a} (S_0 - S_T) ,
\]

where the derivative \(a \partial g^{-2}/\partial a\) is obtained from our explicit parameterization of the relation between the cut-off, \(a\), and the bare coupling, \(g^2\), given in Eq. 6.

The main difficulty for a systematic analysis of \(p\) and \(\epsilon\) on large lattices (large values of \(N_T\)) arises from the fact that the relevant observable, the difference of action densities \((S_0 - S_T)\) drops like \(N^{-4}_T\). A rapidly increasing accuracy in the numerical calculation thus is required. We have calculated the action densities on lattices of size \(16^4\), \(32^4\) as well as \(16^3 \times 4\), \(32^3 \times 6\) and \(8\) for a large number of different couplings. Note that we use large spatial lattices, \(N_\sigma/N_T = (4-5.33)\). Except very close to \(T_c\) this is sufficient for an approximation of the thermodynamic limit [4]. On the basis of results for \(N_T = 6\) and \(8\) we will perform an extrapolation to the continuum \((N_T \rightarrow \infty)\) limit.

In Figure 2 we show the results for \(N_T = 8\), which is statistically the most difficult case. For a calculation of the pressure we have to integrate the action densities with respect to \(\beta\), Eq. 4. For this purpose we use interpolations as shown in Fig. 2. As can be seen from the Figure, \(\Delta S\) rapidly becomes small below the critical coupling.
We thus can use a value $\beta_0$ close to the critical coupling to normalize the free energy density. We then use the relation between the gauge coupling and the lattice cut-off, Eq. 6, to determine the temperature scale. Results obtained for the pressure on lattices with temporal extent $N_\tau = 4, 6$ and 8 are shown in Figure 3a. We clearly see the expected cut-off dependence of the pressure. It qualitatively reflects the $N_\tau$-dependence of the free gluon gas, which is shown by dashed-dotted lines in this figure. Quantitatively, however, we find that the cut-off dependence of the pressure is considerably weaker than suggested by the free gas calculation.

Errors on the numerical results for the pressure arise from ambiguities in determining the temperature scale as well as from errors on our interpolating curves for the action densities. In order to control the latter sources of errors, we have therefore integrated $\Delta S$ also by using straight line interpolations in addition to the smooth interpolation shown in Figure 2. The resulting differences are on the level of a few percent. They are shown as typical error bars in Figure 3a. The ambiguities arising at finite cut-off from the choice of parameterizations of the temperature scale only amount to a shift in the temperature scale. This effect is largest for $N_\tau = 4$ and is shown as dashed curve in Figure 3a. We stress that this ambiguity will not influence the extrapolation to the continuum limit.
Figure 3: The pressure (a) versus $T/T_c$ for $N_\tau = 4, 6$ and 8 integrating the interpolations for the action density. For $N_\tau = 4$ we show two curves, which correspond to the parameterization of the temperature scale using the effective coupling scheme (dashed curve) and the parameterization of the scaling violations of the critical temperature (solid curve), respectively. For $N_\tau = 6, 8$ we only show the latter. Error bars indicate the uncertainties arising from the integration of the raw data for the action differences (See text for further discussion). The horizontal dashed line shows the continuum limit ideal gas value and the dashed-dotted lines give the corresponding values for $N_\tau = 4, 6$ and 8. In Fig.3b we show the difference $(\epsilon - 3p)/T^4$.

A similar analysis was carried out for $(\epsilon - 3p)/T^4$. Results are shown in Figure 3b. Also here we have examined the systematic errors arising from the parameterizations of $a(g^2)$. For $N_\tau = 4$ these errors are about 6% on the peak of $(\epsilon - 3p)/T^4$ and less than 2% everywhere else. Also for $N_\tau = 6, 8$ the errors are on the 2% level.

We note that we did not attempt to separate our data sample in the vicinity of $\beta_c$ in sets belonging two different phases, although we have clear evidence for metastabilities as signal for a first order phase transition at all three values of $N_\tau$. We rather prefer to average over these metastabilities and show continuous curves for $(\epsilon - 3p)/T^4$ as it should be for calculations performed in finite physical volumes.

Based on the analysis of the pressure and energy density on various size lattices we can attempt to extrapolate these quantities to the continuum limit. As discussed above, in the case of a free theory the leading $N_\tau^{-2}$ corrections to the continuum limit
result provide a good description of the actual \( N_\tau \)-dependence only for \( N_\tau \geq 6 \). This is seen qualitatively also in our numerical data. Following Eq.1, in a quadratic fit we thus only use the \( N_\tau = 6 \) and 8 data respectively to extrapolate to the continuum limit,

\[
\left( \frac{p}{T^4} \right)_a = \left( \frac{p}{T^4} \right)_0 + \frac{c_2}{N_\tau^2}.
\]  (9)

In order to control systematic errors resulting from the specific parameterization of the temperature scale used we have performed extrapolations with the two different parameterizations discussed above. The resulting differences have been taken as estimate for a systematic error in \( (p/T^4)_0 \).

The extrapolations of the pressure, energy density and entropy density are shown in Fig. 4. We generally find that the difference between the extrapolated values and the results for \( N_\tau = 8 \) is less than 4\%, which should be compared with the corresponding result for the free gas, where the difference is still about 8\%. This suggests that relative to the ideal gas case more low momentum modes, which are less sensitive to finite cut-off effects, contribute to thermodynamic quantities.

Figure 4: Extrapolation to the continuum limit for the energy density, entropy density and pressure versus \( T/T_c \). The dashed horizontal line shows the ideal gas limit. The hatched vertical band indicates the size of the discontinuity in \( \epsilon/T^4 \) (latent heat) at \( T_c \) [9]. Typical error bars are shown for all curves.
The earlier results for the equation of state derived from lattice calculations on lattices with \( N = 4 \) have been parameterized in terms of various models incorporating non-perturbative effects either through a bag constant, temperature dependent gluon masses or a combination of those \[15\]. We do not intend to go through such analyses of our results at this point. However, we would like to point out a few basic features of our current results for the equation of state of a gluon gas. We find that the energy density rapidly rises to about 85% of the ideal gas value at \( 2T_c \) and then shows a rather slow increase, which is consistent with a logarithmic increase as one would expect from a leading order perturbative correction. The pressure rises much more slowly and still shows sizeable deviations from the ideal gas relation \( \epsilon = 3p \) for \( T \simeq 3T_c \). The trace anomaly, \((\epsilon - 3p)/T^4\), is related to the difference between the gluon condensate at zero and finite temperature \[10\], \( \epsilon - 3p = G(0) - G(T) \). It has a pronounced peak at \( T \simeq 1.1T_c \). Expressed in units of the string tension we find

\[
(\epsilon - 3p)_{\text{peak}} = (0.57 \pm 0.02)\sigma^2 \simeq 2.3 \text{ GeV/fm}^3,
\]

which should be compared with the value of the zero temperature gluon condensate, \( G(0) \simeq 2 \text{ GeV/fm}^3 \). This fulfils the above relation if \( G(T) \simeq 0 \) at \( T \simeq 1.1T_c \).

To conclude, we stress that the systematic analysis of thermodynamic quantitites on different size lattices allowed us to control their distortion due to finite cut-off effects. For the first time, from lattice calculations of the \( SU(3) \) gauge theory at finite temperature, we could extract results for bulk thermodynamic quantitites in the continuum limit.

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