

Precise determination of T_c in QCD from scaling

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Existing lattice data on the QCD phase transition are analyzed in renormalized perturbation theory. In quenched QCD it is found that T_c scales for lattices with only three time slices, and that $T_c/\Lambda_{\overline{\text{MS}}}=1.15 \pm 0.05$. A preliminary estimate in QCD with two flavors of dynamical quarks shows that this ratio depends on the quark mass. For realistic quark masses we estimate $T_c/\Lambda_{\overline{\text{MS}}}=0.49 \pm 0.02$. We also investigate the equation of state in quenched QCD at 1-loop order in renormalized perturbation theory.

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The QCD phase transition temperature (T_c) is a fundamental constant of the hadronic world, and will soon be accessible to experiments. It has also been the target of many lattice computations. Current practice is to express T_c in units of the mass of the rho meson (M_ρ) or the square root of the string tension ($\sqrt{\sigma}$) [1]. However, in the last few years it has become clear that the renormalized QCD coupling α_S measured on fairly coarse lattices [2] yields results comparable to those obtained in precision measurements at the CERN e^+e^- collider LEP and in other experiments [3]. This prompts us to test the approach to the continuum limit of QCD thermodynamics by testing the constancy of $T_c/\Lambda_{\overline{\text{MS}}}$, where $\Lambda_{\overline{\text{MS}}}$ is the QCD scale parameter extracted in the modified minimal subtraction ($\overline{\text{MS}}$) scheme.

In the limit when all quark masses are zero (or infinite), QCD has only one dimensionless parameter—the coupling $\alpha_S=g^2/4\pi$. Quantum corrections transmute it into a momentum scale. This scale is either given explicitly as the QCD parameter Λ , or specified implicitly, as the value of the coupling $\alpha_S(\mu)$ at scale μ .

In the lattice regularization of QCD, the value of the lattice spacing (a) is determined by the bare coupling $\beta=6/g^2$. However, $6/\beta$ is not a good expansion parameter for perturbation theory. It is more appropriate to define the coupling through some physically motivated process. In one definition, called the V scheme [2], α_S at a scale of $3.4018/a$ is found from the logarithm of the plaquette value¹ (\mathcal{P}) through the formula

$$-\ln \mathcal{P} = \frac{4\pi}{3} \alpha_V [1 - (1.1897 + 0.071N_f)\alpha_V]. \quad (1)$$

In another definition, the E scheme [4], the renormalized coupling at scale a is

$$\alpha_E = \frac{3}{4\pi} (1 - \mathcal{P}). \quad (2)$$

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¹ \mathcal{P} is defined to be one third of the real part of the trace of the product of four link matrices taken in order around a plaquette.

We choose to work in these two schemes, as well as the $\overline{\text{MS}}$ scheme whose relation to the V scheme has been worked out [5]. At 2-loop order we can write

$$a\Lambda = kR(1/4\pi\beta_0\alpha_V), \quad \text{where} \quad R^2(x) = \exp(-x)x^{\beta_1/\beta_0^2}. \quad (3)$$

The constant k depends on the scheme, being unity in the E scheme and 3.4018 in the V scheme. The function R is obtained by integrating the two-loop beta function $\bar{\beta}(g) = -\beta_0 g^3 - \beta_1 g^5$.

The QCD phase transition temperature is determined by tuning the bare coupling on lattices with $N_t \ll N_s$ (where N_t is the number of sites in the Euclidean time direction and N_s that in the spatial directions). Then, $T_c = 1/a_c N_t$, where a_c is the lattice spacing at the coupling where the phase transition occurs. Our strategy is to compute the renormalized coupling α_V at these bare couplings and hence determine $T/\Lambda_{\overline{\text{MS}}}$ using Eq. (3), and the known ratio of $\Lambda_{\overline{\text{MS}}}$ and the scale Λ in any other scheme.

In quenched QCD with the usual Wilson action, the critical bare couplings β_c have been determined for $2 \leq N_t \leq 16$ [6]. The main source of systematic uncertainty in the older data arises from the fact that the thermodynamic limit $N_s \rightarrow \infty$ was not taken. Later data [7–9] have taken this limit, and we only used these to study scaling. The statistical errors in these later studies are also much smaller, and hence they are able to test the scaling hypothesis much more stringently.

We extracted α_S from the plaquette values listed in Ref. [9] using Eqs. (1),(2). Values of $\ln \mathcal{P}$ at β_c were obtained by cubic spline interpolation. Statistical errors in the interpolated values were found by propagation. We probed systematic errors in the interpolation by the change in α_S on removal of some of the knot points. The results of our analysis are shown in Fig. 1. $T_c/\Lambda_{\overline{\text{MS}}}$ is constant down to β_c for $N_t=3$. A large part of the error in this ratio comes from the errors in the measurement of \mathcal{P} , which, while small, are exponentiated in Λ .

More detailed results are shown in the right-hand panel of Fig. 1. Small scaling violations at these couplings, seen in measurements at $T=0$, have been attributed to finite lattice spacing errors [10]. On replacing the scaling function R

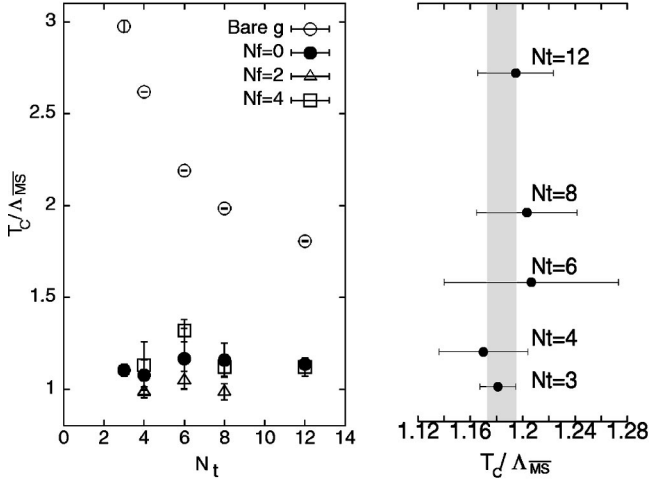


FIG. 1. The panel on the left shows $T_c/\Lambda_{\overline{\text{MS}}}$ as a function of N_t in the V scheme. For $N_f=0$ we show tests of scaling for both the bare lattice coupling and α_V . For the former the errors come only from the determination of the critical coupling, whereas for the latter they also include errors in the determination of \mathcal{P} . For $N_f=2$ with $m/T_c=0.1$ and $N_f=4$ with $m/T_c=0.08$ only the latter is shown. The panel on the right shows details of $T_c/\Lambda_{\overline{\text{MS}}}$ for $N_f=0$ in the $\overline{\text{MS}}$ scheme.

in Eq. (3) by $\bar{R}(\alpha_V)=R(\alpha_V)[1+c_2\hat{a}^2+c_4\hat{a}^4]$, where $\hat{a}=R(\alpha_V)/R(\alpha_V^0)$ and α_V^0 is determined at $\beta=6$, it was found [11] that data on $a\sqrt{\sigma}$ could be quantitatively described down to $\beta=5.4$. As shown in the figure, in the $\overline{\text{MS}}$ -scheme we can fit a constant value of $T_c/\Lambda_{\overline{\text{MS}}}$ using the critical couplings determined for $3\leq N_t\leq 14$ with good confidence— $\chi^2=0.6$ for 4 degrees of freedom. The statistical error in this estimate is about 1%. Taking into account the variation between values obtained in different schemes, and for fits with $N_t\geq 3$ or 4, we quote

$$T_c=(1.15\pm 0.05)\Lambda_{\overline{\text{MS}}} \quad (\text{quenched QCD}). \quad (4)$$

This error estimate now includes not only the statistical errors but also the systematic uncertainties above. Since experiments cannot access a quenched theory, the value of $\Lambda_{\overline{\text{MS}}}$ in MeV units is hard to pin down. When comparing different estimates, in MeV units, of the same scale in quenched QCD this universal problem should be borne in mind (see Fig. 2). Here we convert T_c into physical units using the value $\Lambda_{\overline{\text{MS}}}\approx 250$ MeV as a mean of the values obtained in different schemes in [11] by assuming $\sqrt{\sigma}=465$ MeV. This gives $T_c\approx 285\pm 10$ GeV, in reasonable agreement with other estimates, such as that found in a recent study using an RG-improved action [12].

This analysis leads us to investigate the extraction of thermodynamic quantities in the QCD plasma using renormalized perturbation theory. Failure of scaling would then be a direct signal for lattice artifacts such as power corrections in a . We examine the energy density (E) and the pressure (P). These can be written in terms of the difference $\Delta_i=\mathcal{P}_i-\mathcal{P}_0$

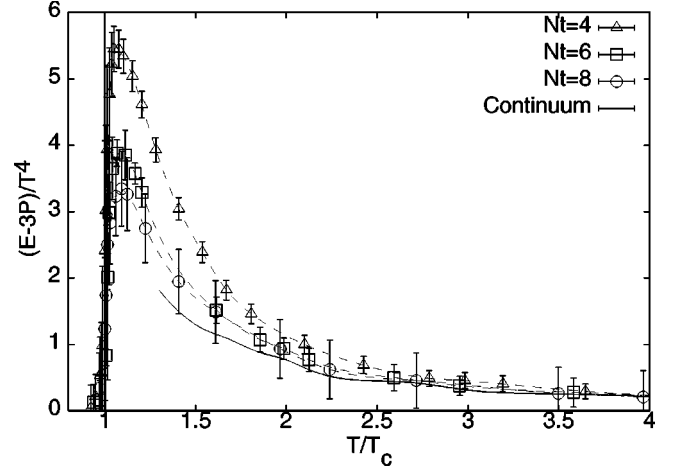


FIG. 2. $(E-3P)/T^4$ for a QCD plasma evaluated as a function of T/T_c at different lattice spacings when $\alpha_{\overline{\text{MS}}}$ sets the scale. The continuum curve is not continued into the region where finite volume effects may be important. Errors on the continuum extrapolation are roughly similar to those at $N_t=8$.

between the spatial ($i=s$) and temporal ($i=t$) plaquettes and their zero temperature counterpart \mathcal{P}_0 . E is defined by the formula

$$\frac{E}{T^4}=6N_cN_t^4\left[\frac{\Delta_s-\Delta_t}{4\pi\alpha_s}-(c'_s\Delta_s+c'_t\Delta_t)\right]. \quad (5)$$

The anisotropy coefficients c'_s and c'_t are known to 1-loop order² [13]. A measure of deviations from ideal gas behavior is

$$\Delta=\frac{E-3P}{T^4}=12N_cN_t^4(c'_s+c'_t)(\Delta_t+\Delta_s), \quad (6)$$

which can be combined with Eq. (5) to give the pressure. The sum rule $g^3(c'_s+c'_t)=\bar{\beta}(g)$ [13], allows us to evaluate Δ beyond 1-loop order. In fact, part of the finite a corrections can be incorporated into Δ by evaluating $\bar{\beta}(g)$ using \bar{R} instead of R . However, we avoid this approach, since we need to use c'_s and c'_t consistently in Eqs. (5),(6). In the following we use only the 1-loop results for these coefficients and work in the $\overline{\text{MS}}$ scheme.

Raw data on $\mathcal{P}_{0,s,t}$ at a range of couplings measured on $N_t\times(4N_t)^3$ lattices ($N_t=4, 6$, and 8) are tabulated in Ref. [8]. We have used these to evaluate thermodynamic quantities only for $T<4T_c$, because the finite spatial volumes of the lattices used may cause spatial deconfinement above $4T_c$. As expected, Δ varies as $1/N_t^2$ at fixed T , i.e., as a^2 .

²At this order the coefficients remain unchanged in going from the lattice scheme, $g^2=6/\beta$, in which they have been computed, to the $\overline{\text{MS}}$ or V scheme, but change in the E scheme. In the absence of a two-loop computation, we have evaluated the renormalized couplings at the scale appropriate to the plaquette.

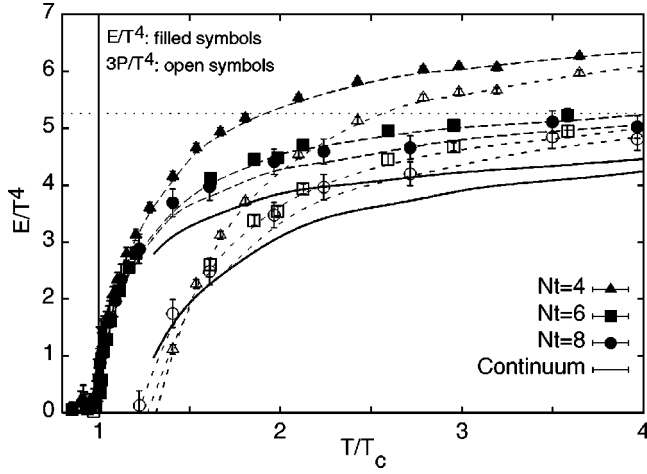


FIG. 3. E/T^4 and $3P/T^4$ for a QCD plasma evaluated as explained in the text, using the data of Ref. [8]. The dashed curves are smooth cubic spline fits. The dotted horizontal line is the ideal gas result in the continuum limit.

This power correction can be removed through the use of improved actions [14]. Δ shows a peak at $T \approx 1.1T_c$ in the continuum limit. However, the location of the peak is uncertain because there is no unique definition of T_c at finite volumes. Different definitions, which all coincide in the thermodynamic limit, give different values of the pseudocritical point on finite volume systems [15]. Using coarse lattices, we have estimated that in $SU(3)$ theory for $N_s = 4N_t$ this inherent uncertainty in the critical coupling may be as much as $\delta\beta \approx 0.005 - 0.01$: much larger than the statistical error for any given definition of the critical point. For similar reasons the value of Δ at the peak cannot be reliably extracted without taking into account finite volume effects. In the range $1.3T_c \leq T \leq 4T_c$, finite volume corrections are expected to be small. For such T , Δ is monotonically decreasing. However, many quantities of interest can be extracted only near T_c . The results of a finite size scaling study which does this will be reported elsewhere.

We have also evaluated E/T^4 and found that it scales to the continuum limit as $a^2 = 1/N_t^2$. In the temperature range where finite volume effects are strong, the large value of Δ gives a negative value to P evaluated using the formulas in Eqs. (5),(6). As we have argued already, an evaluation of thermodynamics in this range of T requires better control over finite volume effects. However, the problem of negative pressures is also avoided if the continuum limit of P is found by combining E/T^4 and Δ in the limit $a = 0$. This gives nearly vanishing P in the region of the peak in Δ .

In Fig. 3 we show our estimates of the continuum limit of E and P in the range $1.3T_c \leq T \leq 4T_c$, where finite volume effects are small. At $4T_c$ our estimate of the energy density is about 15% lower (and the pressure about 19% lower) than for an ideal gas. At this temperature, our estimates of E and P are about 5% lower than the earlier determination which used the integral method [8]. While statistically insignificant at present, this difference is due entirely to the treatment of

the region around the peak of Δ .³ The speed of sound in the QCD plasma (c_s) is slightly lower than the ideal gas value ($c_s^2 = 1/3$) at $4T_c$ (but consistent with it within errors), and falls to $c_s^2 \approx 0.1 \pm 0.025$, at $1.5T_c$.

Our attempt to measure the pressure using perturbatively determined coefficients may seem mysterious when current practice has converged on the use of an “integral” method [8]. As we have mentioned, these two methods agree within error bars for $T > 2T_c$ but differ near T_c . The integral method, by construction, gives a continuous pressure across T_c . However, if true, this is important information and needs independent verification. The latent heat density at the phase transition $\Delta Q/T_c^4 = \Delta S/T_c^3$, where ΔS is the jump in the entropy density at T_c . In general this is not the same as the change in the energy or enthalpy density at the phase transition. These contain an extra term due to the change in specific volume at fixed pressure or the change in pressure at fixed volume. In a quenched lattice simulation, the change in volume is negligible when changing T by an infinitesimal amount across T_c . As a result, the pressure should change discontinuously at T_c . This is analogous to boiling water in a closed vessel—the pressure jumps at the phase transition. Such a jump in pressure is related to the change in specific volume, and hence the slope of the phase boundary in the (P, T) plane through the Clausius-Clapeyron equation. This physics is missed when the integral method is used to extract the pressure. This issue is currently being investigated in a lattice simulation whose results will be reported elsewhere.

While the observation of scaling on coarse lattices is interesting in quenched QCD, the real pay off would be in the study of finite temperature QCD with dynamical light quarks. Since there are inherent difficulties with simulating QCD with dynamical massless quarks, all lattice studies have used quarks with mass $m > 0$. In such theories, scaling should be tested at fixed $m/\Lambda_{\overline{MS}}$ (or equivalently, fixed ratio of m and any hadronic mass scale).

Measurements of β_c in QCD with four flavors of dynamical staggered quarks have been performed for $N_t = 4, 6$ [16] and 8 [17]. This last measurement was done with $m/T_c = 0.08$. The simulations at smaller N_t were done at several values of m , enabling us to find β_c at $m/T_c = 0.08$ by interpolation. Plaquette values were taken from a recent finite temperature simulation at fixed m/T_c [18]. Since it is known that $\Delta_{t,s}/\mathcal{P}_0$ are less than 0.1%, even near T_c , we have used $(\mathcal{P}_s + \mathcal{P}_t)/2$ to determine α_s . The difference of α_s measured using \mathcal{P}_s and \mathcal{P}_t is taken as an estimate of its error. We used Eq. (3) to set the scale. $T_c/\Lambda_{\overline{MS}}$, when determined through the bare coupling, changes from 8.2 to 4.7 in going from $N_t = 4$ to 8. As shown in Fig. 1, when α_V is used, 2-loop scaling works much better.

The phase transition in 2-flavor QCD has been studied in greater detail (see Ref. [1] for a recent compilation of data).

³However, note that our use of the 1-loop expressions for c'_s and c'_t , and the consequent inability to make an optimal choice of scale is the largest uncertainty in this method for $T \geq 1.5T_c$. Such uncertainties can be reduced by appropriate 2-loop computations.

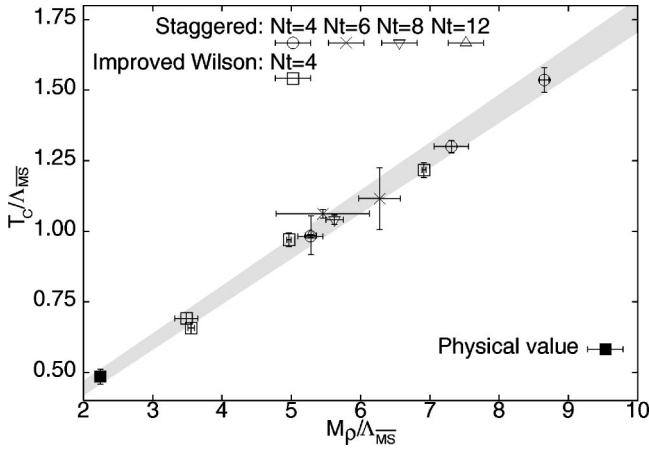


FIG. 4. $T_c/\Lambda_{\overline{\text{MS}}}$ plotted against $M_\rho/\Lambda_{\overline{\text{MS}}}$ and extrapolated to the physical value. The band shows the $1-\sigma$ errors on the best fit line to the measurements.

Measurements of β_c using dynamical staggered quarks exist for $N_f \leq 12$ [19,20]. Earlier simulations with Wilson quarks (which have order a lattice artifacts) showed that pion masses were rather high compared to those obtained with staggered quarks. This problem becomes less acute on using improved actions for Wilson quarks, and finite temperature simulations have now been performed with such improved actions [21,22]. There have also been some studies with domain wall fermions.

We have fixed α_V and set the scale using published plaquette values for staggered quarks at several bare quark masses [20,23]. $T_c/\Lambda_{\overline{\text{MS}}}$ for $N_f=2$ shown in Fig. 1 are based on the subset of the data which uses staggered quarks at $m/T_c=0.1$. In contrast to the near constancy of this ratio as shown in the figure, $T_c/\Lambda_{\overline{\text{MS}}}$ computed from the same data using the bare lattice definition of g falls from 3.9 to 2.8 in going from $N_f=4$ to 8. To extend this test to other values of m/T_c we have to interpolate between plaquette values for various quark masses. An upper limit for the error in this procedure is the actual change in \mathcal{P} between extreme values of the quark masses at which they are measured. This varies between a few parts in a thousand at $\beta=5.26$ to about 2% at $\beta=6$. This uncertainty in \mathcal{P} translates into a similar magnitude of uncertainty in $T_c/\Lambda_{\overline{\text{MS}}}$ and is much smaller than the change when using $6/\beta$ across a similar range of quark masses. Excellent scaling of $T_c/\Lambda_{\overline{\text{MS}}}$ is seen also for other values of m/T_c .

In order to obtain a physically relevant value of T_c , it is necessary to extrapolate $T_c/\Lambda_{\overline{\text{MS}}}$ to measured values of the hadron masses. It would be most interesting to perform this extrapolation in the quark or pion masses. However, this needs control over the critical exponents of the theory—a task we do not attempt here. Instead we choose to extrapolate T_c to the physical region in terms of M_ρ [23]. There are two reasons for this. First, the ratio T_c/M_ρ is known to be nearly constant. Secondly, M_ρ is quite sensitive to finite lattice spacing effects. The linearity of the plot of $T_c/\Lambda_{\overline{\text{MS}}}$ against $M_\rho/\Lambda_{\overline{\text{MS}}}$ in Fig. 4 then indicates that, for the chosen data set, finite lattice spacing effects in M_ρ are under reasonable control. The value of $\Lambda_{\overline{\text{MS}}}$ also needs to be specified. This de-

pends on how many active flavors are present at the scale under consideration. The world average of $\Lambda_{\overline{\text{MS}}}^{(5)}$ (at scales high enough for 5 active flavors) is 219_{-23}^{+25} [3]. At lower scales, with only three active flavors, $\Lambda_{\overline{\text{MS}}}^{(3)}=343_{-28}^{+31}$, using the prescription of Ref. [3] to match across flavor thresholds.

The physical value of T_c is obtained by extrapolating to the real-world value of $M_\rho/\Lambda_{\overline{\text{MS}}}^{(3)}$. This is done by fitting a straight line to the data including staggered and improved Wilson quarks [21]. We have taken the two sets of data together since they both have cutoff effects of order a^2 . The extrapolation gives

$$T_c/\Lambda_{\overline{\text{MS}}}=0.487\pm 0.023 \quad \text{and}$$

$$T_c=167\pm 9_{-14}^{+15} \quad (N_f=2 \text{ QCD}). \quad (7)$$

The error in the ratio above reflects only the statistical errors in various measurements. The first error in T_c is purely from extrapolation and the second set from the errors on $\Lambda_{\overline{\text{MS}}}^{(3)}$. Since they come from independent sources, it is possible to add them in quadrature. This result is consistent with a recent estimate using $O(4)$ critical indices to scale T_c as the pion mass is taken to its physical value [22]. However, there are possibly large systematic uncertainties. Currently the least well understood problem is whether extrapolating one hadron mass to its measured value also takes all other hadron masses to their correct values. Until this issue is settled, all estimates of T_c must be considered preliminary.

We end with a small application of our measurements of $T_c/\Lambda_{\overline{\text{MS}}}$. This addresses the question of the temperature range where dimensional reduction (DR) is expected to be valid. Perturbative matching of the $T>0$ four dimensional theory with DR fixes the effective couplings in the latter [24]. There is good numerical evidence that the $SU(3)$ pure gauge theory agrees with its DR version for $T>2T_c$ [25]. If the value of the strong coupling were the determining factor

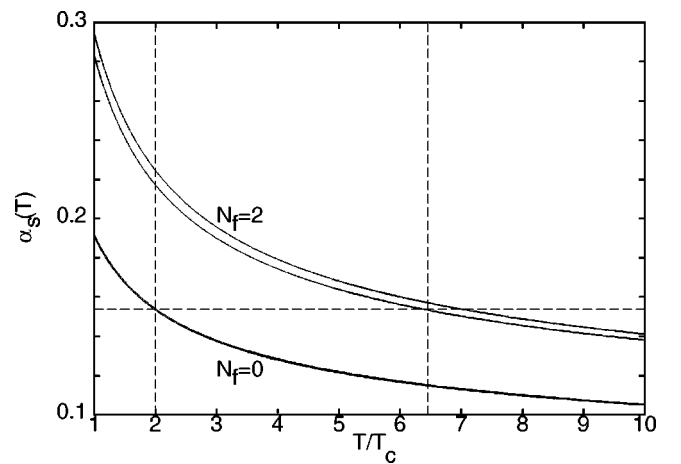


FIG. 5. α_s at 2-loop order in the $N_f=0$ and $N_f=2$ theories at the scale optimized for the three-dimensional gauge coupling in dimensionally reduced theories, shown as a function of the temperature. The bands arise from the quoted errors in the measurement of $T_c/\Lambda_{\overline{\text{MS}}}$. This plot is used to limit the validity of dimensional reduction for $N_f=2$ as explained in the text.

in the agreement, then this would imply that for $N_f = 0$, α_S is small enough at $2T_c$ to trust this expansion. If for $N_f = 2$ no other physics becomes more important, then the matching should be equally reliable when the coupling is as small. Now we ask for the temperature at which α_S in the $N_f = 2$ theory takes on the value that it had at $2T_c$ for $N_f = 0$. Using the values of $T_c/\Lambda_{\overline{\text{MS}}}$ already extracted, we are in a position to do this. The optimal scale choice for α_S has been investigated in Ref. [24]. This depends, of course, on N_f and the quantity for which the perturbation theory is optimized. Choosing the scale which optimizes the three-dimensional gauge coupling we find the dependence of α_S on T shown in Fig. 5. This tells us that for $N_f = 2$ DR can be used only for $T > 6.5T_c$. Using scales optimized for other quantities, and varying the computation of the strong coupling from 2-loop to 3-loop order, we find that the lower limit of the range of validity of DR for $N_f = 2$ varies between $6T_c$ and $8T_c$.

In summary, we demonstrated that the lattice data on

strong interaction thermodynamics obey QCD scaling relations very well and allow some continuum physics to be extracted on fairly coarse lattices. T_c can be measured with precision of about 4%, taking into account both statistical errors as well as systematic uncertainties such as renormalization scheme dependence. Simulations including dynamical quarks, when extrapolated to physical values of the ρ meson mass give statistical errors of about 4% in $T_c/\Lambda_{\overline{\text{MS}}}$. Renormalized perturbation theory at 1-loop order seems to be able to give a good account of the pressure, energy density and the speed of sound for $T > 1.5T_c$, leading to hopes that improved actions and higher loop orders can yield continuum physics at small expense. A study of finite volume effects on thermodynamics closer to T_c will be reported elsewhere.

It is a pleasure to thank Urs Heller for making available the full results of the fits reported in Ref. [11], and Rajiv Gavaï for many discussions.

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