Non-perturbative thermodynamics of SU(N) gauge theories

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The pressure near the deconfinement transition as determined up to now in lattice gauge theories shows unphysical behaviour: it can become negative and may in SU(3) even have a gap at the transition. This has been attributed to the use of only perturbatively known derivatives of coupling constants. We propose a method to evaluate the pressure, which works without these derivatives, and is valid on large lattices. In SU(2) we study the finite-volume effects and show that for lattices with spatial extent $N_\sigma \gtrsim 15$ these effects are negligible. In SU(3) we then obtain a positive and continuous pressure. The influence of non-perturbative corrections to the β-function on the energy density are investigated and found to be important, in particular for the latent heat.

1. Introduction

Monte Carlo simulations of lattice gauge theories have proven to be a powerful tool to analyze the non-perturbative aspects of these theories. This approach also opened for the first time the possibility to study the finite-temperature QCD phase transition from first principles and to obtain quantitative results for the transition temperature. The analysis of other important thermodynamic quantities like energy density, entropy density or pressure have also been studied on the lattice. The operators used to extract these quantities have, however, an essential drawback: they involve in addition to certain matrix elements of the field strength tensor also derivatives of the bare couplings with respect to temperature and/or volume [1]. The relevant derivatives of the space-like (g_σ) and time-like (g_τ) couplings in the standard Wilson action have been calculated perturbatively [2]. One finds to O(g^2) [#1]

$$\left(\frac{\partial g_\sigma^{-2}}{\partial \xi} \right)_{\xi=1} = c_\sigma' + O(g^2) ; \tag{1}$$

[#1] The derivative with respect to the temperature T can be written in terms of the lattice anisotropy $\xi = a/a_\tau$, where a and a_τ are the lattice spacings in the space- and time-like directions, respectively. Details about this and our notation can be found in ref. [1].

$$\left(\frac{\partial g_\tau^{-2}}{\partial \xi} \right)_{\xi=1} = c_\tau' + O(g^2) . \tag{1 cont'd}$$

In most numerical calculations of thermodynamical quantities performed in the past the leading-order weak-coupling expressions for these derivatives (c_σ', c_τ') have been used. Results for thermodynamical quantities obtained in this way are thus not entirely non-perturbative.

Non-perturbative results for the relevant derivatives of the couplings have been calculated at some selected points [3]. These calculations indicate that at least for the SU(3) gauge theory at intermediate couplings ($g^2 \simeq 1$) deviations from the perturbatively calculated values can be large. This does not come as a surprise since it is known that the derivatives of g_σ and g_τ are related to the QCD β-function through

$$a \frac{\mathrm{d}g}{\mathrm{d}a} = g^3 \left(\frac{\partial g_\sigma^{-2}}{\partial \xi} + \frac{\partial g_\tau^{-2}}{\partial \xi} \right)_{\xi=1} . \tag{2}$$

As there are large deviations from the perturbative β-function of the SU(3) gauge theory for $g \gtrsim 1$, it is to be expected that this is also true for the derivatives of g_σ and g_τ.

Another indication of the inadequacy of the perturbative relations for the derivatives $\partial g_{\sigma(\tau)}^{-2} / \partial \xi$ at intermediate couplings comes from recent high-statistics calculations of thermodynamical quantities for

the SU(3) gauge theory on thermal lattices of size $N_\sigma^3 \times 4$ [4,5]. Close to the critical coupling for the first-order deconfinement transition, which on lattices of this size occurs close to $6/g^2 \simeq 5.69$, one observes that the pressure, P, becomes negative. Moreover, P is discontinuous at the critical point. This approach also leads to incompatible results for the latent heat of the transition, if it is extracted either from the interaction measure $\Delta = (\epsilon - 3P)/T^4$ [1], which reflects the deviations of the thermodynamical system from a massless ideal gas, or the enthalpy density, $\epsilon + P$ [4,5]. Monte Carlo simulations for these quantities have thus reached an accuracy where inconsistencies resulting from the usage of operators for thermodynamical observables, which are not entirely non-perturbative, become visible.

2. Thermodynamics

One way of arriving at completely non-perturbative expressions for thermodynamical observables is outlined in ref. [3]: one first calculates the couplings given in eq. (1) non-perturbatively at zero temperature. These results can then be inserted in the standard expressions for the thermodynamical observables.

An alternative approach, which we want to discuss here, is based on a calculation of the free-energy density, f, and the interaction measure Δ. The free energy is related to the partition function via

$$f = -TV^{-1} \ln Z . \tag{3}$$

On the lattice the logarithm of the partition function may be calculated from the expectation value of the standard Wilson action, S, since the derivative with respect to the bare coupling $\beta = 2N/g^2$ is [1]

$$-\partial \ln Z/\partial \beta = \langle S \rangle = 3N_\sigma^3 N_\tau (P_\sigma + P_\tau) , \tag{4}$$

where $P_{\sigma(\tau)}$ is the space (time) plaquette with

$$P = N^{-1} \langle \mathrm{Tr}(1 - UUU^\dagger U^\dagger) \rangle .$$

The physical free-energy density is then obtained up to an integration constant, i.e. the value at β_0, from

$$\left. \frac{f}{T^4} \right|_{\beta_0}^{\beta} = -3N_\tau^4 \int_{\beta_0}^{\beta} \mathrm{d}\beta' \, [2P_0 - (P_\sigma + P_\tau)] . \tag{5}$$

Here we have normalized f, removing the vacuum contribution at approximately $T = 0$ by subtracting the plaquette value P_0 on a symmetric lattice ($N_\tau = N_\sigma$).

The interaction measure Δ can be obtained as [1]

$$\Delta = \frac{\epsilon - 3P}{T^4} = -a \frac{\mathrm{d}g^{-2}}{\mathrm{d}a} 6NN_\tau^4 [2P_0 - (P_\sigma + P_\tau)] . \tag{6}$$

This relation involves the QCD β-function, $a\mathrm{d}g/\mathrm{d}a$. In the past it has been approximated in the leading order by the perturbative weak-coupling expression, eq. (2). However, as discussed above we should take into account deviations from asymptotic scaling in the β-function in order to achieve a truly non-perturbative calculation of the thermodynamical quantities. Starting with a calculation of f and Δ has the advantage that we need to know *only* the non-perturbative form of the β-function and the average plaquette $P_\sigma + P_\tau$, i.e. the expectation value of the action on a lattice with $N_\tau < N_\sigma$ and on the corresponding symmetric lattice with $N_\tau = N_\sigma$.

Other thermodynamical quantities can then be obtained from standard thermodynamical relations, if we assume in addition homogeneity of the system [#2]. This general property can usually be expected to hold in a given phase of a very large system of a single particle type when only isotropic interactions are acting. An important consequence of the homogeneity of the system is then

$$\left. \frac{\partial \ln Z}{\partial V} \right|_T = \frac{\ln Z}{V} , \tag{7}$$

which in fact relates the pressure, P, and the free-energy density, f, through the identity

$$P = -f . \tag{8}$$

Given eq. (8) and the thermodynamic relation

$$f = \epsilon - Ts , \tag{9}$$

we can then determine the entropy density, s, using eqs. (5) and (6) [#3]. In general we can expect eq. (8) to hold in the thermodynamic limit. In a finite vol-

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[#2] An extensive quantity is said to be homogeneous of order one when an increase of the size of the system by a factor λ leads to an increase of the quantity by the same factor.

[#3] We note that the quantity $(\epsilon + P)/T$ calculated on finite lattices is usually taken to be the entropy density, though this is true only for homogeneous systems.

ume, however, this relation is violated due to surface effects. For a derivation of non-perturbative thermodynamics of SU(N) gauge theories on finite lattices we therefore have to look somewhat closer at the properties of the thermodynamical functions:

(1) The relation between P and f given in eq. (8) has to be investigated for finite volumes.

(2) We need a non-perturbative β-function.

We shall discuss these points in the following sections.

3. The free-energy density and pressure

As pointed out above we want to determine the pressure from the free-energy density by simply using eq. (8). A first test of eq. (8) consists in comparing the weak-coupling expansions of P/T^4 and $-f/T^4$. The expansions are obtained from those of the plaquettes, which were calculated up to order g^4 in ref. [6]. Of course, the integration constant to be used in eq. (5) is the value at $g^2=0$, i.e. we can only test the approach to this point. The integrand contains first a g^2-term, which must disappear to leave a finite integral. Indeed, with the values from ref. [6], we find for $N_{\sigma=16}$, $N_\tau=4$ a cancellation of the g^2-factor with an accuracy of 10^{-6}. The next term from the integral and the corresponding one from the pressure weak-coupling expansion (see, e.g., ref. [7]) coincide within 5%.

We have studied the problem of finite-size corrections to eq. (8) at intermediate β-values in the case of SU(2). There we have a large set of data on lattices with $N_\sigma=8$, 12, 18, 26 and $N_\tau=4$ from a finite-size analysis [8] and an investigation of the interaction measure Δ [7]. In addition we have calculated some new points on the $8^3\times4$ lattice below $\beta=2.24$. In fig. 1 we show the pressure data divided by T^4 resulting from the usual formula, ref. [1], involving the perturbative coupling derivatives. Inside the fluctuation of the data points (the error bars have been omitted for clarity, their size is of the order of the fluctuation for the data from each lattice size) the P/T^4 values show no significant finite-size effects. Indeed this is expected from finite-size scaling theory [8]. The corresponding data for $\Delta=(\epsilon-3P)/T^4$ are gathered in fig. 2. They show a considerable finite-size effect in the neighbourhood of the critical cou-
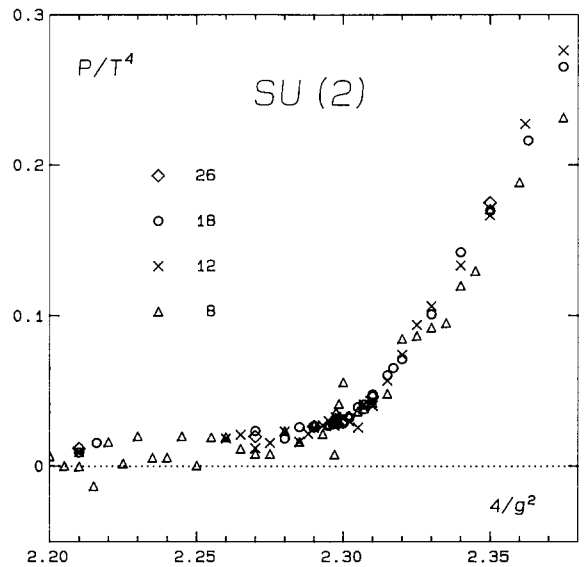

Fig. 1. Pressure divided by T^4 for the SU(2) gauge theory plotted against β on $N_\sigma=8$, 12, 18, 26 and $N_\tau=4$ lattices calculated with the conventional formula involving the perturbative coupling derivatives.
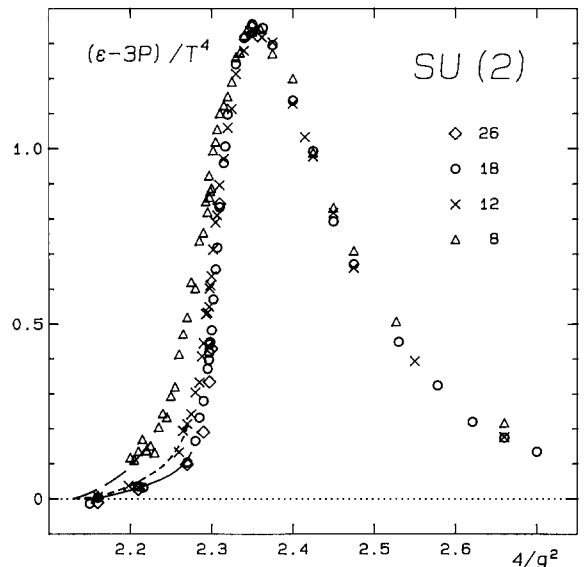

Fig. 2. The interaction measure $\Delta=(\epsilon-3P)/T^4$ for SU(2) gauge theory plotted against β, eq. (6), with adg^{-2}/da calculated from the weak-coupling scaling relation. The lines are fits through the small-β points, used for the integral in eq. (5) for $N_\sigma=8$ (long dashes), 12 (short dashes) and 18 (solid line).

pling, $\beta_c = 2.3$, up to about $\beta = 2.35$. Since Δ is proportional to the integrand in eq. (5) we expect a similar finite-size effect for f/T^4.

We have evaluated f from eq. (5) in two steps: in the regions where our data populations were dense enough, we have used the histogram technique [9] to find the integral contributions from the $N_\sigma^3 \times 4$ lattices, the contributions of the symmetric lattice were calculated from spline fits to high-statistics 16^4 lattice plaquette values in the same β-ranges; in the small-β region we have supplemented the Δ data by fits through the remaining few points (the fits are also shown in fig. 2) and then integrated these fits to obtain the lower integral parts. The errors from the histogram method are difficult to determine. Most probably they are much smaller than the fluctuation of data points, since information from many overlapping histograms (in the case of the $8^3 \times 4$ lattice we had 38, for $18^3 \times 4$ still 20) was used simultaneously. Errors from the fits to Δ and their integrals could shift the free-energy density curves slightly in the y-direction but would not change their shapes.

The resulting curves for $-f/T^4$ on $N_\sigma = 8$, 12, 18 lattices (for $N_\sigma = 26$ too few points were available) are compared in fig. 3 to the direct data for P/T^4 on the $18^3 \times 4$ lattice from fig. 1. We observe a strong volume dependence of the free-energy density indicating that $F = Vf$ is not an extensive quantity on small lattices. On the other hand, the $N_\sigma = 18$ curve is in perfect agreement with the direct data above and already at the transition point, i.e. for SU(2) we see in this region essentially no violation of the perturbative relations for the coupling derivatives. Below the phase transition the direct data should, however, deviate more and more from the true non-perturbative result.

We conclude that for SU(2) on lattices with $N_\sigma \gtrsim 15$ (and $N_\tau = 4$) the finite-size dependence of the free-energy density becomes negligible and therefore that eq. (8) is applicable. For SU(3) gauge theory we expect similar finite-size effects; in contrast to SU(2), however, a noticeable difference to the perturbative calculation is anticipated.

To calculate the pressure via eq. (8) we have taken the SU(3) data on $16^3 \times 4$ and 16^4 lattices from ref. [4]. In fig. 4a we show $N_\tau^4(2P_0 - P_\sigma - P_\tau)$ as obtained from the Δ-data of ref. [4], and the known factors in front of this quantity in eq. (6). The solid
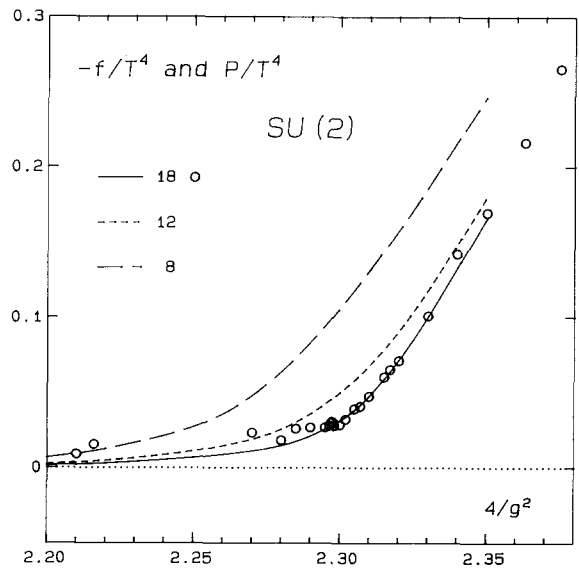

Fig. 3. Finite-size dependence of the free-energy density for the SU(2) gauge theory plotted against β. Compared are $-f/T^4$ from eq. (5) for $N_\sigma = 8$ (long dashes), 12 (short dashes) and 18 (solid line) with P/T^4 (circles) from the direct formula with perturbative coupling derivatives for the $18^3 \times 4$ lattice (same as in fig. 1).

curve in the plot is an interpolation of these data points, with a gap assumed at $\beta = 5.6925$. From this interpolation we evaluated the integral in eq. (5). The resulting non-perturbative P/T^4 is shown in fig. 4b together with the Monte Carlo data of ref. [4], which were calculated with perturbative coupling derivatives. We note that by construction this pressure is always continuous across the deconfinement transition. Evidently, our approach solved the unsatisfactory situation of a negative, discontinuous pressure.

4. Non-perturbative β-function and energy density

Already the early Monte Carlo renormalization group (MCRG) studies [10,11] of the QCD β-function have shown that there are considerable deviations from the weak-coupling scaling relation. In particular in the case of SU(3) large deviations have been observed for $\beta \gtrsim 5.7$, which, however, seem to disappear rapidly above $\beta \gtrsim 6.1$. The numerical results for the discrete β-function, $\Delta\beta(\beta)$, obtained from a stan-
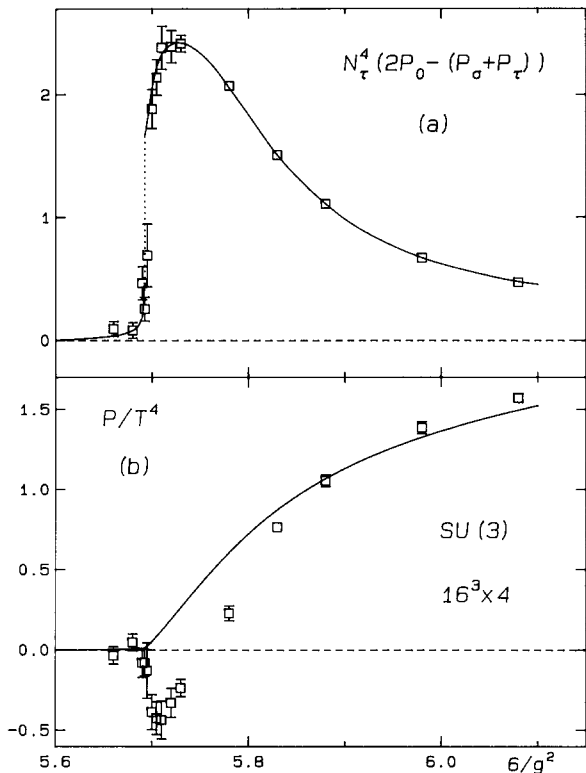
Fig. 4. (a) The difference between plaquette expectation values on asymmetric and symmetric lattices times N_τ^4 from Monte Carlo SU(3) data [4] on $16^3 \times 4$ and 16^4 lattices, respectively. The solid line is an interpolation through these data, used for the integral in eq. (5). (b) The non-perturbative result for the pressure in SU(3) gauge theory as a function of β along with the Monte Carlo data of ref. [4], based on perturbative coupling derivatives.

dard MCRG analysis, have been fitted with Padé approximants, in order to extract a non-perturbative β-function [12,13]. The approximants are chosen such that they are consistent with the perturbative form at large β and reproduce the observed scaling violations down to $\beta \simeq 5.7$. To be specific we use the following parametrization given in ref. [13]:

$$a \frac{\mathrm{d}g}{\mathrm{d}a} = b_0 g^3 \frac{(1 - a_1 g^2)^2 + a_2^2 g^4}{[1 - (a_1 + b_1/2b_0)g^2]^2 + a_3 g^4}, \qquad (10)$$

where $b_0 = 11N/48\pi^2$ and $b_1 = 34N^2/768\pi^4$ are the first two coefficients in the perturbative QCD β-function for SU(N) gauge theories. In the case of SU(3) we use the set of coefficients $\{a_1 = 0.853572, \ a_2 = 0.0000093, a_3 = 0.0157993\}$, given in ref. [13].

We have used this non-perturbative β-function and our interpolation of $N_\tau^4(2P_0 - P_\sigma - P_\tau)$, shown in fig. 4a, to extract the interaction measure Δ from eq. (6). This is plotted in fig. 5a as a solid curve. For comparison we show the unchanged data of ref. [4], which are based on the asymptotic weak-coupling scaling relation. Near the transition point, around $\beta = 5.7$, we observe a drop in Δ by about a factor two, which arises from the non-perturbative β-function. By construction the two results approach each other at higher β-values. The non-perturbative energy density was then found by adding three times the pressure from eq. (8) (solid curve in fig. 4b). In fig. 5b we compare the result (solid curve) again with the unchanged data from ref. [4]. A similar drop as in Δ occurs; in particular the slight peak in ϵ/T^4 near $\beta = 5.83$ has dis-
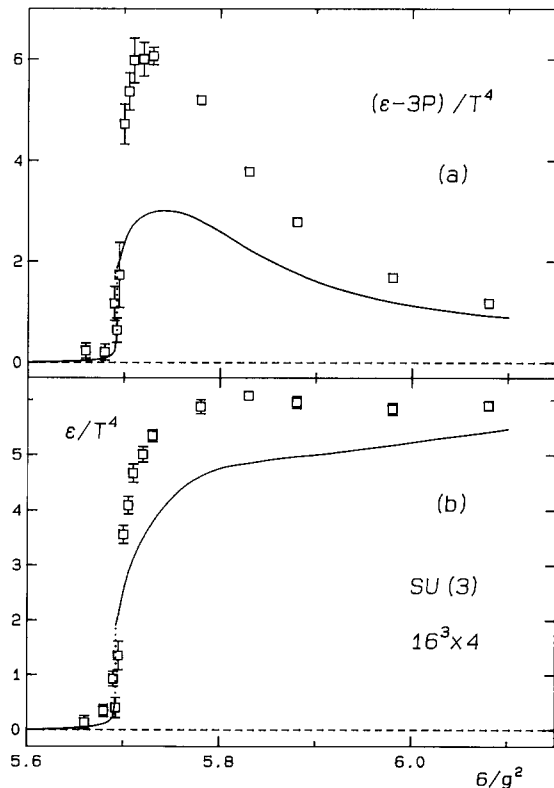

Fig. 5. The interaction measure $\Delta = (\epsilon - 3P)/T^4$, (a), and the energy density divided by T^4, (b), plotted against β for SU(3) gauge theory. The data are from ref. [4] and were calculated using perturbative coupling derivatives. The solid lines show the corresponding results when the pressure is computed from eq. (8) and the non-perturbative β-function, eq. (10), is taken into account.

appeared – the non-perturbative energy density is a very monotonously rising function and the gap $\Delta\epsilon/T^4$ is reduced considerably.

5. Summary and discussion

In summarizing, we have seen that, under the assumption of the homogeneity of the system, it is possible to calculate the pressure non-perturbatively on the lattice. By construction it is also continuous at the first-order transition points and it turns out to be positive everywhere. The information needed on an $N_\sigma^3 \times N_\tau$ lattice is just the expectation value of the average plaquette $(P_\sigma + P_\tau)$ and a corresponding value P_0 on a symmetric N_σ^4 lattice, i.e. essentially the actions.

From the same lattice data, the average plaquettes, one then determines the interaction measure $\epsilon - 3P$ and after that by the simple addition of $3P$ the energy density. In this second step, however, one needs the β-function. The non-perturbative β-function may change the shape of the energy density and the size of the latent heat density in SU(3) considerably. In fact it may resolve the problem of the N_τ-dependence of $\Delta\epsilon/T_c^4$ found in ref. [14]. Because of the continuity of the non-perturbative pressure there is no further ambiguity in the determination of the latent heat density, as is the case in the usual gap calculations from the enthalpy density, $\epsilon + P$, or $\epsilon - 3P$ involving the derivatives c_σ', c_τ' and the asymptotic β-function.

This ambiguity and its origin, the incomplete knowledge of the derivatives of the couplings with respect to the anisotropy ξ, was already noticed in one of the first determinations of the latent heat density in SU(3), ref. [15]. The cure in both refs. [14] and [15] was to impose the condition of continuity of the pressure at the transition point. The two calculations still differ in so far as in ref. [14] the quantity $\epsilon + P$, and in ref. [15] the quantity $\epsilon - 3P$, was used to extract the gap in the energy density. The enthalpy density $\epsilon + P$ depends on the difference of the partial derivatives given in eq. (1), while the interaction measure $\epsilon - 3P$ depends on the sum of these derivatives via eq. (2). If one insists on using perturbative coupling derivatives, the second quantity is to be preferred, because, owing to eq. (2), and the weak-coupling β-function the sum of the derivatives is known up to order g^2, the difference only to order g^0.

In full QCD theory, the same difficulties in the determination of the pressure appear, see, for example, ref. [16]. There too our procedure to obtain a physical pressure is applicable and certainly superior to the conventional approach as long as Monte Carlo simulations for thermodynamic quantities are restricted to rather small temporal lattices $(N_\tau \lesssim 10)$.

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