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On the Phase Diagram of Yang-Mills Theories in presence of a θ parameter

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We study the dependence of the deconfinement temperature on the θ parameter for $SU(N)$ gauge theories, with $N_c = 3, 4$. Results have been obtained for imaginary $\theta = i\theta_I$ and analytically continued to real values of θ in order to determine the curvature of the critical line $T_c(\theta)$. A comparison with reweighting at real θ is performed to check for the validity of analytic continuation. We also discuss the dependence of physical observables on the topological sector around the transition.

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1. Introduction

The possible presence of a θ term in the Lagrangian of Quantum Chromodynamics (QCD) has been widely discussed in the past. This term corresponds to the Lagrangian density

$$\mathscr{L}_{QCD} + \mathscr{L}_\theta = \mathscr{L}_{QCD} - i\theta\, q(x) = \mathscr{L}_{QCD} - i\theta \frac{g_0^2}{64\pi^2} \varepsilon_{\mu\nu\rho\sigma} F^a_{\mu\nu}(x) F^a_{\rho\sigma}(x)\,, \tag{1.1}$$

in which θ multiplies the topological charge density $q(x)$. $\mathscr{L}_\theta$ violates P and CP symmetries and it has intimately non-perturbative effects on the structure of non-Abelian gauge theories. Its value has been stringently bounded from above by experiments, $|\theta| \lesssim 10^{-10}$. Anyhow, the dependence of QCD on θ is very interesting both for theoretical and phenomenological reasons; an example is the solution to the $U(1)_A$ problem, that is related to the mass of the η' meson [1]. In the present study we focus on the effects induced by a non-zero θ term on the deconfinement phase transition of pure gauge Yang-Mills theories. The CP symmetry present at $\theta = 0$ suggests the critical temperature, $T_c(\theta)$, to be an even function of θ. Therefore we parameterize it as

$$T_c(\theta)/T_c(0) = 1 - R_\theta \theta^2 + \mathscr{O}(\theta^4). \tag{1.2}$$

In Section 2 we report our results [2, 3] for the value of the critical line curvature R_θ for the $SU(3)$ pure gauge theory. In our numerical lattice simulations we exploited analytic continuation to avoid the sign problem. We support the hypothesis of analyticity in θ around $\theta = 0$ with a study at small real θ performed via reweighting. In Section 3 we show the nontrivial dependence of the observables on the topological background, in particular close to the deconfinement transition. Finally in Section 4 we discuss preliminary results for $SU(4)$, in view of determining the large$-N_c$ behaviour of R_θ.

2. Critical Temperature dependence on θ in $SU(3)$

What is the fate of the critical deconfining temperature in QCD as the θ parameter is switched on? Computations, performed in the context of various models, indicate that it decreases [2, 4, 5, 6, 7]. The first non-perturbative numerical results for R_θ in the $SU(3)$ pure gauge theory were presented in Ref. [2], where we performed simulations at imaginary values of θ to circumvent the sign problem [8, 9, 10, 11]. In this approach the theory is assumed to be analytic around $\theta = 0$, a fact corroborated by our current knowledge about free energy derivatives with respect to θ at $\theta = 0$ [12, 13, 14, 15, 16, 17]. As for analytic continuation at nonzero μ_B [18, 19], we expect that linear terms in θ^2, hence R_θ, can be reliably determined by analytic continuation of results of simulations performed at imaginary $\theta = i\theta_I$ term, *i.e.* from numerical studies of the lattice partition function

$$\mathscr{Z}_L(T,\theta) = \int [dU]\, e^{-\theta_L Q_L[U] - S_L[U]}. \tag{2.1}$$

$[dU]$ indicates the integration over the gauge link variables $U_\mu(x)$. Q_L and S_L are respectively the lattice discretizations of the topological charge, $Q_L = \sum_x q_L(x)$, and of the pure gauge action. We considered the standard Wilson plaquette action, $S_L = \beta \sum_{x;\, \mu>\nu}(1 - \mathrm{ReTr}\Pi_{\mu\,\nu}(x)/N_c)$, where

$\beta = 2N_c/g_0^2$. The lattice discretized operator $q_L(x)$ is related, in general, to the continuum operator $q(x)$ by a multiplicative renormalization [20]:

$$q_L(x) \overset{a\to 0}{\sim} a^4 Z(\beta) q(x) + \mathcal{O}(a^6), \tag{2.2}$$

where $a = a(\beta)$ is the lattice spacing and $Z \to 1$ when $a \to 0$. The lattice parameter θ_L appearing in Eq. (2.1) is related to the imaginary part of θ by $\theta_I = Z(\beta)\theta_L$. Albeit the associated renormalization is large, a simple definition of $q_L(x)$ allows to keep Monte-Carlo algorithms rather efficient. Hence we use the gluonic definition

$$q_L(x) = \frac{-1}{2^9\pi^2} \sum_{\mu\nu\rho\sigma=\pm 1}^{\pm 4} \tilde{\varepsilon}_{\mu\nu\rho\sigma} \mathrm{Tr}\left(\Pi_{\mu\nu}(x)\Pi_{\rho\sigma}(x)\right), \tag{2.3}$$

where $\tilde{\varepsilon}_{\mu\nu\rho\sigma} = \varepsilon_{\mu\nu\rho\sigma}$ for positive directions and $\tilde{\varepsilon}_{\mu\nu\rho\sigma} = -\varepsilon_{(-\mu)\nu\rho\sigma}$. Standard heat-bath and over-relaxation algorithms over SU(2) subgroups are allowed with this definition of $q_L(x)$ [11]. Since Z_N center symmetry is not broken by the θ-term, we can adopt the Polyakov loop as the order parameter for deconfinement.

We performed simulations on four lattices (see below) to approach the continuum limit. On each lattice we chose $\sim 4-6$ values of θ_L and for each θ_L about 10 values of β close to the transition. The critical couplings $\beta_c(\theta_L)$ have been calculated by performing a Lorentzian fit to the data of the Polyakov loop susceptibility. From $\beta_c(\theta_L)$ we reconstruct $T_c(\theta_L)/T_c(0) = a(\beta_c(0))/a(\beta_c(\theta_L))$ by means of the non-perturbative determination of $a(\beta)$ reported in Ref. [21]. The location of T_c is affected by finite size corrections, which however should be greatly reduced when computing the ratio $T_c(\theta_L)/T_c(0)$. Finally, we converted θ_L into θ_I by exploiting the determination of the renormalizaton $Z(\beta)$ at the critical coupling β_c, which is obtained interpolating the data reported in Ref. [2]. The curvature R_θ was determined on three different lattices, $16^3 \times 4$, $24^3 \times 6$ and $32^3 \times 8$. Around the transition, they correspond to the same spatial volume in physical units and different lattice spacings, $a \simeq (4T_c)^{-1}, (6T_c)^{-1}$ and $(8T_c)^{-1}$. Then, in Ref. [3], we performed simulations on a finer lattice, $40^3 \times 10$, always at the same physical volume and at $a \simeq (10T_c)^{-1}$. The full set of results is reported in Table I of Ref. [3]. Assuming $\mathcal{O}(a^2)$ corrections, our continuum limit extrapolation for the curvature is $R_\theta = 0.0178(5)$.

Presently known techniques to circumvent the sign problem are only approximate and introduce systematic errors. We employ reweighting as an alternative approach in order to compare two independent methods and to cross-check the results. In this case the idea is to move the complex phase factor of the path integral inside the observable O:

$$\langle O \rangle_\theta = \frac{\int [dU]\, e^{-S_L[U]+i\theta Q}\, O}{\int [dU]\, e^{-S_L[U]+i\theta Q}} = \frac{\langle e^{i\theta Q} O\rangle}{\langle \cos(\theta Q)\rangle}. \tag{2.4}$$

The averages without subscript are taken at $\theta = 0$. We used the equality $\langle e^{i\theta Q}\rangle = \langle \cos(\theta Q)\rangle$ which comes from the $Q \to -Q$ symmetry of the topological charge distribution at $\theta = 0$.

The severeness of the sign problem can be estimated by the average phase factor. When $\langle \cos(\theta Q)\rangle$ vanishes unfeasibly large statistics would be needed to have reasonable statistical errors. QCD at finite baryon density is affected by similar problems [22]. Reweighting in θ proved to require larger statistics with respect to the imaginary θ approach. In particular, in order to be able to collect

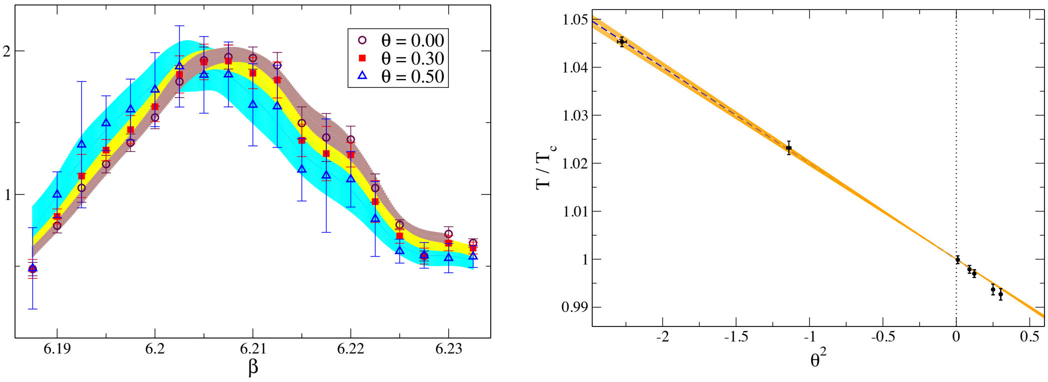

Figure 1: *Left* - The susceptibility of the Polyakov loop as a function of β at $\theta = 0$ and at a few values of real θ obtained via reweighting. The bands represents data reweighted also in β. *Right* - Critical temperature ratio as a function of θ^2, both for real and imaginary θ. The linear fit in θ^2, only on the data at $\theta^2 < 0$, is reported as well.

a sufficiently large sample of measures, we need the determination of the topological charge to be as cheap as possible. We used the cooling algorithm (see Ref. [12]) which provides reliable results on fine enough lattices: that is why we applied the reweighting method only to the $N_t = 10$ lattice. Q has been measured once every 10 cooling steps, up to a maximum of 40 steps. After having checked that the four choices lead to compatible results, we chose to use the results for Q obtained after $n_{cool} = 30$ cooling sweeps.
We discuss now the behavior of observables computed at nonzero θ by reweighting, and make a comparison with results from imaginary θ. We are interested in the modulus of the Polyakov loop,

$$\langle |L| \rangle_\theta = \frac{\langle e^{i\theta Q} |L| \rangle}{\langle e^{i\theta Q} \rangle} = \frac{\langle \cos(\theta Q) |L| \rangle}{\langle \cos(\theta Q) \rangle}, \tag{2.5}$$

and in its susceptibility, $\chi_L(\theta) = V_s(\langle |L|^2 \rangle_\theta - \langle |L| \rangle_\theta^2)$. The errors of χ_L and of the ratio of expectation values in Eq. (2.5) is computed via a jackknife algorithm. We have replaced also in the numerator $e^{i\theta Q}$ with its real part, $\cos(\theta Q)$. This is reasonable because the path integral measure at $\theta = 0$ and L are invariant under parity transformations, under which instead $Q \to -Q$.
In the left panel of Fig. 1, we show our results for the susceptibility as a function of β, obtained after reweighting at $\theta = 0.3$ and 0.5, together with the original data at $\theta = 0$. As θ increases the peak shifts to lower values of β, i.e. to lower temperatures, in agreement with the analytic continuation results. We extract from the susceptibility peaks the critical temperatures and compare them with results at imaginary θ. In the right panel of Fig. 1, we compare reweighted data with the linear extrapolation in θ^2, obtained by fitting results at imaginary θ. The agreement, within statistical errors, supports the validity of analytic continuation.
It would be interesting in the future to compare with results obtained via Langevin dynamics [23].

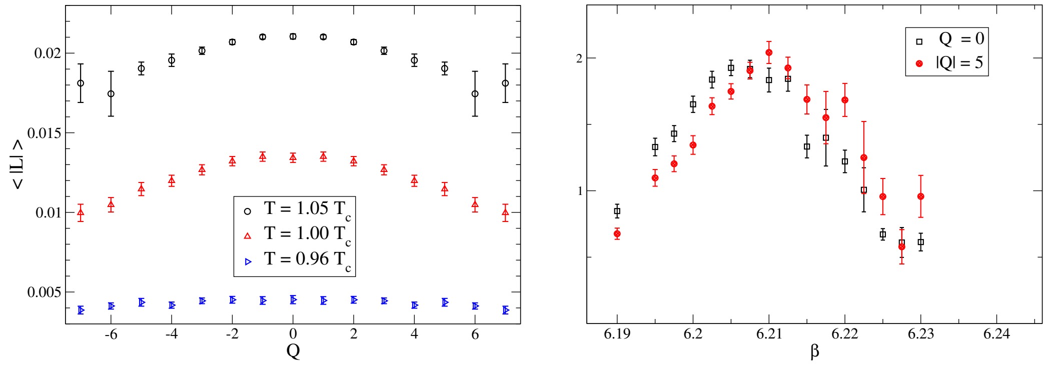

Figure 2: *Left* - Dependence of the modulus of the Polyakov loop on the topological sector Q. Simulations were performed for a few values of T around the transition on the $40^3 \times 10$ lattice. *Right* - Polyakov loop susceptibility for sector $Q = 0$ and $|Q| = 5$ as a function of β.

3. Polyakov Loop at fixed topological background in $SU(3)$

The general expression for a reweighted observable, Eq. (2.4), can be rewritten in the form:

$$\langle O \rangle_\theta = \frac{1}{\langle \cos(\theta Q) \rangle} \sum_{Q=-\infty}^{\infty} e^{i\theta Q} \, \mathscr{P}(Q) \, \langle O \rangle_Q \tag{3.1}$$

where $\langle \cdot \rangle_Q$ means the average in a fixed topological sector and $\mathscr{P}(Q)$ is the topological charge distribution at $\theta = 0$. Equation (3.1) shows that it is possible to have a non-trivial dependence on θ only if the observable depends on Q. The fact that the position of the deconfinement transition changes with θ suggests the physical observables to be Q dependent, especially around T_c. Investigating this kind of dependence is important to understand the possible systematic effects present in numerical simulations at fixed topological sector, e.g. for QCD with overlap fermions. Studies regarding these effects have been performed both at zero and finite T [24, 25, 26]; in particular, Ref. [26] shows that systematic effects in the determination of the topological susceptibility at finite T are under control.

We performed this study at fixed topological background on the finest lattice at our disposal ($40^3 \times 10$) because the determination of the topological charge is most reliable. We have divided the configurations sampled at each β and at $\theta = 0$ according to Q, which has been determined by cooling, as discussed previously. We show, in the left panel of Fig. 2, the behavior of the Polyakov loop as a function of Q for some temperatures around T_c

$$\langle |L| \rangle_{|Q|} = \frac{\sum_{i=1}^{M} |L|_i \, \delta_{|Q|,|Q_i|}}{\sum_{i=1}^{N} \delta_{|Q|,|Q_i|}}, \tag{3.2}$$

where M is the number of measures. In order to reduce statistical errors, we have combined observables in opposite topological sectors, using the symmetry of the Polyakov loop under P. As we can see, the dependence on $|Q|$ is quite mild below T_c, then it becomes stronger at the transition and finally slightly milder above deconfinement. The average plaquette displays a similar behaviour, but the relative variation between two different sectors is modest (never larger than 10^{-4}). Also the susceptibility of the Polyakov loop depends on Q: in the right panel of Fig. 2 it is plotted as a

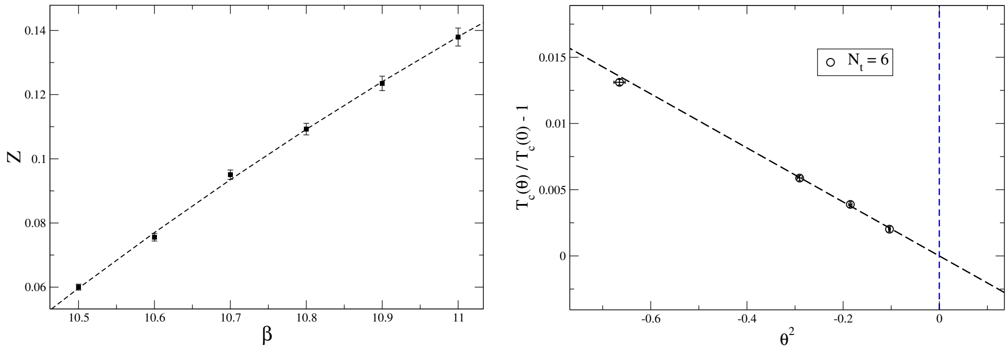

Figure 3: *Left* - Renormalization $Z(\beta)$ of the topological charge operator for $SU(4)$ determined on a 16^4 lattice, together with a quadratic interpolation. *Right* - Critical temperature ratio for $SU(4)$ on a $18^3 \times 6$ lattice as a function of θ^2. The dashed line is the linear fit in θ^2.

function of β for $Q = 0$ and $|Q| = 5$. We learn that deconfinement can be influenced by the overall topological background: the susceptibility peaks are shifting towards higher β (i.e. the critical temperature increases) with $|Q|$. This in qualitative agreement with the imaginary θ simulations: when $\theta_I \neq 0$ the average value of the topological charge $\langle Q \rangle_{\theta_I}$ becomes different from zero and T_c tends to increase. The values of $T_c(Q)$ that we obtained are reported in Table III of Ref. [3].

4. Preliminary results for $SU(4)$

Our determination of R_θ for $SU(3)$ ($R_\theta = 0.0178(5)$) is in rough agreement with the model prediction of Ref. [2], $T_c(\theta)/T_c(0) = 1 - \theta^2 \Delta\chi/(2\Delta\varepsilon) + \mathscr{O}(\theta^4)$, which is based on the fact that the transition is first order. $\Delta\varepsilon$ and $\Delta\chi$ are respectively the jump of the energy density and the drop of the topological susceptibility at the transition. In the large N_c limit, $\Delta\chi$ tends to the topological susceptibility χ computed at $T = 0$ and stays finite, while $\Delta\varepsilon \propto N_c^2$, so that $R_\theta \propto 1/N_c^2$. In particular the model predicts $R_\theta = 0.0281(62)$ for $N_c = 3$ and $R_\theta = 0.0158(35)$ for $N_c = 4$.
It is then interesting to study on the lattice the large$-N_c$ behaviour. We report here first results for $SU(4)$. In Figure 3 we show the multiplicative renormalization of the topological charge defined in Eq. (2.2), computed on a 16^4 lattice as $Z = \langle QQ_L \rangle / \langle Q^2 \rangle$. We determined the critical couplings β_c on a $18^3 \times 6$ lattice for several values of θ_I. The critical temperature ratios $(T_c(\theta) - T_c(0))/T_c(0)$ shown in Fig. 3 were computed using the nonperturbative string tension determination for $SU(4)$ of Ref. [27]. Fitting these data with a linear behaviour in θ^2 we obtained the critical line curvature $R_\theta(N_t = 6) = 0.0204(6)$. It the next future we will perform further simulations with other lattice spacings in order to be able to compute the continuum limit extrapolated value of R_θ in the $SU(4)$ Yang-Mills theory and to check for the validity of the large N_c prediction.

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