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θ-dependence of the deconfinement transition in Yang-Mills theories.

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We investigate the dependence of the deconfinement temperature of $SU(3)$ pure gauge theory on the topological θ parameter, finding that, for small values of θ, it decreases linearly in θ^2. The problem is approached numerically using lattice simulations at imaginary θ, in order to avoid the sign problem present at real θ, then exploiting analytic continuation. The dependence is also studied analytically in the limit of a large number of colors N, based on a simple model for the dependence of the topological susceptibility on T: we find that the critical temperature decreases linearly with θ^2/N^2; model results are comparable with numerical results obtained for $N = 3$.

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1. Introduction

The possible presence of a CP violating topological θ term in the QCD Lagrangian:

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

where $q(x)$ is the topological charge density, is constrained by stringent experimental upper bounds, ($|\theta| \lesssim 10^{-10}$). Nevertheless, the dependence of QCD and of $SU(N)$ gauge theories on θ is of great theoretical and phenomenological interest. θ derivatives of the vacuum free energy, computed at $\theta = 0$, enter various aspects of hadron phenomenology. An example is the topological susceptibility $\chi \equiv \langle Q^2 \rangle / V$ ($Q \equiv \int d^4x\, q(x)$ and V is the space-time volume), which enters the solution of the so-called $U(1)_A$ problem [1, 2].

In the present study we focus on the effects that a non-zero θ induces on the deconfinement phase transition of pure Yang-Mills theories. The CP symmetry present at $\theta = 0$ implies that the critical temperature, $T_c(\theta)$, must be an even function of θ, therefore we parameterize it as follows

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

In the following we will determine R_θ for the $SU(3)$ pure gauge theory by means of numerical lattice simulations, obtaining $R_\theta > 0$. Then we will discuss the results of a model computation, valid in the large N limit, showing that R_θ is expected to be $O(1/N^2)$.

2. Numerical approach: analytic continuation

Lattice simulations are the ideal tool to study non-perturbative effects related to θ dependence. Nevertheless, the Euclidean path integral representation of the partition function

$$Z(T,\theta) = \int [dA]\, e^{-S_{QCD}[A] + i\theta Q[A]} = e^{-V_s f(\theta)/T}, \tag{2.1}$$

is not suitable for Monte-Carlo simulations, because the measure is complex when $\theta \neq 0$. In Eq. (2.1) S_{QCD} is the pure gauge action, $f(\theta)$ is the free energy density and V_s is the spatial volume.

A similar sign problem appears for QCD at finite baryon chemical potential μ_B. In that case, a possible but not exhaustive solution is to study the theory at imaginary μ_B, where the measure is positive, then exploiting analytic continuation to infer the dependence at real μ_B, at least for small values of μ_B/T [3]. The approach proposed in Refs. [4, 5, 6, 7] for exploring a non-zero θ is identical in principle. As for $\mu_B \neq 0$ one assumes the theory to be analytical around $\theta = 0$: this fact is supported by our present knowledge about free energy derivatives at $\theta = 0$ [8, 9, 10, 11, 12].

As it happens for analytic continuation at nonzero μ_B [13], we expect that linear terms in θ^2, hence R_θ, can be determined reliably by analytic continuation from an imaginary $\theta \equiv i\theta_I$ term, i.e. from numerical studies of the lattice partition function:

$$Z_L(T,\theta) = \int [dU]\, e^{-S_L[U] - \theta_L Q_L[U]}, \tag{2.2}$$

where $[dU]$ is the integration over the elementary gauge link variables U_μ; S_L and Q_L are the lattice discretizations of respectively the pure gauge action and the topological charge, $Q_L = \sum_x q_L(x)$. We consider the Wilson plaquette action, $S_L = \beta \sum_{x,\mu>\nu}(1 - \mathrm{ReTr}\,\Pi_{\mu\nu}(x)/N)$, where $\beta = 2N/g_0^2$.

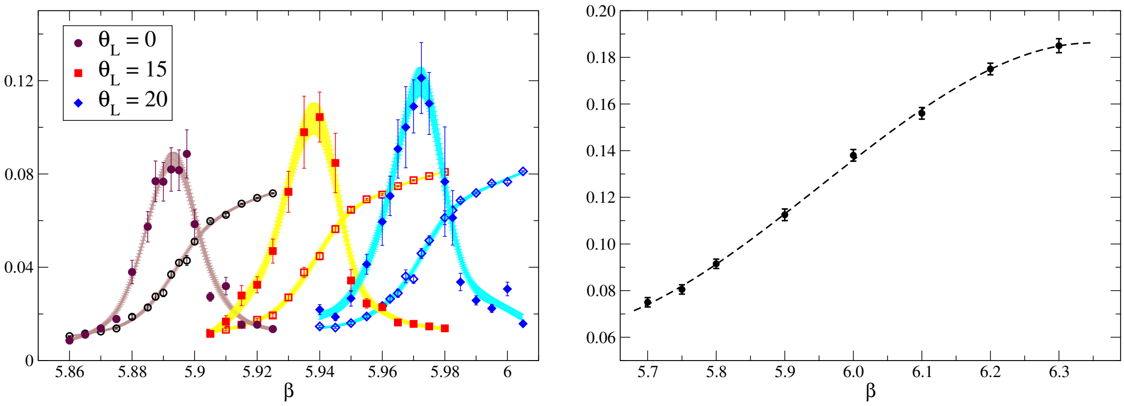

Figure 1: Left panel: Polyakov loop and its susceptibility as a function of β on a $24^3 \times 6$ lattice and for a few θ_L values. The susceptibility values have been multiplied by a factor 250. Right Panel: Determination of the renormalization constant Z on a 16^4 lattice. The dashed line is a cubic interpolation of data.

The lattice discretized operator $q_L(x)$ is linked, in general, to the continuum operator $q(x)$ by a finite multiplicative renormalization [14]

$$q_L(x) \overset{a\to 0}{\sim} a^4 Z(\beta) q(x) + O(a^6) \,, \tag{2.3}$$

where $a = a(\beta)$ is the lattice spacing and $\lim_{a\to 0} Z = 1$; therefore the imaginary part of θ is related to the lattice parameter θ_L appearing in Eq. (2.2) as follows: $\theta_I = Z\theta_L$. It is important, in order to keep the Monte-Carlo algorithm efficient enough, to choose a simple definition of $q_L(x)$, even if the associated renormalization is large. Following Ref. [7], we adopt the gluonic definition

$$q_L(x) = \frac{-1}{2^9 \pi^2} \sum_{\mu\nu\rho\sigma=\pm 1}^{\pm 4} \tilde{\varepsilon}_{\mu\nu\rho\sigma} \mathrm{Tr}\left(\Pi_{\mu\nu}(x)\Pi_{\rho\sigma}(x)\right) \,, \tag{2.4}$$

where $\tilde{\varepsilon}_{\mu\nu\rho\sigma} = \varepsilon_{\mu\nu\rho\sigma}$ for positive directions and $\tilde{\varepsilon}_{\mu\nu\rho\sigma} = -\tilde{\varepsilon}_{(-\mu)\nu\rho\sigma}$. That allows for a standard heat-bath + over-relaxation algorithm over $SU(2)$ subgroups [7].

The Z_N center symmetry, corresponding to gauge transformations which are periodic in the Euclidean time direction only up to a center group element, is exact for $SU(N)$ pure gauge theories and is spontaneously broken at their deconfinement transition. It remains exact also at finite θ_L, since $q_L(x)$ is a sum over closed local loops, hence we still expect Z_N spontaneous breaking and we can adopt the Polyakov loop and its susceptibility as probes for deconfinement

$$\langle L \rangle \equiv \frac{1}{V_s} \sum_{\vec{x}} \frac{1}{N} \langle \mathrm{Tr} \prod_{t=1}^{N_t} U_0(\vec{x},t) \rangle \qquad \chi_L \equiv V_s \left(\langle L^2 \rangle - \langle L \rangle^2 \right) \rangle \,, \tag{2.5}$$

where N_t is the number of sites in the temporal direction.

We have performed simulations on three different lattices, $16^3 \times 4$, $24^3 \times 6$ and $32^3 \times 8$, corresponding, around T_c, to equal spatial volumes (in physical units) and three different lattice spacings $a \simeq 1/(4T_c)$, $a \simeq 1/(6T_c)$ and $a \simeq 1/(8T_c)$. That permits us to perform a continuum limit extrapolation of our results. On each lattice, different series of simulations at fixed θ_L and variable β have been performed, with typical statistics of $10^5 - 10^6$ measurements, each separated by 4 over-relaxation + 1 heat-bath sweeps, for each θ_L. In Fig. 1 we show results for the Polyakov loop

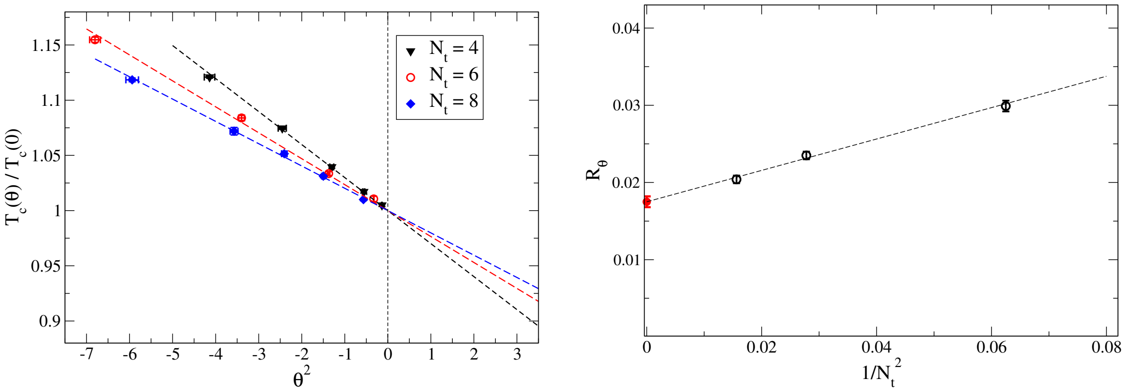

Figure 2: Left panel: $T_c(\theta)/T_c(0)$ as a function of θ^2 for different values of N_t. Dashed lines are the result of linear fits, as reported in the text, then extrapolated to $\theta^2 > 0$. Right panel: R_θ as a function of $1/N_t^2$. The point at $1/N_t = 0$ is the continuum limit extrapolation, assuming $O(a^2)$ corrections.

modulus and its susceptibility as a function of β for a few values of θ_L on a $24^3 \times 6$ lattice; we also show data obtained after reweighting in β.

The critical coupling $\beta_c(\theta_L)$ has been located at the maximum of the susceptibility after a Lorentzian fit to unreweighted data. We checked that the values obtained at $\theta_L = 0$ coincide, within errors, with those found in previous works [15]. 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. [15]. Notice that most finite size effects in the determination of $\beta_c(\theta_L)$ are expected to cancel when computing the ratio $T_c(\theta_L)/T_c(0)$. A complete set of results is reported in Table 1 of Ref. [16].

Finally, we need to convert θ_L into the continuum parameter $\theta = i\,\theta_I$. Possible methods for a non-perturbative determination of the renormalization constant $Z(\beta)$ are based on the assumption that the ultraviolet fluctuations responsible for Z are independent of the topological background [17]; here, following Ref. [7], we obtain Z in terms of averages over the thermal ensemble:

$$Z = \langle Q Q_L \rangle / \langle Q^2 \rangle \tag{2.6}$$

where Q is, configuration by configuration, the integer closest to the topological charge obtained after cooling. Z has been determined for a set of β values on a symmetric 16^4 lattice (see Fig. 1), then obtaining Z at the critical values of β by a cubic interpolation. A check for systematic effects has been done by changing the number of cooling sweeps (15, 30, 45 and 60 sweeps) and, at the highest explored value of β, by exploring also a larger 24^4 lattice. In this way we finally obtain $\theta_I(\beta_c(\theta_L)) = Z(\beta_c(\theta_L))\,\theta_L$. The values of θ_I we have obtained are reported in the 4th column of Table 1 in Ref. [16]. Final results for $T_c(\theta_I)/T_c(0)$ and for the three different lattices explored are reported in Fig. 2. In all cases a linear dependence in θ^2, according to Eq. (1.2), nicely fits data. In particular we obtain $R_\theta = 0.0299(7)$ for $N_t = 4$ (χ^2/d.o.f. $\simeq 0.3$), $R_\theta = 0.0235(5)$ for $N_t = 6$ (χ^2/d.o.f. $\simeq 1.6$) and $R_\theta = 0.0204(5)$ for $N_t = 8$ (χ^2/d.o.f. $\simeq 0.7$). Assuming $O(a^2)$ (i.e. $O(1/N_t^2)$) corrections, we can extrapolate the continuum value $R_\theta = 0.0175(7)$, χ^2/d.o.f. $\simeq 0.97$ (see Fig. 2). We conclude that T_c decreases in presence of a real non-zero θ, in agreement with arguments based on model [18, 19] and semi-classical [20] computations.

3. Large N estimate

A first order transition is the point where the free energies of two different phases get the same value. Let $f_{d/c}$ be the free energies associated to the deconfined/confined phase of $SU(N)$ gauge theories. around T_c they can be expanded, apart from a common constant, in terms of $t = (T - T_c)/T_c$: $f_{c/d}/T = A_{c/d}\,t + O(t^2)$. The slope difference is related to the latent heat $\Delta\varepsilon = T_c(A_c - A_d)$.

At $\theta \neq 0$ both free energies get an additional contribution which, at the lowest order in θ, reads $\chi(T)\theta^2/T$, where $\chi(T)$ is the topological susceptibility at $\theta = 0$. Our model exploits the fact that in the large N limit $\chi(T) = \chi(0) \equiv \chi$ for $T < T_c$ and $\chi(T) = 0$ for $T > T_c$ [21, 22, 23], hence

$$f_c/T = A_c\,t + \chi\theta^2/2T + O(t^2) \qquad f_d/T = A_d\,t + O(t^2)$$

From this argument one can obtain $T_c(\theta)$ by finding the temperature at which $f_c = f_d$, the result is

$$\frac{T_c(\theta)}{T_c(0)} = 1 - \frac{\chi}{2\Delta\varepsilon}\theta^2 + O(\theta^4) = 1 - \frac{0.253(56)}{N^2}\theta^2 + O(1/N^4) \tag{3.1}$$

where $\Delta\varepsilon$ is again the latent heat of the transition $\theta = 0$. The coefficient of the quadratic term have been determined numerically using the results in [8, 22, 24]. We can extrapolate such result to $SU(3)$, getting $R_\theta \simeq 0.0282(62)$: this is larger than our determination, but we expect that since, for $SU(3)$, our assumption for a sharp drop of χ at T_c is not true, the actual behavior being smoother [21]. It would be interesting to extend our numerical results to $N > 3$, in order to check Eq. (3.1), as well as to $N = 2$, to compare with the results of Ref. [20]. From Eq. (3.1) we read that R_θ scales as $1/N^2$ in the large N limit, in agreement with general arguments predicting the free energy to be a function of θ/N [25]: therefore in the large N limit T_c should be θ independent.

4. Conclusions and speculations

We have discussed the $\theta-$dependence of the deconfinement temperature in $SU(3)$ pure gauge theories. Exploiting analytic continuation from imaginary to real θ, we have deduced that T_c decreases with θ, the curvature of the critical line being $R_\theta = 0.0175(7)$ at $\theta = 0$. As it happens for the $T - \mu_B^2$ plane case, other transition lines may be present in the $T - \theta^2$ plane. For $\mu_B^2 < 0$ one finds unphysical transitions, known as Roberge-Weiss lines [26], associated with the periodicity of the theory in imaginary μ_B. In the case of the $T - \theta^2$ diagram the situation is different but similar in some sense: no periodicity is expected for imaginary θ, CP being explicitely broken for any nonzero θ_I, hence we cannot predict other possible transitions for $\theta^2 < 0$. A $2\pi-$periodicity is instead expected for real θ, with a possible phase transition at $\theta = \pi$ where CP breaks spontaneously. Our simulations give evidence only for a deconfinement transition line, which is linear in θ^2 at least for small real θ: non-trivial corrections may appear as θ approaches π. However, following Ref. [25] and the arguments above, we speculate that, at least for large N, $T_c(\theta)$ be a multibranched function, dominated by the quadratic term also down to $\theta = \pi$

$$T_c(\theta)/T_c(0) \simeq 1 - R_\theta \min_k (\theta + 2\pi k)^2 \tag{4.1}$$

where k is a relative integer. Periodicity in θ implies cusps for the function $T_c(\theta)$ at $\theta = (2k+1)\pi$, where the deconfinement line could meet the CP breaking transition present also at $T = 0$. A similar situation has been described in Ref. [19]. Therefore, analogies may be present between the real θ case and what found at imaginary μ_B.

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