\( \theta \)-dependence of the deconfinement temperature in Yang-Mills theories.

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We determine the \( \theta \) dependence of the deconfinement temperature of SU(3) pure gauge theory, finding that it decreases in presence of a topological \( \theta \) term. We do that by performing lattice simulations at imaginary \( \theta \), then exploiting analytic continuation. We also give an estimate of such dependence in the limit of a large number of colors \( N \), and compare it with our numerical results.

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The possible effects of a CP violating term in Quantum ChromoDynamics (QCD) have been studied since long. Such term enters the Euclidean lagrangian as follows:

\[
\mathcal{L}_\theta = \mathcal{L}_{\text{QCD}} - i \theta q(x)
\]

\[
q(x) = \frac{g_0^2}{64 \pi^2} \epsilon_{\mu\nu\rho\sigma} F^a_{\mu\nu}(x) F^a_{\rho\sigma}(x)
\]

where \( q(x) \) is the topological charge density.

Experimental upper bounds on \( \theta \) are quite stringent (\( |\theta| \lesssim 10^{-10} \)), suggesting that such term may be forbidden by some mechanism. Nevertheless, the dependence of QCD and of SU(\( N \)) gauge theories on \( \theta \) is of great theoretical and phenomenological interest. \( \theta \) derivatives of the vacuum free energy, computed at \( \theta = 0 \), enter various aspects of hadron phenomenology; an example is the topological susceptibility \( \chi \equiv (Q^2)/V \) \( (Q = \int d^4x \; q(x) \) and \( V \) is the space-time volume), which contains the solution of the so-called \( U(1)_A \) problem \[3\] \[4\]. Moreover it has been proposed \[3\] that topological charge fluctuations may play an important role at finite temperature \( T \), especially around the deconfinement transition, where local effective variations of \( \theta \) may be detectable as event by event \( P \) and CP violations in heavy ion collisions.

In the present work we study the effect of a non-zero \( \theta \) on the critical deconfining temperature \( T_c \), considering the case of pure Yang-Mills theories. Due to the symmetry under CP at \( \theta = 0 \), the critical temperature \( T_c(\theta) \) is expected, similarly to the free energy, to be an even function of \( \theta \). Therefore we parameterize \( T_c(\theta) \) as follows

\[
\frac{T_c(\theta)}{T_c(0)} = 1 - R_\theta \theta^2 + O(\theta^4)
\]

In the following we shall determine \( R_\theta \) for the SU(3) pure gauge theory, obtaining \( R_\theta > 0 \), and compare it with a simple model computation valid in the large \( N \) limit, showing that \( R_\theta \) is expected to be \( O(1/N^2) \).

The method – Effects related to the topological \( \theta \) term are typically of non-perturbative nature, hence numerical simulations on a lattice represent the ideal tool to explore them. However, it is well known that the Euclidean path integral representation of the partition function

\[
Z(T, \theta) = \int [dA] \; e^{-S_{\text{QCD}}[A] + i \theta Q[A]} = e^{-V_t f(\theta)/T},
\]

is not suitable for Monte-Carlo simulations because the measure is complex when \( \theta \neq 0 \). \( S_{\text{QCD}} = \int d^4x \; \mathcal{L}_{\text{QCD}} \) and periodic boundary conditions are assumed over the compactified time dimension of extension \( 1/T \); \( f(\theta) \) is the free energy density and \( V_t \) is the spatial volume.

A similar sign problem is met for QCD at finite baryon chemical potential \( \mu_B \), where the fermion determinant becomes complex. In that case, a possible partial solution is to study the theory at imaginary \( \mu_B \), where the sign problem disappears, and then make use of analytic continuation to infer the dependence at real \( \mu_B \), at least for small values of \( \mu_B/T \) \[4\]. An analogous approach has been proposed for exploring a non-zero \( \theta \) \[3\] \[8\]; as for \( \mu_B \neq 0 \), also in this case one assumes that the theory is analytic around \( \theta = 0 \), a fact supported by our present knowledge about free energy derivatives at \( \theta = 0 \) \[3\] \[10\].

Various studies have shown that the dependence of the critical temperature on the baryon chemical potential, \( T_c(\mu_B) \), can be determined reliably up to the quadratic order in \( \mu_B \), while ambiguities related to the procedure of analytic continuation may affect higher order terms \[11\]. It is natural to assume that a similar scenario takes place for analytic continuation from an imaginary \( \theta = i \theta_t \) term, i.e. that \( R_\theta \) can be determined reliably from numerical studies of the lattice partition function:

\[
Z_L(T, \theta) = \int [dU] \; e^{-S_L[U] - \theta L Q_L[U]},
\]

where \( [dU] \) is the integration over the elementary gauge link variables \( U_{\mu} \); \( S_L \) 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 will consider the Wilson action, \( S_L = \beta \sum_{x,\mu>\nu} (1 - \text{Re} \text{Tr} \Pi_{\mu\nu}(x)/N) \) where \( \beta = 2N/g_0^2 \) and \( \Pi_{\mu\nu} \) is the plaquette operator.
Various choices are possible for the lattice operator $q_L(x)$, which in general are linked to the continuum $q(x)$ by a finite multiplicative renormalization \[ q_L(x) \sim a^d Z(\beta) q(x) + O(a^6), \] where $a = a(\beta)$ is the lattice spacing and $\lim_{\beta \to 0} Z = 1$. Hence, as the continuum limit is approached, the imaginary part of $\theta$ is related to the lattice parameter $\theta_L$ appearing in Eq. (4) as follows: $\theta = Z \theta_L$.

Since $q_L(x)$ enters directly the functional integral measure, it is important, in order to keep the Monte-Carlo algorithm efficient enough, to choose a simple definition, even if the associated renormalization is large. Therefore, following Ref. [8], we adopt the gluonic definition

\[ q_L(x) = \frac{-1}{24\pi^2} \sum_{\mu, \nu, \rho, \sigma = \pm 1} \varepsilon_{\mu \nu \rho \sigma} \text{Tr} \left( \Pi_{\mu \nu}(x) \Pi_{\rho \sigma}(x) \right), \] where $\varepsilon_{\mu \nu \rho \sigma} = \varepsilon_{\mu \nu \rho \sigma}$ for positive directions and $\tilde{\varepsilon}_{\mu \nu \rho \sigma} = -\varepsilon_{\mu \nu (-\rho) \sigma}$. With this choice gauge links still appear linearly in the modified action, hence a standard heat-bath algorithm over $SU(2)$ subgroups, combined with overrelaxation, can be implemented.

Finite temperature $SU(N)$ pure gauge theories possess the so-called center symmetry, corresponding to a multiplication of all parallel transports at a fixed time by an element of the center $Z_N$. Such symmetry is spontaneously broken at the deconfinement transition and the Polyakov loop is a suitable order parameter. Since $q_L(x)$ is a sum over closed loops, the modified action $S_L + \theta_L Q_L$ is also center symmetric, hence we still expect $Z_N$ spontaneous breaking and we will adopt the Polyakov loop and its susceptibility as probes for deconfinement

\[ \langle L \rangle \equiv \frac{1}{V_s} \frac{1}{N} \text{Tr} \left( \prod_{t=1}^{N_t} U_0(x, t) \right), \]
\[ \chi_L \equiv V_s \left( \langle L^2 \rangle - \langle L \rangle^2 \right), \] where $N_t$ is the number of sites in the temporal direction.

**Results** – In the following we present results obtained 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 will permit us to extrapolate $R_D$ to the continuum limit.

We have performed, on each lattice, several series of simulations at fixed $\theta_L$ and variable $\beta$. Typical statistics have been of $10^5 - 10^6$ measurements, each separated by a cycle of 4 over-relaxation + 1 heat-bath sweeps, for each run; autocorrelation lengths have gone up to $O(10^4)$ cycles around the transition. In Fig. 1 we show results for the Polyakov loop modulus and its susceptibility as a function of $\beta$ for a few values of $\theta_L$ on a $24^3 \times 6$ lattice; we also show data obtained after reweighting in $\beta$. We notice a slight increase in the height of the susceptibility peak as $\theta_L$ increases, however any conclusion regarding the influence of $\theta$ on the strength of the transition would require a finite size scaling analysis and is left to future studies.

The critical coupling $\beta_c(\theta_L)$ is located at the maximum of the susceptibility through a Lorentzian fit to unweighted data: values obtained at $\theta_L = 0$ coincides within errors with those found in previous works [13]. 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. [13]. Notice that most finite size effects in the determination of $\beta_c(\theta_L)$ should cancel when computing the ratio $T_c(\theta_L)/T_c(0)$.

A complete set of results is reported in Table I.

**TABLE I:** Collection of results obtained for $\beta_c$ and $T_c$.

| Lattice | $\theta_L$ | $\beta_c$ | $\theta_L$ | $T_c(\theta_L)/T_c(0)$ |
|---------|------------|-----------|------------|--------------------------|
| $16^3 \times 4$ | 0 | 5.6911(4) | 0 | 1 |
| $16^3 \times 4$ | 5 | 5.6934(6) | 0 | 0.409(10) |
| $16^3 \times 4$ | 10 | 5.6990(7) | 0.747(15) | 1.0171(12) |
| $16^3 \times 4$ | 15 | 5.7092(7) | 1.141(20) | 1.0395(11) |
| $16^3 \times 4$ | 20 | 5.7248(6) | 1.566(30) | 1.0746(10) |
| $16^3 \times 4$ | 25 | 5.7447(7) | 2.035(30) | 1.1290(10) |
| $24^3 \times 6$ | 0 | 5.8929(8) | 0 | 1 |
| $24^3 \times 6$ | 5 | 5.8985(10) | 0.750(90) | 1.0105(24) |
| $24^3 \times 6$ | 10 | 5.9105(5) | 1.168(12) | 1.0335(18) |
| $24^3 \times 6$ | 15 | 5.9394(8) | 1.836(18) | 1.0834(23) |
| $24^3 \times 6$ | 20 | 5.9717(8) | 2.600(24) | 1.1534(24) |
| $32^3 \times 8$ | 0 | 6.0622(6) | 0 | 1 |
| $32^3 \times 8$ | 5 | 6.0684(3) | 0.753(8) | 1.0100(11) |
| $32^3 \times 8$ | 8 | 6.0813(6) | 1.224(15) | 1.0312(14) |
| $32^3 \times 8$ | 10 | 6.0935(11) | 1.551(20) | 1.0515(21) |
| $32^3 \times 8$ | 12 | 6.1095(21) | 1.890(24) | 1.0719(34) |
| $32^3 \times 8$ | 15 | 6.1337(27) | 2.437(30) | 1.1201(17) |

FIG. 1: Polyakov loop and its susceptibility as a function of $\beta$ on a $24^3 \times 6$ lattice and for a few $\theta_L$ values. The susceptibility values have been multiplied by a factor 250.
parameter $\theta = i \theta_1$. A well known method for a non-perturbative determination of the renormalization constant $Z = Z(\beta)$ is that based on heating techniques [14]. Here we follow the method proposed in Ref. [8], giving $Z$ in terms of averages over the thermal ensemble:

$$Z = \langle QQ_L \rangle / \langle Q^2 \rangle$$  \hspace{1cm} (8)

where $Q$ is, configuration by configuration, the integer closest to the topological charge obtained after cooling. Such method assumes, as usual, that UV fluctuations responsible for renormalization are independent of the topological background. $Z$ has been determined for a set of $\beta$ values on a symmetric $16^4$ lattice, as reported in Fig. 2 then obtaining $Z$ at the critical values of $\beta$ by a cubic interpolation. Typical statistics have been of $10^6$ measurements, each separated by 5 cycles of 4 over-relaxation + 1 heat-bath sweeps, for each $\beta$; the autocorrelation length of $Q$ has reached a maximum of $10^3$ cycles at the highest value of $\beta$. A check for systematic effects has been done by repeating the determination with a different number of cooling sweeps to obtain $Q$ (15, 30, 45 and 60) or, at the highest explored value of $\beta$, on a larger $24^4$ lattice. In this way we finally obtain $\chi(\beta_c(\theta_L)) = Z(\beta_c(\theta_L)) \theta_L$, as reported in the 4th column of Table I. The results for $T_c(\theta)$ and for the three different lattices explored are reported in Fig. 3. In all cases a linear dependence in $\theta^2$, according to Eq. (2), nicely fits the data. In particular we obtain $R_0 = 0.0299(7)$ for $N_t = 4$ ($\chi^2$/d.o.f. $\simeq 0.3$), $R_0 = 0.0235(5)$ for $N_t = 6$ ($\chi^2$/d.o.f. $\simeq 1.6$) and $R_0 = 0.0204(5)$ for $N_t = 8$ ($\chi^2$/d.o.f. $\simeq 0.7$).

We have performed various tests to check the stability of our fits. If we change the fit range, e.g. by excluding, for each $N_t$, the 1-2 largest values of $\theta_1$, results for $R_\theta$ are stable within errors. If we assume a generic power like behavior $T_c(\theta)/T_c(0) = 1 + A \theta^\alpha$, we always obtain that $\alpha$ is compatible with 2 within errors; if we fix $\alpha$ to values which would imply a non-analyticity at $\theta = 0$, e.g. $\alpha = 1$, we obtain a $\chi^2$/d.o.f. of $O(10)$ or larger.

Assuming $O(a^2)$ corrections we extrapolate the continuum limit $R_\theta = 0.0175(7)$, $\chi(0)$, $\chi^2$/d.o.f. $\simeq 0.97$ (see Fig. 1). Our result is therefore that $T_c$ decreases in presence of a real non-zero $\theta$ parameter. This is in agreement with the large $N$ expectation that we discuss in the following, as well as with arguments based on the semi-classical approximation discussed in Ref. [13] for $N = 2$ and with model computations [16].

Large $N$ estimate – We present now a simple argument to estimate the dependence of $T_c$ on $\theta$ in the large $N$ limit. Since the transition is first order, around the critical temperature we can define two different free energy densities, $f_c(T)$ and $f_d(T)$, corresponding to the two different phases, confined and deconfined, which cross each other at $T_c$ with two different slopes. The slope difference is related to the latent heat. Indeed the energy density

$$\epsilon = -T^2 \frac{\partial f(T)}{\partial T} \log Z ; \; \; Z = \exp \left( - \frac{V_s f(T)}{T} \right)$$  \hspace{1cm} (9)

hence $\epsilon = -T^2 \frac{\partial f(T)}{\partial T}$. Close enough to a first order transition we may assume, apart from constant terms, $f_c(T) = A_c T + O(t^2)$ and $f_d(T) = A_d t + O(t^4)$, where $t \equiv (T - T_c)/T_c$ is the reduced temperature. The latent heat is therefore $\Delta \epsilon = \epsilon_d - \epsilon_c = T_c(A_c - A_d)$.

A non-zero $\theta$ modifies the free energy, at the lowest order, as follows:

$$f(T, \theta) = f(T, \theta = 0) + \chi(T) T^2 / 2 \; + \; O(\theta^4)$$  \hspace{1cm} (10)

where $\chi(T)$ is the topological susceptibility. $\chi(T)$ is in general different in the two phases, dropping at deconfinement [17,19], hence the condition for free energy equilibrium, $f_c = f_d$, which gives the value of $T_c$, will change
as a function of \( \theta \). The dependence of \( \chi \) on \( T \) simplifies in the large \( N \) limit, being independent of \( T \) in the confined phase and vanishing in the deconfined one \(^{[18, 19]} \). Hence we can write, for \( N \to \infty \),

\[
f_c/T \simeq A_c t + (\chi/T) \theta^2/2; \quad f_d/T \simeq A_d t \quad (11)
\]

where \( \chi \) is, from now on, the \( T = 0 \) topological susceptibility. The equilibrium condition then reads \((A_c - A_d) t = (\chi/T) \theta^2/2 + O(\theta^4)\), giving

\[
T_c(\theta)/T_c(0) = 1 - \frac{\chi}{2\Delta_c} \theta^2 + O(\theta^4) \quad (12)
\]

In the large \( N \) limit we have \(^{[18, 20]} \),

\[
\frac{\chi}{\sigma^2} \simeq 0.0221(14); \quad \frac{\Delta_c}{N^2 T_c} \simeq 0.344(72); \quad T_c/\sqrt{\sigma} \simeq 0.5970(38)
\]

apart from \( 1/N^2 \) corrections, hence we get

\[
R_\theta = \frac{\chi}{2\Delta_c} \simeq \frac{0.253(56)}{N^2} + O(1/N^4) \quad (13)
\]

The leading \( 1/N \) estimate for \( SU(3) \) is then \( R_\theta \simeq 0.0281(62) \). This is larger than our determination, even if marginally compatible with it: a possible interpretation is that for \( SU(3) \) the behavior of \( \chi \) at \( T_c \) is smoother than the sharp drop to zero that we have assumed.

Notice that the \( 1/N^2 \) dependence of \( R_\theta \) is in agreement with general arguments \(^{[21]} \) predicting the free energy to be a function of the variable \( \theta^2/N \) as \( N \to \infty \) (see also Refs. \(^{[4, 15]} \)). For the same reason we expect \( O(\theta^2) \) corrections to Eq. (12) to be of \( O(1/N^4) \): they are indeed related to \( O(\theta^4) \) corrections to the free energy, which have been measured at \( T = 0 \) by lattice simulations \(^{[22, 24]} \) and are known to be small and of order \( 1/N^2 \).

It would be interesting to extend the present study to \( N > 3 \), in order to check the prediction in Eq. (13), and to \( N = 2 \), in order to compare with the results of Ref. \(^{[15]} \).

We conclude with a few remarks and speculations regarding the phase structure in the \( T - \theta^2 \) plane. In Fig. 3 we have drawn the critical line, for different \( N_c \) and up to \( \theta^2 \) terms, as fitted from \( \theta^2 < 0 \) simulations, and its continuation to \( \theta^2 > 0 \); however other transition lines may be present, as it happens for the \( T - \mu_B^2 \) plane. For \( \mu_B^2 < 0 \) one finds unphysical transitions, known as Roberge-Weiss lines \(^{[22]} \), which are linked to the periodicity of the theory in terms of imaginary \( \mu_B \). In the case of a \( \theta \) parameter, no periodicity is expected for imaginary \( \theta \), \( CP \) invariance being explicitly broken for any \( \theta \neq 0 \), hence we cannot predict other possible transitions for \( \theta^2 < 0 \). A \( 2\pi \) periodicity is instead expected for real values of \( \theta \), with the possible presence of a phase transition at \( \theta = \pi \) where \( CP \) breaks spontaneously.

Our simulations have given evidence, for \( \theta^2 < 0 \), only for a deconfinement transition line, describable by a \( \theta^2 \) behavior up to \( |\theta| \approx \pi \). We expect continuity of such behavior, at least for small real \( \theta \), while non-trivial corrections may appear as \( \theta \) approaches \( \pi \). However, following Ref. \(^{[21]} \) and the arguments above, we speculate that, at least for large \( N \), \( T_c(\theta) \) be a multibranched function, dominated by the quadratic term down to \( \theta = \pi \)

\[
T_c(\theta)/T_c(0) \simeq 1 - R_\theta \min (\theta + 2\pi k)^2
\]

where \( k \) is a relative integer; in this case periodicity in \( \theta \) implies cusps for \( T_c(\theta) \) at \( \theta = (2k + 1) \pi \), where the deconfinement line could meet the CP breaking transition present also at \( T = 0 \). Therefore the phase diagram at real \( \theta \) could have some analogies with that found at imaginary \( \mu_B \).

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