θ Dependence of the Deconfinement Temperature in Yang-Mills Theories

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We determine the θ dependence of the deconfinement temperature of $SU(3)$ pure gauge theory, finding that it decreases in the presence of a topological θ term. We do that by performing lattice simulations at imaginary θ, 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 for a long time. Such a term enters the Euclidean Lagrangian as follows:

$$\mathcal{L}_\theta = \mathcal{L}_{\rm QCD} - i\theta q(x), \qquad q(x) = \frac{g_0^2}{64\pi^2}\epsilon_{\mu\nu\rho\sigma}F^a_{\mu\nu}(x)F^a_{\rho\sigma}(x), \tag{1}$$

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

Experimental upper bounds on θ 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 θ is of great theoretical and phenomenological interest. The 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]. 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 θ 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 nonzero θ 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 θ. Therefore we parameterize $T_c(\theta)$ as follows

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

In the following we shall determine R_θ 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_θ is expected to be $O(1/N^2)$.

The method.—Effects related to the topological θ term are typically of a nonperturbative 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

$$Z(T,\theta) = \int [dA]e^{-S_{\rm QCD}[A]+i\theta Q[A]} = e^{-V_s f(\theta)/T} \tag{3}$$

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

A similar sign problem is met for QCD at finite baryon chemical potential μ_B, where the fermion determinant becomes complex. In that case, a possible partial solution is to study the theory at imaginary μ_B, where the sign problem disappears, and then make use of analytic continuation to infer the dependence at real μ_B, at least for small values of μ_B/T [4]. An analogous approach has been proposed for exploring a nonzero θ [5–8]; 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 $\theta = 0$ [9,10].

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 μ_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 $\theta \equiv i\theta_I$ term, i.e., that R_θ can be determined reliably from numerical studies of the lattice partition function,

$$Z_L(T,\theta) = \int [dU]e^{-S_L[U]-\theta_L Q_L[U]}, \tag{4}$$

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 will consider the Wilson action

$S_L = \beta\sum_{x,\mu>\nu}(1 - \mathrm{Re\,Tr}\Pi_{\mu\nu}(x)/N)$, 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 [12]

$$q_L(x) \overset{a\to 0}{\sim} a^4 Z(\beta) q(x) + O(a^6), \tag{5}$$

where $a = a(\beta)$ is the lattice spacing and $\lim_{a\to 0} Z = 1$. Hence, as the continuum limit is approached, the imaginary part of θ is related to the lattice parameter θ_L appearing in Eq. (4) as follows: $\theta_I = Z\theta_L$.

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

$$q_L(x) = \frac{-1}{2^9\pi^2} \sum_{\mu\nu\rho\sigma=\pm 1}^{\pm 4} \tilde{\epsilon}_{\mu\nu\rho\sigma} \mathrm{Tr}(\Pi_{\mu\nu}(x)\Pi_{\rho\sigma}(x)), \tag{6}$$

where $\tilde{\epsilon}_{\mu\nu\rho\sigma} = \epsilon_{\mu\nu\rho\sigma}$ for positive directions and $\tilde{\epsilon}_{\mu\nu\rho\sigma} = -\tilde{\epsilon}_{(-\mu)\nu\rho\sigma}$. With this choice gauge links still appear linearly in the modified action; hence, a standard heat-bath algorithm over $SU(2)$ subgroups, combined with over relaxation, 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 local 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

$$\langle L \rangle \equiv \frac{1}{V_s}\sum_{\vec{x}} \frac{1}{N}\left\langle \mathrm{Tr}\prod_{t=1}^{N_t} U_0(\vec{x}, t)\right\rangle,$$
$$\chi_L \equiv V_s(\langle L^2\rangle - \langle L\rangle^2)), \tag{7}$$

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_θ to the continuum limit.

We have performed, on each lattice, several series of simulations at fixed θ_L and variable β. 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 $O(10^3)$ cycles around the transition. In Fig. 1 we show results for the Polyakov loop 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. We notice a slight increase in the height of the susceptibility peak as θ_L increases; however, any conclusion regarding the influence of θ on the strength of the transition would require a finite size scaling analysis and is left to future studies.

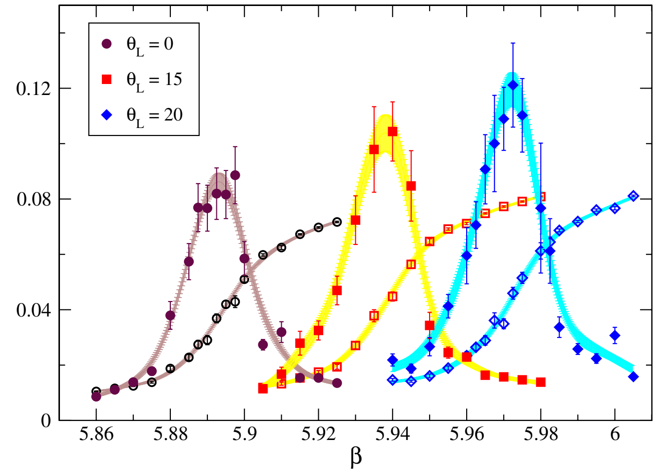

FIG. 1 (color online). Polyakov loop and its susceptibility as a function of β on a $24^3 \times 6$ lattice and for a few θ_L values. The susceptibility values have been multiplied by a factor of 250.

The critical coupling $\beta_c(\theta_L)$ is located at the maximum of the susceptibility through a Lorentzian fit to unreweighted 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 nonperturbative 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.

As a final step, we need to convert θ_L into the physical parameter $\theta = i\theta_I$. A well known method for a nonperturbative 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:

$$Z = \frac{\langle QQ_L\rangle}{\langle Q^2\rangle}, \tag{8}$$

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 β values on a symmetric 16^4 lattice, as reported in Fig. 2, then obtaining Z at the critical values of β by a cubic interpolation. Typical statistics have been of 10^5 measurements, each separated by 5 cycles of 4 over-relaxation +1 heat-bath sweeps, for each β; the autocorrelation length of Q has reached a maximum of 10^3 cycles at the highest value of β. A check for systematic effects has been done by

TABLE I. Collection of results obtained for β_c and T_c.

Lattice	θ_L	β_c	θ_I	$T_c(\theta_I)/T_c(0)$
$16^3 \times 4$	0	5.6911(4)	0	1
$16^3 \times 4$	5	5.6934(6)	0.370(10)	1.0049(11)
$16^3 \times 4$	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)	1.1209(10)
$24^3 \times 6$	0	5.8929(8)	0	1
$24^3 \times 6$	5	5.8985(10)	0.5705(60)	1.0105(24)
$24^3 \times 6$	10	5.9105(5)	1.168(12)	1.0335(18)
$24^3 \times 6$	15	5.9364(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	6.1059(21)	1.890(24)	1.0719(34)
$32^3 \times 8$	15	6.1332(7)	2.437(30)	1.1201(17)

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 β, on a larger 24^4 lattice. In this way we finally obtain $\theta_I(\beta_c(\theta_L)) = Z(\beta_c(\theta_L))\theta_L$, as reported in the 4th column of Table I.

Final results for $T_c(\theta_I)/T_c(0)$ and for the three different lattices explored are reported in Fig. 3. In all cases a linear dependence in θ^2, according to Eq. (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. $\simeq 0.7$).

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 θ_I, results for R_θ 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 α is compatible with 2 within errors; if we fix α to values which would imply a nonanalyticity at $\theta = 0$, e.g., $\alpha = 1$, we obtain a χ^2/d.o.f. of $O(10)$ or larger.

Assuming $O(a^2)$ corrections we can extrapolate the continuum value $R_\theta = 0.0175(7)$, χ^2/d.o.f. $\simeq 0.97$ (see Fig. 4). Our result is therefore that T_c decreases in presence of a real nonzero θ parameter. This is in agreement with the large N expectation that we discuss in the following, as well as with arguments based on the semiclassical approximation discussed in Ref. [15] 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 θ 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 is

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

hence, $\epsilon = -T^2 \partial(f/T)/\partial T$. Close enough to a first order transition we may assume, apart from constant terms, $f_c/T = A_c t + O(t^2)$ and $f_d/T = A_d t + O(t^2)$, 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 nonzero θ modifies the free energy, at the lowest order, as follows:

$$f(T,\theta) = f(T,\theta = 0) + \chi(T)\theta^2/2 + O(\theta^4), \qquad (10)$$

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

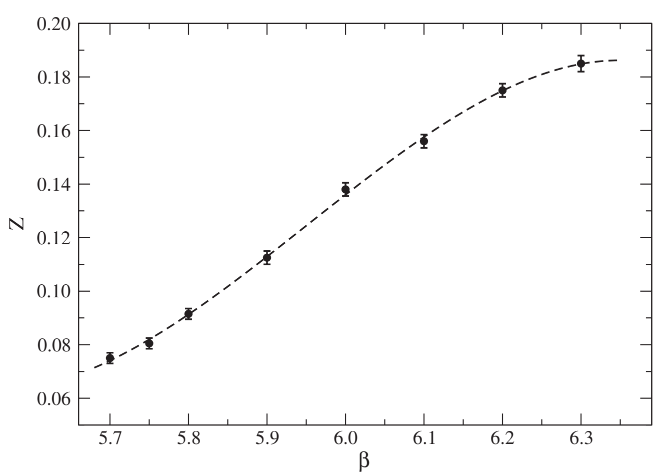

FIG. 2. Determinations of the renormalization constant Z on a 16^4 lattice. The dashed line is a cubic interpolation of data.

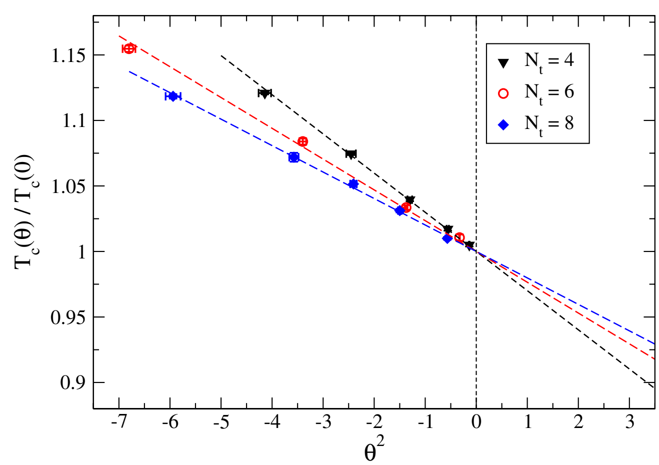

FIG. 3 (color online). $T_c(\theta)/T_c(0)$ as a function of θ^2 for different values of N_t. Dashed lines are the result of linear fits, as reported in the text, then extrapolated to $\theta^2 > 0$.

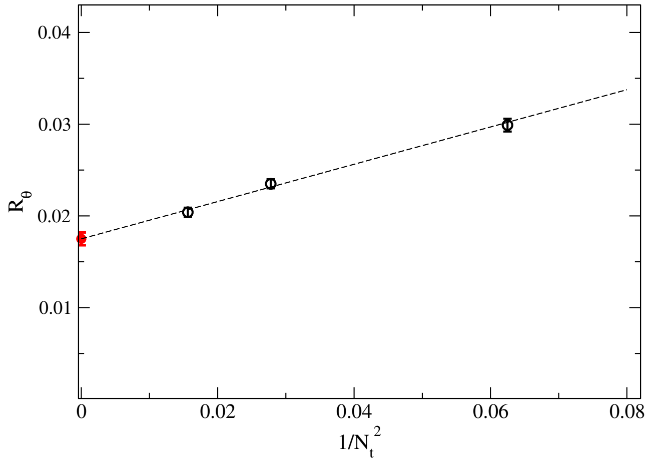

FIG. 4 (color online). R_θ as a function of $1/N_t^2$. The point at $1/N_t = 0$ is the continuum limit extrapolation, assuming $O(a^2)$ corrections.

$f_c = f_d$, which gives the value of T_c, will change as a function of θ. The dependence of χ 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 $N \to \infty$,

$$f_c/T \simeq A_c t + (\chi/T)\theta^2/2; \qquad f_d/T \simeq A_d t, \qquad (11)$$

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

$$\frac{T_c(\theta)}{T_c(0)} = 1 - \frac{\chi}{2\Delta\epsilon}\theta^2 + O(\theta^4). \qquad (12)$$

In the large N limit we have [9,18,20],

$$\frac{\chi}{\sigma^2} \simeq 0.0221(14); \qquad \frac{\Delta\epsilon}{N^2 T_c^4} \simeq 0.344(72);$$
$$\frac{T_c}{\sqrt{\sigma}} \simeq 0.5970(38)$$

apart from $1/N^2$ corrections; hence, we get

$$R_\theta = \frac{\chi}{2\Delta\epsilon} \simeq \frac{0.253(56)}{N^2} + O(1/N^4). \qquad (13)$$

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 χ at T_c is smoother than the sharp drop to zero that we have assumed.

Notice that the $1/N^2$ dependence of R_θ is in agreement with general arguments [21] predicting the free energy to be a function of the variable θ/N as $N \to \infty$ (see also Refs. [9,15]). For the same reason we expect $O(\theta^4)$ 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_t and up to θ^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 [25], which are linked to the periodicity of the theory in terms of imaginary μ_B. In the case of a θ parameter, no periodicity is expected for imaginary θ, CP invariance being explicitly broken for any $\theta_I \neq 0$; hence, we cannot predict other possible transitions for $\theta^2 < 0$. A 2π periodicity is instead expected for real values of θ, 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 θ^2 behavior up to $|\theta| \sim \pi$. We expect continuity of such behavior, at least for small real θ, while nontrivial corrections may appear as θ approaches π. 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 $\theta = \pi$

$$T_c(\theta)/T_c(0) \simeq 1 - R_\theta \min_k (\theta + 2\pi k)^2, \qquad (14)$$

where k is a relative integer: in this case periodicity in θ 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 θ could have some analogies with that found at imaginary μ_B.

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