Phase Diagram of Yang-Mills Theories in the Presence of a $\theta$ Term

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We study the phase diagram of non-Abelian pure gauge theories in the presence of a topological $\theta$ term. The dependence of the deconfinement temperature on $\theta$ is determined on the lattice both by analytic continuation and by reweighting, obtaining consistent results. The general structure of the diagram is discussed on the basis of large-$N$ considerations and of the possible analogies and dualities existing with the phase diagram of QCD in presence of an imaginary baryon chemical potential.

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I. INTRODUCTION

The possible presence of a non-zero $\theta$ parameter in the langrangian of Quantum Chromodynamics (QCD) has been discussed since long. Such parameter is coupled to the topological charge density,

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

which violates $P$ and $CP$ symmetries, and its effects on the structure of non-Abelian gauge theories are intimately non-perturbative.

Experimental upper bounds on it are quite stringent, $|\theta| \lesssim 10^{-10}$. Nevertheless, the dependence of QCD on $\theta$ is quite interesting, from both a theoretical and a phenomenological point of view; think for instance of the solution to the $U(1)_A$ problem, regarding the mass of the $\eta'$ meson [1, 2].

The study of $\theta$ related issues is particularly interesting when one investigates the behavior of non-Abelian gauge theories at finite temperature $T$. Modifications in $\theta$ dependence are a probe of the changes in the non-perturbative properties of the theory and of the approach to the semiclassical regime expected at asymptotically high temperatures [3-5]. Topological charge fluctuations may be relevant, also from a phenomenological point of view, 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 [6].

The purpose of the present paper is to discuss some general features of the phase diagram of pure $SU(N)$ Yang-Mills theories in presence of a $\theta$ term. Unfortunately, the addition of such a term makes the Euclidean action complex, hindering direct numerical lattice simulations, like it happens for QCD at finite baryon chemical potential. For that reason, most of the present knowledge is based on model studies, on the computations of $\theta$ derivatives at $\theta = 0$ or on other methods which partially circumvent the sign problem, like analytic continuation from imaginary chemical potentials [7-12].

In Ref. [11] we have already discussed about the dependence of the critical deconfining temperature on $\theta$, providing an estimate of such dependence in the large $N$ limit and a numerical computation for $N = 3$, based on analytic continuation from results obtained at imaginary values of $\theta$, for which the action is real. The main result is that $T_c$ decreases as a function of $\theta$, being a linear function of $\theta^2$ for small $\theta$ values: such fact is in agreement with predictions coming from continuity based semiclassical approximations [13-15] and model computations [16-19], and can be simply interpreted by considering that the free energy of the confined phase increases, as a function of $\theta$, more than what happens for the deconfined phase (since the topological susceptibility drops at $T_c$ [20-22]), so that the deconfined phase becomes more and more favorable as $\theta$ increases [11].

The first purpose of the present study is to provide stronger numerical evidence regarding the determination of $T_c(\theta)$. Apart from presenting, in Section IIA new data at imaginary $\theta$ on a finer lattice, corresponding to a temporal extent $N_t = 10$, which confirm the continuum limit extrapolation of Ref. [11], we will obtain, in Section IIIB an independent determination of $T_c(\theta)$ for small values of $\theta$, based on reweighting of data at $\theta = 0$, showing that it is consistent with the determination from imaginary $\theta$, hence that systematic effects are under control for both methods. Consistency between analytic continuation and reweighting will be demonstrated also for the dependence on $\theta$ of other physical observables, like the Polyakov loop.

A question which is naturally related to previous topics is how physical quantities depend on the topological sector $Q$, especially around the deconfinement transition.

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Such issue, which is discussed in Section II C, is of particular interest for the related information about the systematic effects involved in numerical simulations carried out within a fixed topological sector, like those exploiting overlap fermions. The problem has been investigated by recent literature [23-25], showing that, for some quantities, systematic effects are well under control, see for instance Ref. [25] for a study regarding the pure gauge topological susceptibility at finite $T$. We will show that for other quantities, like the Polyakov loop, effects on finite volumes can be larger, especially around $T_c$, and that even small deviations of $T_c$ itself are detectable when switching from one sector to the other.

In the last part of the paper, which is contained in Section III, we will discuss the general properties of the phase diagram in the $T_c - \theta$ plane. Unfortunately, presently available numerical methods, like analytic continuation or reweighting, do not permit to obtain much reliable information, apart from the curvature of the critical line $T_c(\theta)$ at $\theta = 0$. Therefore, part of the discussion is based on known large-$N$ considerations and model predictions [26-33], as well as recent numerical evidence [34] regarding the change in the realization of $\theta$ dependence and periodicity, which takes place at the deconfinement transition. Particular emphasis will be placed on the analogy that we draw between the $T_c - \theta$ diagram and the phase diagram of QCD in presence of an imaginary baryon chemical potential $\mu_B$: we will speculate about the duality between the two diagrams, in the sense of an analogy that we draw between the $\theta$ dependence of physical quantities and $T_c(\theta)$ itself are expected to be even functions of $\theta$, i.e.,

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

if the theory is analytic around $\theta = 0$.

A decreasing $T_c(\theta)$ means that the curvature $R_{\theta}$ is positive. A possible argument to understand such decrease has been given in Ref. [11]. The free energy increases as a function of $\theta$, and the coefficient of the lowest order term, which is quadratic in $\theta$, is given by $\chi/2$, where $\chi$ is the topological susceptibility ($\chi \equiv \langle Q^2 \rangle/(a^4V)$ and $a^4V$ is the physical spatial volume). Due to the sharp drop of $\chi$ across the deconfinement transition [20-22], the increase of free energy in the confined phase is larger than that in the deconfined phase; hence, as $\theta$ increases, it becomes more and more favorable to the system to stay in the deconfined phase, so that the deconfining temperature moves to lower temperatures. In particular, for a first order transition, which is the case for $SU(N)$ pure gauge theories with $N \geq 3$, one finds [11]:

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

where $\Delta \epsilon$ and $\Delta \chi$ are respectively the jump of the energy density and the drop of the topological susceptibility at the transition. In the large $N$ limit, $\Delta \chi$ tends to $\chi$ computed at $T = 0$ and stays finite, while $\Delta \epsilon \propto N^2$, so that $R_{\theta} \propto 1/N^2$.

The first numerical results regarding $R_{\theta}$ have been given in Ref. [11] for the $SU(3)$ pure gauge theory, exploiting the idea of performing simulations at imaginary values of $\theta$ in order to avoid the sign problem [7-10]. The approach is the same adopted for QCD at finite baryon chemical potential $\mu_B$, where purely imaginary values of $\mu_B$ avoid complex values of the fermion determinant: one can then make use of analytic continuation to infer the dependence at real $\mu_B$, at least for small values of $\mu_B/T$ [37]; in particular the critical temperature can be reliably estimated up to the quadratic order in $\mu_B$, while ambiguities related to the procedure of analytic continuation may affect higher order terms [38]. The same approach can be used to explore physics at non-zero $\theta$, if one assumes that the theory is analytic around $\theta = 0$, a fact supported by our present knowledge about free energy derivatives at $\theta = 0$ [39-43].

In Ref. [11], the curvature $R_{\theta}$ has been determined by analytic continuation on three different lattice sizes, $16^3 \times 4, 24^3 \times 6$ and $32^3 \times 8$, corresponding to the same physical spatial volume and different lattice spacings, $a \simeq (4T_c)^{-1}, (6T_c)^{-1}$ and $(8T_c)^{-1}$, around the transition. That has permitted us to extrapolate the curvature to the continuum limit, obtaining $R_{\theta} = 0.0175(7)$, a value which is in rough agreement with the model prediction in Eq. (2) [11].

In the present study we make progress by performing new numerical simulations, both at zero and non-zero imaginary $\theta$, on a $40^3 \times 10$ lattice. On the one hand, in Section II A we obtain a new determination of $R_{\theta}$ by analytic continuation, on a finer lattice, which permits us to check and improve the continuum extrapolation of Ref. [11]. On the other hand, the determination of the topological background $Q$ of configurations sampled at $\theta = 0$ will permit us to obtain direct information at real $\theta$ by reweighting techniques, as illustrated in Section II B in this way we shall be able to check the reliability of analytic continuation and to put the numerical determination of $R_{\theta}$ on a more solid basis. Finally Section II C is devoted to investigate the dependence of physical quantities, including the critical temperature, on the topological sector.
A. Results from imaginary $\theta$

The partition function of lattice $SU(N)$ gauge theories in presence of an imaginary theta term reads

$$Z_L(T, \theta_L) = \int [dU] \ e^{-S_L[U] - \theta_L Q_L[U]} , \quad (3)$$

where $U$ stands for a configuration of gauge link variables, $U_\mu(n)$, while $S_L$ and $Q_L$ are the lattice discretizations of respectively the pure gauge action and the topological charge, $Q_L = \sum_x q_L(x)$. As in Ref. [11], we consider the Wilson plaquette action and a simple discretization for $q_L$:

$$q_L(x) = \frac{-1}{2a^2} \sum_{\mu\nu\rho\sigma=\pm 1} \hat{\theta}_{\mu\nu\rho\sigma} \text{Tr} (\Pi_{\mu\nu}(x)\Pi_{\rho\sigma}(x)) , \quad (4)$$

where $\Pi_{\mu\nu}$ is the plaquette operator, $\hat{\theta}_{\mu\nu\rho\sigma} = \epsilon_{\mu\nu\rho\sigma}$ for positive directions and $\hat{\theta}_{\mu\nu\rho\sigma} = -\epsilon_{(-\mu)\nu\rho\sigma}$. 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; that would not be possible for different improved choices of $q_L$, like for instance smeared or fermionic operators.

In general, the lattice operator $q_L(x)$ is linked to the continuum $q(x)$ by a finite multiplicative renormalization [44]

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

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 $\theta$ is related to the lattice parameter $\theta_L$ appearing in Eq. (3) as follows: $\theta_L = Z \theta_L$.

Knowledge about $Z(\beta)$ is essential to fix the working physical value of $\theta_L$. It is important to stress that other renormalizations, linked to the choice of the lattice operator $q_L$, may affect the free energy, e.g. in the form of additive renormalizations stemming from two (or more) point correlators of $q_L$. Such UV terms, however, are continuous across the phase transition, hence they do not play any role in the determination of $T_c$ as a function of $\theta_L$; this is confirmed by the fact that, as shown in Ref. [11] and in the present manuscript, a consistent extrapolation to the continuum can be taken for $R_\theta$.

Here we will make use of the non-perturbative determination of $Z$ reported in Ref. [11], see in particular Fig. 2 reported therein. That has been obtained by measuring, on symmetric $T = 0$ lattices, the following quantity [10]

$$Z \equiv \frac{\langle Q Q_L \rangle}{\langle Q^2 \rangle} , \quad (6)$$

where $Q$ is, configuration by configuration, the integer closest to the topological charge obtained after cooling [32]. [45]. The idea is similar to that used by heating techniques [40], where the average value of $Q_L$ is determined within a fixed topological sector.

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**FIG. 1:** Polyakov loop susceptibility as a function of $\beta$ on the $40^3 \times 10$ lattice for some explored values of $\theta_L$.

| lattice | $\theta_L$ | $\beta_L$ | $\beta_T(\theta_L)/\beta_T(0)$ |
|---------|------------|------------|---------------------------------|
| $16^3 \times 4$ | 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) | 1.0399(11) |
| $16^3 \times 4$ | 20 | 5.7228(6) | 1.566(30) | 1.0470(10) |
| $16^3 \times 4$ | 25 | 5.7477(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) | 0.570(20) | 1.0105(24) |
| $24^3 \times 6$ | 10 | 5.9105(5) | 1.168(12) | 1.0353(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 | 6.1099(17) | 1.890(24) | 1.0719(24) |
| $32^3 \times 8$ | 16 | 6.1332(7) | 2.437(30) | 1.1201(17) |
| $40^3 \times 10$ | 0 | 6.2082(4) | 0 | 1 |
| $40^3 \times 10$ | 6 | 6.2236(8) | 1.068(7) | 1.0232(14) |
| $40^3 \times 10$ | 8 | 6.2381(5) | 1.509(10) | 1.0453(10) |
| $40^3 \times 10$ | 13.4 | 6.2821(9) | 2.461(22) | 1.1144(16) |

**TABLE I:** Collection of results obtained for $\beta_L$ and $T_c$. Results for $N_t = 4, 6, 8$ are taken from Ref. [11] and reported for completeness.

The new set of numerical simulations on the $40^3 \times 10$ lattice have been carried out at four different values of $\theta_L$, $\theta_L = 0.0, 6.0, 8.4$ and 13.4. We have performed several series of simulations at fixed $\theta_L$ and variable $\beta$. Typical statistics have been of $O(10^5)$ measurements per $\beta$ at $\theta = 0$ and of $O(10^4)$ measurements per $\beta$ at $\theta \neq 0$, each separated by an updating cycle of 4 over-relaxation + 1 heat-bath sweeps. The somewhat larger statistics at $\theta = 0$ is justified in view of the further analysis reported in the
The modified action, an order parameter, is a related one. In general the location of the critical coupling \( \beta_c \), which is obtained by interpolation of the susceptibility \( \chi \) at the deconfinement transition temperature, we have considered the Polyakov loop and its susceptibility

\[
L \equiv \frac{1}{V_s} \sum_x \frac{1}{N} \text{Tr} \prod_{t=1}^{N_t} U_0(x,t)
\]

\[
\chi L \equiv V_s \left( \langle |L|^2 \rangle - \langle |L| \rangle^2 \right)
\]

where \( V_s \) is the spatial volume and \( |L| \) is the Polyakov loop modulus. Center symmetry, which corresponds to a multiplication of all parallel transports at a fixed time by an element of the center of the SU(\( N \)) gauge group, \( Z_{N_t} \), is spontaneously broken at the deconfinement transition and the Polyakov loop, which is not invariant under center transformations, is a related order parameter. The modified action \( S_L + \theta_L Q_L \) is also center symmetric, hence the Polyakov is an exact order parameter also at \( \theta \neq 0 \).

The Polyakov loop susceptibility is plotted as a function of \( \beta \) in Fig. 1 together with data obtained after reweighting in \( \beta \). As \( \theta_L \) increases, the susceptibility peak moves to higher values of \( \beta \), i.e., to higher temperatures \( T = 1/(a(\beta)N_t) \).

The critical couplings \( \beta_c(\theta_L) \) have been obtained by performing a Lorentzian fit to the unrewighted data of the 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. [47]; in general the location of \( T_c \) is affected by finite size corrections, which however should almost cancel when computing the ratio \( T_c(\theta_L)/T_c(0) \). Finally, \( \theta_L \) must be converted into \( \theta_f \) by exploiting the determination of \( Z \) at the critical coupling \( \beta_c \), which is obtained by interpolation of data reported in Ref. [11]. All results are shown in Table I where we also report, for the reader’s convenience, data obtained on different lattices in Ref. [11].

The values obtained for \( T_c(\theta_f)/T_c(0) \) can be fitted according to Eq. (1), with \( \theta_f^2 = -\theta^2 \). If we restrict to \( \theta_f < 2 \), we get \( R_{\theta} = 0.0200(5) \), with \( \chi^2/\text{d.o.f.} \simeq 0.11 \). As a final step, we can put the value of \( R_{\theta} \) together with those obtained for smaller values of \( N_t \) in Ref. [11], see Fig. 2. An extrapolation to the continuum limit assuming \( O(a^2) \) corrections, \( R_{\theta}(N_t) = R_{\theta}^{\text{cont}} + b/N_t^2 \), yields \( R_{\theta}^{\text{cont}} = 0.0178(5) \), with \( \chi^2/\text{d.o.f.} \simeq 0.6 \). That is consistent with the continuum extrapolation reported in Ref. [11], and in rough agreement with the leading \( 1/N \) estimate for \( SU(3) \), \( R_{\theta} = 0.0286(11) \). The most significant correction to the large-\( N \) prediction can be attributed to the fact that, for finite \( N \), the susceptibility does not drop sharply to zero at the transition, i.e. \( \Delta \chi \) in Eq. (2) is less than the value of \( \chi \) in the confined phase.

B. Comparison with reweighting at real \( \theta \)

Presently known solutions to the sign problem are only approximate and typically introduce assumptions and systematic errors. In the case of analytic continuation an obvious assumption is that of analyticity around \( \theta = 0 \). A possible way to keep such effects under control is to compare different, independent methods, cross-checking results.

A method alternative to analytic continuation, which has been largely used in QCD at finite baryon chemical potential, is reweighting. The idea is to sample configurations at \( \theta = 0 \) and to move the complex factor of the path integral measure into the observable , i.e., for a
The generic quantity $O$, 
\[ \langle O\rangle_\theta = \frac{\int [dU] e^{-S_L[U]+i\theta Q} O}{\int [dU] e^{-S_L[U]+i\theta Q}} = \frac{\langle e^{i\theta Q} O \rangle}{\langle \cos(\theta Q) \rangle}, \tag{8} \]
where averages without subscript are taken as usual at $\theta = 0$, and the equality $\langle e^{i\theta Q} \rangle = \langle \cos(\theta Q) \rangle$ has been used, which derives from the symmetry under $Q \rightarrow -Q$ of the distribution at $\theta = 0$. The major drawback of reweighting is that configurations sampled at $\theta = 0$ may not be representative enough of the physics at $\theta \neq 0$; such problem gets worse and worse as $\theta$ increases and as the thermodynamical limit is approached. A measure of the severity of the problem is given by the average phase factor in the denominator of Eq. (8): as $\langle \cos(\theta Q) \rangle$ vanishes, one would need unfeasibly large statistics to keep statistical errors under control. Such problems are well known from QCD at finite baryon density [48]; a partial improvement can be achieved by reweighting in more than one parameter [49].

Since in the reweighting method the topological charge does not enter the sampling algorithm directly, one can make use of smoothed gluonic or fermionic definitions of $Q$, in order to avoid issues related to renormalization. However, the implementation must be cheap enough to permit the collection of a sufficiently large sample of measures. We have adopted cooling, in particular the implementation outlined in Ref. [39], which is known to provide reliable results on fine enough lattices. This is the reason why we have decided to apply the reweighting method only to configurations sampled on the $N_t = 10$ lattice. $Q$ has been measured once every 4 updating cycles; we will show results for $Q$ obtained after $n_{\text{cool}} = 30$ cooling sweeps, however we have checked that different choices lead to compatible results.

Let us start the discussion of our results by showing, in Fig. 4, the behavior of the average phase factor, $\langle \cos(\theta Q) \rangle$, as a function of $\theta$, for 3 different bare couplings, $\beta = 6.1600, 6.2075, \text{ and } 6.2475$, corresponding to $T \simeq 0.93 T_c, T_c$ and $1.06 T_c$ respectively. In Fig. 5 we also show $\langle \cos(\theta Q) \rangle$ as a function of $n_{\text{cool}}$ for a few values of $\theta$ at $T \simeq 1.06 T_c$, which nicely demonstrates the stability of results under different choices of $n_{\text{cool}}$.

\begin{figure}[h]
\centering
\includegraphics[width=\textwidth]{fig4}
\caption{Dependence of $\langle \cos(\theta Q) \rangle$ on the number of cooling steps for $T \simeq 1.06 T_c$ and three values of $\theta$.}
\end{figure}

\begin{figure}[h]
\centering
\includegraphics[width=\textwidth]{fig5}
\caption{Dependence of the Polyakov loop modulus on $\theta^2$ for $T \simeq 1.055 T_c$ on the $40^3 \times 10$ lattice. The dashed line is a best fit according to a linear dependence on $\theta^2$.}
\end{figure}

The regions where $\langle \cos(\theta Q) \rangle$ becomes very small are hardly accessible to reweighting. It is clear that the situation is worse in the confined phase, where only $\theta \lesssim 0.2 \pi$ seems accessible, than in the deconfined phase, where $\theta \sim 0.5 \pi$ seems reachable. That can be understood in terms of the much lower topological activity present in the deconfined phase. It should be stressed, however, that as the thermodynamical limit, $V_s \rightarrow \infty$, is taken, arbitrarily large fluctuations of the global charge $Q$ are expected in both phases, so that $\langle \cos(\theta Q) \rangle$ must drop to zero for any $\theta \neq 0$.

Let us now discuss the behavior of physical quantities computed at nonzero $\theta$ via reweighting, and compare it with results obtained at imaginary $\theta$. We are interested, in particular, in the Polyakov loop modulus,
\[ \langle |L| \rangle_\theta = \frac{\langle e^{i\theta Q}|L| \rangle}{\langle e^{i\theta Q} \rangle} = \frac{\langle \cos(\theta Q)|L| \rangle}{\langle \cos(\theta Q) \rangle} \]
and in its susceptibility, $\chi_L(\theta) = V_s(\langle |L|^2 \rangle_\theta - \langle |L| \rangle^2_\theta)$. The ratio of expectation values in Eq. (9) is computed via a jackknife algorithm. We have replaced $e^{i\theta Q}$ with $\cos(\theta Q)$ also in the numerator, since $L$, as well as the path integral measure at $\theta = 0$, is invariant under parity transformations, under which instead $Q \rightarrow -Q$.

In Fig. 5 we show the dependence of the Polyakov loop on $\theta^2$ for a selected value of the bare coupling, $\beta = 6.245$, corresponding to $T \simeq 1.055 T_c$. Results at $\theta^2 \leq 0$ derive from direct simulations, while those at $\theta^2 > 0$ have been obtained via reweighting from $\theta = 0$ data. All data can be nicely fitted by a linear dependence in $\theta^2$, as shown in the figure, demonstrating that analyticity around $\theta = 0$.
that there is indeed agreement, within statistical errors, to lower temperatures, as \( \theta \) is changed, leads us to suspect that the dependence of physical observables on \( \theta \) is limited on the right by the feasibility of reweighting, while on the left one must avoid the crossing of the deconfining transition, which moves to higher values of \( T \) as \( \theta^2 \) decreases (see Fig. 7).

The increasing behavior of \( \langle |L| \rangle \) can be understood considering that one moves deeper and deeper into the deconfined phase as \( \theta^2 \) increases; the quadratic behavior in \( \theta^2 \) is consistent with analyticity around \( \theta^2 = 0 \) and with the fact that \( \langle |L| \rangle \) is a \( P \)-even quantity. We notice that both features are consistent with the results of Ref. [15].

Finally, in Fig. 6 we show results for the susceptibility as a function of \( \beta \), obtained after reweighting at \( \theta = 0.3 \) and 0.5, together with the original data at \( \theta = 0 \). It is clear that the peak moves to lower values of \( \beta \), i.e. to lower temperatures, as \( \theta \) increases, in agreement with results from analytic continuation. From the susceptibility peaks we can extract the critical temperatures (see Table II), and compare them with results at imaginary \( \theta \). It does not make sense to fit reweighted data directly, since they are obtained from the same data sample and are therefore correlated; instead, in Fig. 7 we compare reweighted data with the extrapolation linear in \( \theta^2 \) obtained by fitting results at imaginary \( \theta \), showing that there is indeed agreement, within statistical errors 1.

1 If one wants to extract the curvature from reweighting, taking into account that results at different real values of \( \theta \) are strongly correlated, then a reasonable estimate is obtained by considering only the point at the largest feasible value of \( \theta \), i.e. \( \theta = 0.55 \). That yields, assuming that such a value is in the linear region, i.e. that \( R_\theta \simeq (1 - T_c(\theta)/T_c(0))/\theta^2 \), the value \( R_\theta = 0.024(4) \), in agreement with the estimate from analytic continuation for \( N_t = 10 \), \( R_\theta = 0.0200(5) \).

![FIG. 6: Polyakov loop susceptibility as a function of \( \beta \) and after reweighting at a few values of real \( \theta \). The shaded bands correspond to data reweighted also in \( \beta \).](image)

| lattice | \( \theta \) | \( \beta_c \) | \( T_c(\theta)/T_c \) |
|---------|-------------|---------------|---------------------|
| \( 40^4 \times 10 \) | 0.10 | 6.2081(4) | 0.9999(8) |
| \( 40^4 \times 10 \) | 0.30 | 6.2068(4) | 0.9979(8) |
| \( 40^4 \times 10 \) | 0.50 | 6.2062(5) | 0.9970(8) |
| \( 40^4 \times 10 \) | 0.70 | 6.2040(6) | 0.9970(11) |
| \( 40^4 \times 10 \) | 0.55 | 6.2033(7) | 0.9927(12) |

TABLE II: Results obtained for \( \beta_c \) and \( T_c \) at real \( \theta \) by the reweighting technique on the \( 40^4 \times 10 \) lattice. The ratios of critical temperatures have been calculated using the \( \theta = 0 \) critical \( \beta \) reported in Table I.

![FIG. 7: Critical temperature as a function of \( \theta^2 \): we report the result of the linear fit in \( \theta^2 \) obtained from simulations at \( \theta^2 < 0 \).](image)

That gives further support to the validity of analytic continuation, at least for small values of \( \theta \).

C. Deconfinement and the Polyakov loop at fixed topological background.

The general expression for a reweighted observable, Eq. (8), can be rewritten in the following form:

\[
\langle O \rangle_\theta = \frac{1}{\langle \cos(\theta Q) \rangle} \sum_{Q=-\infty}^{\infty} e^{iQ \mathcal{P}(Q)} \langle O \rangle_Q \tag{10}
\]

where \( \langle \cdot \rangle_Q \) stands for the average in a given topological sector and \( \mathcal{P}(Q) \) is the topological charge distribution at \( \theta = 0 \). It shows that a non-trivial dependence on \( \theta \) is possible only if the observable has a non-trivial dependence on \( Q \). This is quite natural, since \( \theta \) and \( Q \) are conjugate quantities, like the particle density and the chemical potential.

The fact that, as we have shown, the location of deconfinement moves as \( \theta \) is changed, leads us to suspect that the dependence of physical observables on \( Q \) may be significant around \( T_c \). Investigating such dependence is
quite important for various reasons, for instance to understand the possible systematic effects involved in numerical simulations carried out in a fixed topological sector, like it happens when investigating QCD with overlap fermions. Studies regarding such effects have been reported, both at zero and finite $T$ \cite{22, 23}; in particular, a recent study shows that systematic effects in the determination of the topological susceptibility at finite $T$ are well under control \cite{25}. In the present subsection we will discuss about the dependence on $Q$ of quantities directly related to deconfinement, in particular the Polyakov loop and its susceptibility, showing that in this case systematic effects, even if disappearing in the thermodynamical limit, can be more significant.

Such study is best performed on the finest lattice at our disposal, i.e. the $40^3 \times 10$, where the determination of the topological background is most reliable. For that reason we have divided the set of configurations sampled at each $\beta$ according to the value of $Q$ obtained via cooling, as discussed in the previous subsection. The expectation value $\langle |Q| \rangle$ is obviously independent of $\theta$ since, in a fixed topological background, $\theta$ only adds an irrelevant overall phase factor, hence in principle one may think of combining equal $Q$ configurations sampled at different imaginary values of $\theta$. However, one must consider that the lattice charge operator entering Eq. (3) contains irrelevant discretization terms, which are not constant over a given topological sector and may lead to a residual dependence on $\theta_L$. For that reason, in the following we will consider only configurations sampled at $\theta = 0$.

Let us start by showing, in Fig. 8, the behavior of the Polyakov loop as a function of $Q$ for a few temperatures around $T_c$

$$\langle |L| \rangle = \frac{\sum_i N \delta_{Q_i |Q|} |L_i|}{\sum_i N \delta_{Q_i |Q|}}$$

(11)

where $i$ runs over the $N$ measures and we have combined measures from opposite topological sectors, exploiting the symmetry of the Polyakov loop under parity transformations, in order to reduce statistical errors. The exact symmetry visible in Fig. 8 is therefore artificial, however we have verified that the symmetry holds, within errors, even before such combination. We observe that, while below the transition the dependence on $|Q|$ is quite mild, it gets stronger at the transition and becomes only slightly milder above $T_c$. A similar behavior is observed for the average plaquette, even if in this case the relative variation from one sector to the other is always modest and never larger than $10^{-4}$.

The dependence on $Q$ is quite visible also in the susceptibility of the Polyakov loop, which is shown in Fig. 9 as a function of $\beta$ for $Q = 0$ and $|Q| = 5$. The shift of the susceptibility peaks tells us that even the transition temperature can be influenced by the overall topological background. In particular, in Table III we report the values of $T_c(Q)$, obtained by fitting such peaks with Lorentzian functions. The critical temperature tends to increase as $|Q|$ increases; this is qualitatively consistent with what found when adding an imaginary $\theta$ term, which has the effect of shifting the average value of the topological charge distribution towards non-zero values.

One expects that systematic effects present in a fixed sector $Q$ disappear as the thermodynamical limit is approached. In order to verify that, we have performed, for a given value of $T \simeq 1.018 T_c$ ($\beta = 6.22$), simulations on lattices with different spatial volumes ($L^3_t \times L_s$ with $L_t = 10$ and $L_s = 16, 18, 20, 25, 30, 35, 40$), then combining measures obtained within different topological sectors $Q$ as described above. In Fig. 10 we show how the difference of the Polyakov loop modulus in the $Q = 0$ sector, taken with respect to its average over all sectors, changes as a function of the volume $V = L_t L_s^3$. The difference clearly approaches zero linearly in $1/V$, as one indeed expects on general grounds.

We will now try to better describe the observed dependence of the Polyakov loop on $Q$ by a very simplified model, which is based on the instanton gas approximation and follows the analysis reported in Ref. \cite{22}. Let us consider a generic, extensive quantity, like the average Polyakov loop times the volume $V$: we assume that it receives a given, fixed contribution by each topological sector.

![Figure 8: Dependence of the Polyakov loop modulus on the topological sector $Q$, determined on the $40^3 \times 10$ lattice and for a few values of $T$ around the transition.](image)

![Figure 9: Symmetry of the Polyakov loop under parity transformation.](image)

![Figure 10: Difference of the Polyakov loop modulus in the $Q = 0$ sector, taken with respect to its average over all sectors, as a function of the volume $V = L_t L_s^3$.](image)

![Table III: Results obtained for $\beta_c$ and $T_c$ at fixed topology calculated with $\beta_c = 6.2082(4)$.](image)
object, instanton or anti-instanton, and that the topological objects are distributed according to the instanton gas approximation, i.e. that the probability of having \( n \) instantons and \( \bar{n} \) anti-instantons is given by

\[
P(n, \bar{n}) = e^{-2\lambda} \frac{\lambda^n \bar{n}^{\bar{n}}}{n! \bar{n}!}
\]  

(12)

where \( 2\lambda = \langle Q^2 \rangle = V \chi_l \) and \( \chi_l = a^4 \chi \). The relevant quantity, to describe the behavior as a function of \( Q = n - \bar{n} \), is the average of the total number of topological objects which are found at fixed \( Q \), \( \langle n + \bar{n} \rangle_Q \), which can be extracted as a constrained average starting from the double Poissonian distribution in Eq. (12). The result obtained at the lowest order in \( Q^2/(2\lambda) = Q^2/\langle Q^2 \rangle \), which is the relevant expansion parameter when approaching the thermodynamical limit, is

\[
\langle n + \bar{n} \rangle_Q \simeq 2\lambda - \frac{1}{2} \left( 1 - \frac{Q^2}{2\lambda} \right).
\]  

(13)

The prediction for \( \langle |L| \rangle_Q \), which follows from our simplified model, is then

\[
\langle |L| \rangle_Q = \text{const} - \frac{\gamma}{V} \langle n + \bar{n} \rangle_Q
\]

\[
\simeq \langle |L| \rangle + \frac{\gamma}{2V} \left( 1 - \frac{Q^2}{2\chi_l} \right).
\]  

(14)

where we have defined as \( -\gamma \) the contribution to \( V|L| \) coming from each (anti)instanton and we have exploited the fact that the expression in parentheses vanishes when taking the average over all sectors.

Eq. (14), which is expected to be valid as the thermodynamical limit is approached, predicts \( \langle |L| \rangle_Q \sim \langle |L| \rangle \) to vanish linearly in \( 1/V \). This is confirmed by the behavior shown in Fig. 10 and a linear fit to data on the larger volumes, which is shown in the same figure, gives back \( \gamma \approx 6 \times 10^2 \). It is interesting that, once fixed \( \gamma \) and knowing from the average over the whole ensemble that \( \chi_l = \langle Q^2 \rangle / V \approx 0.947 \times 10^{-5} \), the behavior of the Polyakov loop as a function of \( Q \) in the large volume limit is completely fixed by the model, in particular

\[
\langle |L| \rangle_{Q=0} - \langle |L| \rangle_{Q=\bar{Q}} \approx \gamma Q^2/(2\chi_l^2).
\]  

(15)

In order to check that, in Fig. 10 we plot the quantity

\[
\Sigma(|Q|) = \frac{\langle |L| \rangle_{Q=0} - \langle |L| \rangle_{Q=\bar{Q}}}{\langle |L| \rangle_{Q=0}},
\]

which gives the relative deviation of the Polyakov loop from the value it takes in the trivial topological sector (the error on \( \Sigma(|Q|) \) has been obtained by a jackknife algorithm). In particular, we plot \( \Sigma(|Q|) \) as a function of \( |Q|/V \) for \( |Q| = 1, 2, 3 \) and for all the explored volumes, together with the model prediction, which has no more free parameters left. The fair agreement observed for small values of \( |Q|/V \) is therefore highly non-trivial, given the crudeness of the model: part of the success can be ascribed to the rapid approach to the instanton gas approximation which takes place right above \( T_c \), as demonstrated by the results of Ref. 36. As \( |Q|/V \) increases, however, the topological background is not dilute enough and the model prediction fails.

It would be nice to study the interplay between topological activity and the holonomy in more detail, in particular approaching the deconfining transition from above, and compare with model studies about the same issue (see, e.g., Ref. 50), however that goes beyond the purpose of our present investigation.

Finally, it is important to stress that, despite the fact that the approach to the thermodynamical limit of \( \langle |L| \rangle_Q \) seems to be well understood and that systematic effects vanish as \( 1/V \), from Fig. 10 we learn that they are still appreciable, and of the order of 10%, even on the largest...
III. PHASE DIAGRAM IN THE T - θ PLANE: GENERAL FEATURES AND ANALOGIES WITH THE DIAGRAM AT IMAGINARY µ_B

After studying $T_c(\theta)$, it is tempting to draw a sketch of the whole phase diagram in the $T$-θ plane. On the imaginary side, $\theta = i \theta_I$, no particular structure is expected a priori, since CP symmetry is explicitly broken whenever $\text{Im}(\theta) \neq 0$. Indeed, we have not observed any transition, apart from the deconfining one, in the range of explored values of $\theta_I$, even if we cannot exclude the presence of new phase structures at larger values of $\theta_I$.

The situation is quite different for real $\theta$, which plays the role of an angular variable. Periodicity in $\theta$ must reflect in some way in the structure of the phase diagram in the $T$-θ plane, which is then expected to be non-trivial. It is interesting to notice that this is very similar to what happens in presence of an imaginary baryon chemical potential $\mu_B$, and indeed many analogies can be found between the $T$-$\theta$ phase diagram and the phase structure at imaginary $\mu_B$ [11, 17, 19, 51]. It is convenient, for the following discussion, to introduce the parameter $\theta_B \equiv \text{Im}(\mu_B)/T$, since in terms of it analogies appear more clearly.

The purpose of the present Section is to discuss such analogies, also in a large $N$ perspective, with a particular emphasis on duality, in the sense of an inversion between the high and low temperature regions, between the $T$-$\theta$ and $T$-$\theta_B$ phase diagrams, which can be suggestive of the possible dual role played by the respective relevant degrees of freedom.

We will start by giving a rapid overview about the $T$-$\theta_B$ phase diagram, in order to highlight aspects which may have a direct correspondence with the case of the $T$-θ plane, which is discussed afterwards.

A. Phase diagram in the T-$\theta_B$ plane

Let us consider QCD with $N$ colors and its partition function at non-zero baryon chemical potential,

$$Z(T, \mu_B) = \text{Tr} \exp \left( -\frac{H - \mu_B B}{T} \right),$$

where $H$ is the QCD Hamiltonian and $B$ is the baryon number operator. For purely imaginary values of $\mu_B$, which are often considered to avoid the sign problem, the partition function becomes

$$Z(T, \theta_B) = \text{Tr} \left( e^{-\frac{H}{T}} e^{i\theta_B B} \right)$$

where $\theta_B = \text{Im}(\mu_B)/T$.

It is clear that $\theta_B$ plays the role of an angular variable, however the actual dependence of the free energy on $\theta_B$ depends on the phase of the theory. In the confined phase, $\theta_B$ couples only to physical degrees of freedom which have integer baryon charge $B$, hence the free energy is a function of $\theta_B$ with period $2\pi$. In the deconfined phase, instead, new physical degrees of freedom appear, quarks, carrying a fractional baryon charge, in particular in units of $1/N$: as a consequence the free energy is expected to be a function of $\theta_B/N$.

One may expect then that the periodicity in $\theta_B$ be $2\pi N$, but instead it is easy to prove that, independently of the relevant degrees of freedom, the partition function must be periodic in $\theta_B$ with period $2\pi$. Indeed, in the path integral representation of the partition function

$$Z = \int \mathcal{D}A e^{-S_g[A]} \text{det} M[A],$$

where $\text{det} M[A]$ is the quark determinant, the imaginary chemical potential enters as a twist, by a phase factor $\exp(i\theta_B/N)$, in the boundary conditions for quark fields. However, for $\theta_B = 2\pi k$, with $k$ integer, such twist can be cancelled exactly by a center transformation on the gauge fields i.e. by a gauge transformation periodic in time up to a global element of $\mathbb{Z}_N$, the center of the gauge group, $\exp(-2\pi k/N)$, under which the pure gauge action is invariant. As a consequence, the partition function and the free energy must be always periodic in $\theta_B$, with period $2\pi$.

How is it possible to reconcile such periodicity with the expected dependence on $\theta_B/N$ in the deconfined phase? This is done by a non-analytic, multi-branched behavior of the free energy, as a function of $\theta_B$, in the high temperature deconfined phase, with phase transitions happening at $\theta_B^{(RW)} = (2n+1)\pi$ ($n$ being a relative integer) and known as Roberge-Weiss (RW) transitions [52].
The relevant symmetry is the universality class is that of the 3D Ising model, since the universality class is that of the 3D Ising model, since of large or small quark masses [54–56]. In the former case for intermediate quark masses and first order in the limit and the three-flavor theory, the endpoint is second order studies collected up to now is that, both for the two-flavor depends on the quark mass spectrum: evidence from lattice spond to a discontinous jump in the order parameter, the is actually a triple point, with two further first order [54x-1998]

When crossing such values, gauge fields jump discontinuously from one center sector to the other, characterized by a different global alignment of the Polyakov loop. One has, therefore, \( N \) different branches, which are not equivalent from the point of view of the order parameter, \( \langle L \rangle \), but whose free energies are identical, modulo a shift \( \theta_B \rightarrow \theta_B + 2\pi \), by virtue of the invariance of the pure gauge action under center transformations.

Let us try to better clarify the role played by center symmetry. \( Z_N \) is broken explicitly by the presence of the quark determinant; however, a residual \( Z_2 \) symmetry exists for particular values of \( \theta_B \), \( \theta_B = k\pi \), with \( k \) relative integer. Such residual symmetry can be identified, modulo a phase rotation, with charge conjugation \( C \). It stays always unbroken for even values of \( k \); on the contrary, it breaks spontaneously, in the high \( T \) phase, for odd values of \( k \), for which the effective potential of the Polyakov loop has two equivalent, degenerate minima, corresponding to adjacent center sectors [52].

The RW transitions and their connection with the deconfining, chiral restoring (pseudo)-critical line \( T_c(\theta_B) \) have been widely studied both by numerical lattice simulations and by effective model computations [53–68]. The resulting diagram in the \( T-\theta_B \) plane is sketched in Fig. 12.

The RW transition lines are first order and correspond to a discontinuous jump in the order parameter, the Polyakov loop. The order of their endpoint, instead, depends on the quark mass spectrum: evidence from lattice studies collected up to now is that, both for the two-flavor and the three-flavor theory, the endpoint is second order for intermediate quark masses and first order in the limit of large or small quark masses [54–58]. In the former case the universality class is that of the 3D Ising model, since the relevant symmetry is \( Z_2 \); in the latter, the endpoint is actually a triple point, with two further first order lines departing from it, which can be identified with part of the (pseudo)critical lines \( T_c(\theta_B) \) corresponding to chiral symmetry restoration and deconfinement. The line \( T_c(\theta_B) \) is therefore a multibranched function itself, with cusps which can be conjectured to coincide with the RW endpoints, as depicted in Fig. 12 that is also consistent with available numerical evidence.

**B. Phase diagram in the \( T-\theta \) plane**

In presence of a real \( \theta \) term, gauge configurations are weighted, in the path integral representation of the partition function, by a factor \( \exp(i \theta Q) \). The topological charge \( Q \) is globally integer for finite action configurations, hence the partition function and the free energy must be periodic in \( \theta \), with period \( 2\pi \).

However, if one searches for a \( \theta \) dependence which stays non-zero at the leading order in \( 1/N \), as required by the solution to the axial \( U(1) \) problem, one needs that the free energy be a function of \( \theta/N \), instead of \( \theta \), otherwise \( \theta \) dependence would be suppressed exponentially in \( N \).

Also in this case, the only possible way to reconcile periodicity in \( \theta \) and dependence on \( \theta/N \) is to admit that the free energy density \( f(\theta) \) is a multibranched function of \( \theta/(2\pi) \), scaling in the large \( N \) limit as follows [26–28]:

\[
f(\theta) = N^2 \min_k h \left( \frac{\theta + 2\pi k}{N} \right)
\]

(19)

where \( k \) runs over all relative integers. For each value of \( \theta \) the system chooses the branch which minimizes the free energy. The function \( h \) can be chosen so as to have its minimum in zero [69], so that the branch relevant to \( \theta \sim 0 \) corresponds to \( k = 0 \). Moreover, the invariance under \( CP \), present at \( \theta = 0 \), imposes that \( h \) is an even function of \( \theta \).
A shift $\theta \to \theta + 2\pi$ corresponds to a passage from one branch to the other, which, according to the large $N$ scaling in Eq. (19), must happen discontinuously, in points where the free energies of the two adjacent branches cross with different (opposite) derivatives, i.e. through a first order transition. For symmetry reasons that happens for $\theta = \pm \pi$, or odd multiples of such values. $CP$ symmetry, which is exact in correspondence of such points, is broken spontaneously by the choice of one of the two equivalent branches, which are not invariant under $CP$, but instead exchanged into each other. $CP$ is of course exact also for $\theta = 0$ and for integer multiples of $2\pi$, but there no spontaneous breaking happens.

The scenario depicted above is true only for sufficiently low temperatures. Indeed, in the opposite limit of high $T$, the instanton gas approximation must set in, which predicts a smooth, periodic behavior in $\theta$, but with an exponential suppression in the limit of large $N$ \[ 2, 4 \] \footnote{The same approximation does not work in the low $T$ region, because of infrared divergences.}

Actually, it has been conjectured \[ 22, 23 \] and recently proven by lattice simulations \[ 33 \] that the change in $\theta$ dependence happens exactly in correspondence of the deconfinement transition. Therefore, while the confined phase is characterized by a smooth, periodic dependence on $\theta/N$ and a non-analytic periodicity in $\theta$, induced by the multi-branched structure of the free energy, the deconfined phase is characterized by a smooth, periodic dependence on $\theta$, but suppressed like $e^{-N}$ in the large $N$ limit, which very rapidly approaches the instanton gas prediction\footnote{Evidence from Ref. \[ 33 \], extracted by looking at higher order cumulants of the topological charge distribution, is that the instanton gas approximation sets in around $T \sim 1.1 T_c$ for the $SU(3)$ pure gauge theory.}: in this case, of course, no $CP$ breaking transition is expected at $\theta = \pi$. Hence, the $CP$ breaking transition lines, present for $\theta^{(CP)} = (2n + 1)\pi$ and for low enough temperatures, must end at some temperature around $T_c$, as for the case of the RW lines, since the relevant symmetry is again $Z_2$, their endpoint can be either first order or second order in the 3D Ising universality class.

The scenario described above is reproduced in Fig. \[ 13 \] where we have drawn a sketch of the $T$-$\theta$ phase diagram. We have not made any discussion yet regarding the deconfinement line, $T_c(\theta)$, but let us stop for while to comment on the analogy with the periodic structure in the $T$-$\theta_B$ plane, which now appears quite clearly. The analogy actually implies an exchange between the high $T$ and the low $T$ regions of the two diagrams, i.e. $T \to 1/T$, which is suggestive of the possible dual role played by the relevant degrees of freedom in the two cases.

We have already discussed how the analytic or non-analytic periodic structure of the $T$-$\theta_B$ can be understood in terms of a dependence of the free energy on $\theta_B$ (low $T$) or $\theta_B/N$ (high $T$), which in its turn stems from the relevant degrees of freedom being hadrons with integer baryon charge $B$, or quarks carrying fractional baryon charge in unit of $1/N$. If one wants to apply a similar, intuitive picture to the $T$-$\theta$ plane, one has to conjecture that the relevant topological degrees of freedom carry integer values of $Q$ in the high $T$, deconfined phase (in agreement with the instanton gas picture), but instead fractional charges, in units of $1/N$, in the low $T$, confined phase.

Actually, such hypothesis is not new. Indeed, the possible existence of topological objects with fractional charge, which sometimes are called instanton quarks, and their possible role in the confined phase, have been conjectured since long \[ 34, 35, 70, 80 \]. In the high $T$, deconfined phase, they are expected to be localized and confined into larger objects carrying integer topological charge, like instantons and calorons. Instead in the low $T$, confined phase, they are expected to be free and delocalized topological objects.

Apart from the $CP$ breaking lines, the conjectured diagram sketched in Fig. \[ 13 \] is completed by the deconfinement line, $T_c(\theta)$, that we have discussed for $SU(3)$ and small values of $\theta$ in the previous Section. It is reasonable to assume, also based on the large $N$ model of Ref. \[ 11 \], that $T_c(\theta)$ is fixed by the interplay between thermodynamics and topological properties of the theory: since topology is exponentially suppressed in the deconfined phase, the leading dependence of $T_c(\theta)$ must derive from the topological properties of the confined phase, hence we expect \[ 11 \] that also $T_c(\theta)$ be a multibranched function of $\theta/N$, dominated, at the leading order in $1/N$, by the quadratic term

\[
\frac{T_c(\theta)}{T_c(0)} \simeq 1 - R_\theta \min_k (\theta + 2\pi k)^2
\]

where $k$ is a relative integer and $R_\theta$ is $O(1/N^2)$.

Therefore, our expectation is that, at least for large enough $N$, the deconfinement temperature tends to a finite, non-zero value at $\theta = \pi$ or odd multiples of it (actually, $\theta$ independence is expected as $N \to \infty$). Periodicity in $\theta$ implies the presence of cusps for $T_c(\theta)$ at $\theta = (2k + 1)\pi$. Notice that the phase structure may be more complicated in presence of dynamical fermions, which have not been considered in this context: one can still predict the presence of a zero temperature, CP breaking transition at $\theta = \pi$ \[ 34, 35 \], however the interplay between chiral symmetry breaking and confinement can lead to a richer diagram, with the possibility of considering also quark chemical potentials or external fields \[ 16, 19, 36, 38 \].

There is one feature of the sketch in Fig. \[ 13 \] which is pure speculation, stimulated by the analogy with the $T$-$\theta_B$ plane: the curve $T_c(\theta)$ hits the $CP$ breaking lines exactly at their endpoints, as it happens for $T_c(\theta_B)$ with the RW lines. If such speculation were correct, then, since $T_c(\theta)$ is first order at least for large $N$, it would be reasonable to assume that also the endpoint of the $CP$
lines is first order, i.e. a triple point with two departing first order lines, coinciding with the \( T_c(\theta) \) line in the two adjacent branches. The picture could be modified by the presence of dynamical fermions, because of the possible change in the order of the transition at \( \theta = 0 \) and the possible appearance of critical endpoints in the phase diagram. Unfortunately such scenario is not easily testable by lattice simulations since, contrary to what happens for the \( T-\theta_B \) plane, it regards a region affected by a severe sign problem.

**IV. CONCLUSIONS**

We have presented a discussion regarding the phase diagram of pure gauge \( SU(N) \) Yang-Mills theories in presence of a topological \( \theta \) term, based both on numerical results and on considerations related to the large-\( N \) dependence of the theory.

First, we have discussed the behavior of the deconfinement temperature as a function of \( \theta, T_c(\theta) \). The determination presented in Ref. [11], based on the method of analytic continuation from imaginary values of \( \theta \), has been improved by performing new simulations on a finer lattice with \( N_t = 10 \) (which confirms the continuum extrapolation of the curvature at \( \theta = 0 \) reported in Ref. [11]) and has been compared with new results obtained by reweighting configurations sampled at \( \theta = 0 \). As a result, we can conclude that systematic effects related to analytic continuation and to reweighting are under control, at least regarding the determination of the curvature of the critical line \( R_\theta \). The final, continuum value that we estimate for \( N = 3 \) is \( R_\theta = 0.0178(5) \).

As a byproduct of our numerical analysis, we have explored the dependence of physical observables on the topological sector \( Q \), showing that it is somewhat stronger around the transition, in particular for quantities directly related to deconfinement, like the Polyakov loop, and that the transition temperature itself can depend on the topological background. That may be a warning for lattice QCD studies performed in a fixed topological background.

Finally, in the last part of the paper, we have discussed the general features of the \( T-\theta \) diagram. Most of the discussion has been inspired by the possible analogies and dualities (in the sense of an inversion of the low and high-\( T \) regions) existing, also in a large \( N \) perspective, with the phase diagram of QCD in presence of an imaginary baryon chemical potential. Periodicity in \( \theta \) is smoothly realized in the high-\( T \) phase and is instead associated to a multibranch structure in the low temperature phase, where the relevant dependence is on \( \theta/N \), implying first order transitions which are met at odd multiples of \( \theta = \pi \). Such transitions are the analogues of the Roberge-Weiss transitions in the high-\( T \) phase of QCD in presence of an imaginary baryon chemical potential, in both cases the change in the realization of periodicity can be associated to a change in the relevant degrees of freedom, carrying (topological or baryon) charge \( 1 \) or \( 1/N \).

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