θ dependence in trace deformed SU(3) Yang-Mills theory: A lattice study

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In this paper we investigate, by means of numerical lattice simulations, the topological properties of the trace deformed SU(3) Yang-Mills theory defined on $S_1 \times \mathbb{R}^3$. More precisely, we evaluate the topological susceptibility and the b_2 coefficient (related to the fourth cumulant of the topological charge distribution) of this theory for different values of the lattice spacing and of the compactification radius. In all the cases we find results in good agreement with the corresponding ones of the standard SU(3) Yang-Mills theory on \mathbb{R}^4 .

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I. INTRODUCTION

The strongly interacting dynamics of non-Abelian gauge theories at low energy eluded so far any first-principle analytical description, although several nonperturbative approximation schemes have been developed during the years in order to improve our analytical control over this problem, like the expansion in the number of colors N_c or in the number of flavors N_f/N_c [1,2], instanton calculus [1,3] and holographic approaches [4], just to name a few. These approaches gave invaluable hints and helped in clarifying some aspects of the strongly interacting theory; however they typically provide only qualitative or semiquantitative results. Reliable quantitative estimates can still be obtained only numerically, by means of lattice simulations, or by using effective theories that encode from the beginning some nonperturbative features, like chiral perturbation theory.

A complementary strategy that has been proposed consists in deforming the original theory in such a way as to drive the dynamics towards tractable regimes. For this strategy to be usable one has to ensure that physical observables are analytic in the deformation, in order to have the possibility of going back smoothly to the original nondeformed case once results have been obtained in the deformed theory.

One of the first possibilities that may come to mind is to introduce a new scale in the theory by changing the topology of the space-time from \mathbb{R}^4 to $S_1 \times \mathbb{R}^3$, where

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 S_1 stands for a circumference of length *L*. By varying *L* we switch between the original theory on \mathbb{R}^4 (case $L \gg \Lambda^{-1}$, with Λ being a typical energy scale of the theory) and a regime in which perturbation theory and instanton calculus can be applied (case $L \ll \Lambda^{-1}$).

What remains to be shown, in order to advocate the compactification on $S_1 \times \mathbb{R}^3$ as useful in this paradigm, is that physical properties change smoothly when varying the compactificaton length *L*. This is however generically not the case: the compactified theory resembles very much (and for some choice of boundary conditions it is) finite temperature field theory, and a phase transition is likely to happen at finite temperature.

From now on we consider the specific case of SU(3)Yang-Mills theory compactified on $S_1 \times \mathbb{R}^3$ with periodic boundary conditions. In this setup the length of the compactified direction is nothing but the inverse temperature and it is well known that for $L \approx 0.7$ fm (corresponding to a temperature $T_c \simeq 270$ MeV) a first order phase transition is present [5], separating the low temperature confined phase from the high temperature deconfined one. It is clear that in such a situation it is hopeless to obtain reliable results for the large L case by studying the small L case. To proceed further with this approach we have to smoothen or remove the phase transition and here the trace deformation of the action enters.

Let us remind the reader that the deconfinement phase transition at finite temperature is associated with the spontaneous symmetry breaking (SSB) of the Z_3 center symmetry, whose order parameter is the mean value of the trace of the Polyakov loop $P(\vec{x}) = \mathcal{P} \exp (i \int_0^L A_0(\vec{x}, t) dt)$, which vanishes in the confined phase ($\langle \text{Tr}P \rangle = 0$) while it is different from 0 for $T > T_c$ ($\langle \text{Tr}P \rangle = \alpha e^{i2\pi n/3}$, with $n \in \{0, 1, 2\}$ and $\alpha > 0$).

In order to remove the Z_3 SSB that prevents a smooth connection between large and small L regimes, it was suggested in [6] to add to the SU(3) Yang-Mills action a

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new term, explicitly dependent on the Polyakov loop and disfavoring configurations with $\text{Tr}P \neq 0$ in the path integral. Inspired by the perturbative form of the Polyakov loop effective action at high temperature [7], the authors of [6] suggested the following form for the new term:

$$S_{\rm td} = h \int |\mathrm{Tr} P(\vec{x})|^2 \mathrm{d}^3 x, \qquad (1)$$

where *h* is a new parameter and the subscript "td" stands for "trace deformation" [higher powers of $P(\vec{x})$ have also to be added in $SU(N_c)$ theories with $N_c > 3$, see [6]]. Several works followed this approach, but possible alternatives, like the introduction of adjoint fermions or the use of nonthermal boundary conditions, have also been proposed [8–25]. In the present work we restrict ourselves to the case of the deformation in Eq. (1).

It has been shown in [26], using numerical lattice simulations, that the new term S_{td} indeed moves to smaller values the critical compactification length at which deconfinement happens, but it also introduces a new phase (called "skewed") that has no equivalent in the nondeformed theory. A systematic study of the changes induced by S_{td} on observables different from $\langle TrP \rangle$ has however never been undertaken so far and the present work is a first step in this direction.

The reason for performing such a study is that there is no way of excluding *a priori* the possibility that the deformation term S_{td} generates some spurious phase transition in observables uncorrelated with center symmetry. From a more general perspective we can ask: are we sure that what really matters in the low-energy dynamics of SU(3) Yang-Mills is *just* the fact that center symmetry in not spontaneously broken? Since we have no definite answer to this fundamental question, the best thing we can do is to study the trace deformed theory by means of lattice simulations and investigate the behavior of not-center-related physical observables as functions of *h*.

In the present work we concentrate on two observables related to θ dependence: the topological susceptibility χ and the coefficient b_2 , related to the fourth order cumulant of the topological charge distribution (see, e.g., [27]). These observables appear to be perfectly suited to our purposes; since their value is fixed only by nonperturbative physics, they are very sensitive to the deconfinement transition [28–32] and they do not appear to be tightly related to center symmetry [33,34].

II. NUMERICAL SETUP

The standard Wilson action [35] with bare coupling $\beta = 6/g^2$ was used to discretize the theory and the addition of the term S_{td} presents no difficulties, but for the fact that now the action is nonlinear in the temporal links. For this reason a simple Metropolis scheme [36] had to be used to update temporal links, while links directed along other directions could be updated by heat bath and

over-relaxation algorithms [37–39] implemented à *la* Cabibbo-Marinari [40].

To measure the topological content of the gauge configurations we used cooling [41–45] to remove fluctuations at the scale of the lattice spacing (see [46–51] for discussions on the practical equivalence of different smoothing algorithms) and we measured the topological charge $Q = \int q(x) d^4x$ on the smoothed configurations using the discretization of q(x) introduced in [52,53]

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

where $\Pi_{\mu\nu}$ denotes the plaquette operator, $\tilde{\epsilon}_{\mu\nu\rho\sigma}$ coincides with the Levi-Civita tensor for positive entries and is fixed by complete antisymmetry and $\tilde{\epsilon}_{\mu\nu\rho\sigma} = -\tilde{\epsilon}_{(-\mu)\nu\rho\sigma}$ otherwise.

The topological susceptibility χ and the b_2 coefficient parametrize up to $O(\theta^4)$ the θ dependence of the vacuum energy density [27],

$$\Delta E(\theta) \equiv E(\theta) - E(0)$$

= $\frac{1}{2}\chi\theta^2(1 + b_2\theta^2 + b_4\theta^4 + \cdots),$ (3)

and they can be related to the cumulants of the topological charge distribution at $\theta = 0$ by the relations [27]

$$\chi = \frac{\langle Q^2 \rangle_{\theta=0}}{\mathcal{V}}, \qquad b_2 = -\frac{\langle Q^4 \rangle_{\theta=0} - 3\langle Q^2 \rangle_{\theta=0}^2}{12\langle Q^2 \rangle_{\theta=0}}, \qquad (4)$$

where \mathcal{V} is the four-dimensional volume. These expressions can be used to compute χ and b_2 using simulations performed at $\theta = 0$.

While $\theta = 0$ simulations represent the optimal strategy if one is interested in χ , to determine b_2 there is a better possibility: simulations performed at imaginary values (to avoid the sign problem) of θ can be used to obtain a better estimator, with improved signal-to-noise ratio on large volumes [54–56]. In this approach one adds to the discretized Lagrangian density a term $\mathcal{L}_{\theta} = -\theta_L q_L(x)$, where θ_L is the lattice θ parameter (related to its continuum counterpart by a finite renormalization, $\theta = Z\theta_L$ [57]) and $q_L(x)$ is defined in Eq. (2). The values of Z, χ and b_2 can then be obtained by fitting the cumulants of the distribution of the topological charge extracted from simulations performed at $\theta_L \neq 0$, i.e.,

$$\langle Q \rangle_{\theta_L} = \mathcal{V}\chi Z \theta_L (1 - 2b_2 Z^2 \theta_L^2 + \cdots),$$

$$\langle Q^2 \rangle_{\theta_L} - \langle Q \rangle_{\theta_L}^2 = \mathcal{V}\chi (1 - 6b_2 Z^2 \theta_L^2 + \cdots);$$
 (5)

see [55] for more details. The first four cumulants of the topological charge measured at $\theta_L \neq 0$ were used in this work to provide precise estimates of b_2 .

III. RESULTS

Before presenting our results for χ and b_2 in the deformed theory, let us make a few comments on the way in which center symmetry can be realized in Yang-Mills theory and in its deformed counterpart. In ordinary Yang-Mills theory the fact that $\langle \text{Tr}P \rangle = 0$ does not imply that $\langle |\text{Tr}P(\vec{n})|^2 \rangle$ has to be small; i.e., fluctuations of the Polyakov loop are not severely constrained in the confined region. In the confined phase of the deformed theory at small *L*, where $\langle \text{Tr}P \rangle = 0$ is enforced by the new term in Eq. (1), fluctuations of Tr*P* are instead strongly suppressed.

In Fig. 1 we report data for $\langle |\text{Tr}P(\vec{n})|^2 \rangle$ (related to the trace of P in the adjoint representation) measured on a 8×32^3 lattice for two values of the bare coupling β and of the parameter h controlling the deformation. Without deformation (h = 0 case) the system is in the confined phase at $\beta = 5.8$ but not at $\beta = 6.2$; for h = 1.10 center symmetry is restored also at $\beta = 6.2$. We see that $\langle |\text{Tr}P(\vec{n})|^2 \rangle \simeq 1$ in the standard confined phase (h = 0)while it gets significantly smaller, $\langle |\text{Tr}P(\vec{n})|^2 \rangle \simeq 0.5$, when the deformation is switched on (h = 1.1). This is a possible indication that the confined phase of the original and of the deformed theory are different from the dynamical point of view. Will this difference persist in observables of more direct physical relevance? To elucidate this point we now describe the results obtained for the θ dependence in the two cases.

In Fig. 2 we show the behavior of the topological susceptibility as a function of *h*, obtained from simulations performed at $\theta = 0$ on an 8×32^3 lattice at coupling $\beta = 6.4$. The lattice spacing is fixed by the value of the Sommer parameter r_0 [58], determined in [59], whose value in physical units is $r_0 \simeq 0.5$ fm. For $\beta = 6.4$ and



FIG. 1. Time histories of $|\text{Tr}P(\vec{n})|^2$ for two values of the bare coupling ($\beta = 5.8$ and 6.2) and two values of the deformation parameter (h = 0 and 1.1), measured on a 8×32^3 lattice. The two sets of data corresponding to $\beta = 5.8$, 6.2 at h = 1.1 are graphically indistinguishable.



FIG. 2. Topological susceptibility χ and Re $\langle \text{Tr}P \rangle/3$ measured on a 8×32^3 lattice at bare coupling $\beta = 6.4$ as a function of *h*. The value obtained in standard *SU*(3) Yang-Mills theory [27] is also shown for reference (horizontal band).

temporal extent $N_t = 8$ the system is deconfined at h = 0and χ is very small [28–31]. By increasing the value of hthe topological susceptibility quickly gets larger, until it reaches a plateau starting around $h \approx 0.3$, which is approximately the value at which center symmetry starts to be restored (see the behavior of Re $\langle TrP \rangle$ in Fig. 2).

In Fig. 2 the value of χ obtained in standard SU(3) Yang-Mills theory is also reported for reference and it can be noted that this value is consistent with that in the plateau region of the deformed theory; the same happens in all the explored cases. Two different physical values of *L* have been studied, $L^{-1} \simeq 370$ MeV and $L^{-1} \simeq 495$ MeV, and for each of these values two sets of simulations (at $\theta = 0$) have been performed, corresponding to two values of the coupling β and 16 values of *h* in the range $0 \le h \le 1.5$. The qualitative behavior observed for χ as a function of *h* is the same as that shown in Fig. 2 and the plateau values are reported in Fig. 3, again together with the standard SU(3)



FIG. 3. Plateau values of χ extracted from simulations performed on lattices of different temporal extent ($N_t = 6, 8$, with $N_s = 32$) and using different couplings ($\beta = 6.0, 6.2, 6.4$). We also report the inverse compactification size in physical units.

value. From this figure we can exclude the presence of sizable lattice artefacts in the χ plateau values, which are always compatible with the standard SU(3) value and remarkably insensitive to L.

Up to now we have tacitly assumed the lattice spacing to be independent of the deformation parameter h. We can improve on this in two different ways: by explicitly setting the scale at $h \neq 0$ or by looking at dimensionless observables, whose expectation values are independent of the scale setting.

In order to directly test the independence of the lattice spacing on h we determined the scale t_0 , defined by gradient flow and introduced in [60]. While this scale is not associated to the value of a physical observable of direct experimental relevance (like r_0 or the string tension), it has the advantage of being easily measurable with good accuracy on the lattice (see e.g., the discussion in [61]). To extract the value of t_0/a^2 we integrated the flow equations using the Runge-Kutta integrator described in Appendix C of [60] with step size $\epsilon = 0.01$, using a statistics of O(100) independent configurations generated on symmetric lattices. The results obtained are reported in Table I and the outcome is that t_0/a^2 is indeed practically independent of h in the explored range: data coincide with those at h = 0 up to less than 1%, i.e., well within the statistical errors on γ .

Finally, let us discuss results for the dimensionless coefficient b_2 , defined in Eqs. (3) and (4). As previously discussed, to obtain precise results for this observable it is convenient to perform simulations at imaginary values of the θ parameter, which are however significantly slower than the $\theta = 0$ ones: a single simulation is slower than the corresponding one at $\theta = 0$ by a factor $2 \div 3$ and several θ values have to be simulated to extract a single determination of b_2 . For this reason we concentrated on just a couple of points, well in the plateau region of χ : simulations were performed for $\beta = 6.4$ at two values of the deformation parameter (h = 1.10 and 1.20) using 8×32^3 lattices. Seven values of θ_L (the lattice imaginary θ parameter) were

TABLE I. Values of t_0/a^2 with and without the trace deformation. Values at h = 0 have been computed in [60], results at $\beta = 5.96$ have been extracted using 24⁴ lattices, while 32⁴ lattices have been used at $\beta = 6.17$.

β	h	t_0/a^2
5.96	0.0	2.7854(62)
5.96	1.0	2.8087(69)
5.96	2.0	2.8063(74)
β	h	t_0/a^2
6.17	0.0	5.489(14)
6.17	1.0	5.530(16)

investigated, in the range $0 \le \theta \le 16$, and the stability of the results was tested against changes of the fit range adopted. In all the cases the $O(\theta^6)$ dependence of the vacuum energy density come out to be negligible (as in ordinary Yang-Mills [55]) and in the fit we thus used $b_4 = 0$ [see Eq. (3)].

Results obtained for b_2 are shown in Fig. 4 together with the standard SU(3) result of [55]. To appreciate the effectiveness of the imaginary θ approach, a point is also shown obtained by using simulations at $\theta = 0$ only, which required about the same CPU time as the imaginary θ ones. Also for b_2 there is very good agreement between the values at the plateau for the deformed theory and the values known for the confined Yang-Mills theory [55,62–65], in this case without any assumption on the lattice spacing, since b_2 is dimensionless.

For comparison, in Fig. 4 we also indicate two values of b_2 typical of particular regimes. The first is that in which the dominant topological excitations have integer charges and are weakly interacting. Such a regime is well described by the DIGA [7], in which $\Delta E(\theta) \propto 1 - \cos \theta$ and $b_2 = -1/12$. This value is typical of Yang-Mills theory in the deconfined phase [32] and it is clearly incompatible with the results obtained in this work.

Another interesting case is that in which excitations are still weakly interacting but have fractional topological charges $1/3 [1/N_c \text{ for } SU(N_c)]$. This regime corresponds to the functional form $\Delta E(\theta) \propto 1 - \cos(\theta/3)$ of the vacuum energy, characterized by $b_2 = -1/108$, and it is expected to well describe the deformed theory in the limit of asymptotically small L values [6,66,67]: this sort of fractional instanton gas approximation is related to the fact that Abelian degrees of freedom are dominant in the deformed theory in the limit of small L [6,66,67]. From Fig. 4 we see that our results are inconsistent also with this value. A possible interpretation is that, for the explored



FIG. 4. Results obtained for b_2 in the deformed theory using 8×32^3 lattices. The horizontal band denotes the standard SU(3) value [55], dashed lines denote the value $b_2 = -1/12$ [dilute instanton gas approximation (DIGA)] and $b_2 = -1/108$ (fractional instanton gas approximation).

values of L, the deformed theory resembles the actual Yang-Mills vacuum more closely than for asymptotically small values of L, so that non-Abelian degrees of freedom are still relevant, leading to nontrivial interactions between the fractionally charged objects, hence to a value of b_2 which is not equal to the asymptotically predicted one; however, it is also not far from it, supporting the idea that corrections due to residual interactions might be small, and maybe analytically computable. Following the same line of reasoning, based on the virial expansion, discussed in Ref. [32], one might infer that the residual interactions between the fractionally charged objects are repulsive, because the deviation of b_2 from the asymptotic prediction is negative.

IV. CONCLUSIONS

In this paper we investigated, by means of Monte Carlo simulations, the nonperturbative dynamics of the trace deformed SU(3) gauge theory, in which the term in Eq. (1) is added to the action. Such a deformation term inhibits the spontaneous symmetry breaking of center symmetry in the presence of a compactified direction and, in principle, opens the way to the possibility of investigating the low-energy physics of Yang-Mills theory using perturbative/semiclassical methods. For such an ambitious goal to be achievable it is fundamental that physical observables behave smoothly, as functions of β and h, up to small values of the compactification length L. In this paper we investigated the behavior of observables related to the θ -dependence to inquire this point.

Our numerical results for the topological susceptibility and the coefficient b_2 , obtained using compactification lengths $L^{-1} \approx 370$ MeV and $L^{-1} \approx 495$ MeV, are perfectly compatible with the known values for the nondeformed SU(3) theory. Given the completely nonperturbative origin of these quantities, this is a strong indication that the compactified theory indeed conserves intact a significant part of the dynamics of the original Yang-Mills theory.

The values obtained for b_2 show that, at least for the L values explored, low-energy physics cannot be described as a gas of weakly interacting objects of integer or fractional $(1/N_c)$ topological charge. This is again the same thing that happens in ordinary Yang-Mills, but it is at odds with what is expected to happen at very small compactification radii in the deformed theory. A possible interpretation of this result is the following: the nonperturbative dynamics of the deformed theory is so similar to that of the original Yang-Mills one that analytical computations that go beyond the known leading order semiclassical approximations are required to quantitatively describe our numerical data. Indeed the fact that the L dependence is smooth is not enough to guarantee leading order results to be reliable down to $L \approx 500$ MeV. This is a point that surely deserves further studies, specifically targeted at investigating the small L regime and the way in which the large N_c limit is approached. Another interesting topic that could be relevant to better understand this point is the nature of the topological excitations in the deformed theory, which have to be substantially different from that of Yang-Mills theory, because of the compactified direction, but nevertheless with a similar distribution. The study of other not- θ -related observables is also something of the utmost importance to get a complete picture of the physical effects of the deformation.

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