\(\theta\) 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 \(\mathbb{R}^4\).

Introduction - The strongly interacting dynamics of nonabelian 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 flavours \(N_f/N_c\). Instanton calculus and holographic approaches, 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 semi-quantitative 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 non deformed case once results have been obtained in the deformed theory.

One of the first possibility 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 \(S_1\) 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 \(\Lambda\) 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 compactification radius \(L\). 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 will 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 compactification radius is nothing but the inverse temperature and it is well known that for \(L \approx 0.7\) fm (corresponding to a temperature \(T_c \approx 270\) 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 \(P(\vec{x}) = \mathcal{P} \exp \left( i \int_0^L A_0(\vec{x}, t) dt \right)\), which vanishes in the confined phase \((\langle \text{Tr} P \rangle = 0)\) while it is different from zero for \(T > T_c\) \((\langle \text{Tr} P \rangle = \alpha e^{i 2\pi n/3}\), 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 new term, explicitly dependent on the Polyakov loop and disfavouring 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 \([8]\), the authors of \([6]\) suggested the following form for the new term:

\[
S_{\text{td}} = h \int |\text{Tr} P(\vec{x})|^2 d^3x , 
\]

where \(h\) is a new parameter and the subscript “\(\text{td}\)” 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 \([8]\)). Several works followed this approach, but possible alternative, like the introduction of adjoint fermions or the use of non-thermal boundary conditions, have also been proposed \([3, 25]\). In the present work we will restrict ourselves to the case of the deformation in Eq. \((1)\).

It has been shown in \([24]\), using numerical lattice simulations, that the new term \(S_{\text{td}}\) indeed moves to smaller values the critical compactification radius at which deconfinement happens, but it also introduces a new phase (called “skewed”) that has no equivalent in the non deformed theory. A systematic study of the changes induced by \(S_{\text{td}}\) on observables different from \(\langle \text{Tr} P \rangle\) 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 $S_{ld}$ 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 is 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 $\theta$ dependence: the topological susceptibility $\chi$ 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 non-perturbative 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].

**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 $S_{ld}$ 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 heatbath and overrelaxation 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]:

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

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

The topological susceptibility $\chi$ and the $b_2$ coefficient parameterize up to $O(\theta^4)$ the $\theta$ dependence of the vacuum energy density [27]:

$$\Delta E(\theta) \equiv E(\theta) - E(0) = \frac{1}{2} \chi \theta^2 (1 + b_2 \theta^2 + b_4 \theta^4 + \cdots) \quad (3)$$

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

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

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

While $\theta = 0$ simulations represent the optimal strategy if one is interested in $\chi$, to determine $b_2$ there is a better possibility: simulations performed at imaginary values (to avoid the sign problem) of $\theta$ 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 $\theta_L$ is the lattice $\theta$ 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 $Z$, $\chi$ 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.

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

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

see [53] 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 $b_2$.

**Results** - Before presenting our results for $\chi$ 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 $\langle (\text{Tr} P(n))^2 \rangle$ 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 $\text{Tr} P$ are instead strongly suppressed.

In Fig. 1 we report data for $\langle |\langle (\mathcal{P}\mathcal{T}P(\bar{\nu})^2 \rangle \rangle \rangle$ (related to the trace of $P$ in the adjoint representation) measured on a $8 \times 32^3$ lattice for two values of the bare coupling $\beta$ 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 $\langle |\langle (\mathcal{P}\mathcal{T}P(\bar{\nu})^2 \rangle \rangle \rangle \simeq 1$ in the standard confined phase ($h = 0$) while it gets significantly smaller, $\langle |\langle (\mathcal{P}\mathcal{T}P(\bar{\nu})^2 \rangle \rangle \rangle \simeq 0.5$, 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 $\theta$ dependence in the two cases.

In Fig. 2 we show the behavior of the topological susceptibility $\chi$ and $\text{Re} \langle \text{Tr} P \rangle / 3$ measured on a $8 \times 32^3$ lattice at bare coupling $\beta = 6.4$ as a function of $h$. The value obtained in standard $SU(3)$ Yang-Mills theory $\chi_L$ is also shown for reference (horizontal band).

In Fig. 3 the value of $\chi$ 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, $L^{-1} \approx 370 \text{ MeV}$ and $L^{-1} \approx 495 \text{ MeV}$, and for each of these values two sets of simulations (at $\theta = 0$) have been performed, correspond-

| $h$ | $t_0/a^2$ | $\beta$ | $h$ | $t_0/a^2$ |
|-----|-----------|-------|-----|-----------|
| 5.96 | 0.0 | 2.7854(62) | 5.96 | 0.0 | 5.489(14) |
| 5.96 | 1.0 | 2.8087(69) | 6.17 | 1.0 | 5.530(16) |
| 5.96 | 2.0 | 2.8063(74) | 6.17 | 2.0 | 5.498(16) |

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 $24^4$ lattices, while $32^4$ lattices have been used at $\beta = 6.17$. 

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

FIG. 3. Plateau values of $\chi$ 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.

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 App. C of [60] with stepsize $\epsilon = 0.01$, using
and the stability of the results was tested against changes with the standard negligible (as in ordinary Yang-Mills [55]) and in the fit dependence of the vacuum energy density come out to be

Finally, let us discuss results for the dimensionless coefficient $b_2$, defined in Eqs. (3)-(4). As previously discussed, to obtain precise results for this observable it is convenient to perform simulations at imaginary values of the $\theta$ parameter, which are however significantly slower than the $\theta = 0$ ones. For this reason we concentrated on just a couple of points, well in the plateau region of $\chi$: simulations were performed for $\beta = 6.4$ at two values of the deformation parameter ($h = 1.10$ and 1.20) using $8 \times 32^3$ lattices. Seven values of $\theta_L$ (the lattice imaginary $\theta$ parameter) were investigated, in the range $0 \leq \theta \leq 16$, and the stability of the results was tested against changes of the fit range adopted. In all the cases the $O(\theta^3)$ dependence of the vacuum energy density come out to be negligible (as in ordinary Yang-Mills [54]) 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 [53]. To appreciate the effectiveness of the imaginary $\theta$ approach, a point is also shown obtained by using simulations at $\theta = 0$ only, which required about the same CPU-time as the imaginary $\theta$ 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 [51],[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 dilute instanton gas approximation (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 $1/3 (1/N_c$ for $SU(N_c))$. This regime is expected to well describe the deformed theory in the limit of very small $L$ values [6, 66, 67] and corresponds to $\Delta E(\theta) \propto 1 - \cos(\theta/3)$ and $b_2 = -1/108$. From Fig. 4 we see that our results are inconsistent also with this value.

Conclusions - In this paper we investigated, by means of Monte-Carlo simulations, the non-perturbative 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 $\beta$ and $h$, up to small values of the compactification length $L$. In this paper we investigated the behavior of observables related to the $\theta$-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 non-deformed $SU(3)$ 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. This is a point that surely deserves further studies, specifically targeted at investigating the small $L$ regime, the large $N_c$ limit and the nature of the topological excitations, which have to be substantially different from that of Yang-Mills theory, nevertheless with a similar distribution. The study of other not-$\theta$-related observables is also something of the utmost importance to get a complete picture of the physical effects of the deformation.

Acknowledgement We thank J. Greensite, M. Unsal and T. Sulejmanpasic for useful discussions. Numerical simulations have been performed at the Scientific Computing Center at INFN-PISA and on the MARCONI machine at CINECA, based on the agreement between INFN and CINECA (under project INF18_mpqd).
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