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The imaginary-θ dependence of the SU(N) spectrum

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In this talk we will report on a study of the θ-dependence of the string tension and of the mass gap of four-dimensional SU(N) Yang–Mills theories. The spectrum at $N = 3$ and $N = 6$ was obtained on the lattice at various imaginary values of the θ-parameter, using Parallel Tempering on Boundary Conditions to avoid topological freezing at fine lattice spacings. The coefficient of the $O(\theta^2)$ term in the Taylor expansion of the spectrum around $\theta = 0$ could be obtained in the continuum limit for $N = 3$, and on two fairly fine lattices for $N = 6$.

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1. Introduction

The study of systems described by a Yang-Mills (YM) action augmented with a θ-term has provided, historically, several interesting results. Classically speaking, the addition of a θ-term does not alter the classical equations of motion. Yet, its theoretical and phenomenological implications are far reaching, once the quantum fluctuations are taken into account. The θ-dependence lies at the heart of the Witten–Veneziano solution of the η-η' puzzle [1–4] and it is the starting point for the Peccei–Quinn hypothetical solution to the strong-CP problem based on axions. Accordingly, the study of θ-dependence in a variety of different settings has attracted a great deal of attention in the past years. Starting from QCD, SU(N) and Sp($2N$) models [5–7] in $4d$, to CP^{N-1} models [8, 9] and U(N) models [10–12] in $2d$, to quantum mechanical models [13–15].

So far, the main target of investigation has been the free energy of the system and its θ-dependence, both at zero and finite temperature. Using analytical methods, it is possible to obtain theoretical predictions for the θ-dependence of the QCD vacuum energy either using effective theories close to the chiral limits for low temperatures [16–19], where the θ-dependence of the vacuum energy essentially stems from the θ-dependence of the pion mass (the θ-dependence of the mass of some light resonances has also been investigated in [20]); or for the θ-dependence of the QCD free energy via perturbative and semi-classical arguments for asymptotically-high temperatures [6, 7, 21]. Away from these regimes, the θ-dependence of the vacuum energy has been investigated by means of numerical Monte Carlo simulations of the lattice-discretized theory, both in QCD [22–29] and in SU(N) pure-gauge theories [30–47], with particular focus on the large-N limit of these models, due to its relation with the Witten–Veneziano mechanism [1–4]. Concerning two-dimensional models, the θ-dependence of $2d$ CP^{N-1} models is amenable to be exactly computed using analytical methods in the large-N limit up to the next-to-leading-order in the $1/N$ expansion [8, 45, 48–50], and such predictions have been verified to be supported by numerical evidence [11, 12, 51–53]. The θ-dependence of $2d$ CP^{N-1} models has also been studied numerically [54, 55] in the limit $N \to 2$, as these theories reduce to the $2d$ O(3) non-linear σ model in this limit (see also [56, 57]), whose θ-dependence is theoretically interesting due to its connection with the Haldane conjecture. Finally, also the θ-dependence of $2d$ U(N) Yang–Mills theories can be exactly computed analytically [10–12].

The θ-dependence of the spectrum of the theory has received comparatively less attention, with only one exploratory lattice study [49] present in the literature. Our main goal is to bridge that gap. In particular, we report on our study [58] of the θ-dependence of the spectrum of glueballs and fluxtubes of pure-gauge SU(N) models in $4d$. The results that we have obtained constitute a substantial improvement over the previously available results. This could be achieved with the combination of the imaginary-θ method and of the Parallel Tempering on Boundary Conditions (PTBC) algorithm. The former enables us to improve the signal-to-noise ratio compared to the standard Taylor expansion approach, and the latter enabled us to avoid the freezing of topology, especially at large-N.

This proceeding is organized as follows. In Sec. 2 we describe our numerical setup. In Sec. 3 we present the main results of [58]. Finally, in Sec. 4 we draw our conclusions.

2. Numerical Setup

Direct lattice simulations of the Yang–Mills theory at non-zero values of θ are hindered by the infamous sign problem, as the topological term is purely imaginary, thus yielding a complex action. A popular technique to bypass the sign-problem is to resort to simulations of imaginary-values of $\theta_{\rm I} \equiv \mathrm{i}\theta$, characterized by a purely-real action. Assuming analyticity around $\theta = 0$ it is possible to use analytic continuation and infer the dependence on the real parameter θ from the observed dependence on the imaginary one $\theta_{\rm I}$, at least for small enough values of θ. The imaginary-θ method has been shown to be extremely effective in improving the signal-to-noise-ratio of the higher-order coefficients in the θ-expansion of several quantities, compared to simulations at $\theta = 0$ alone [38, 44–47, 52, 53, 57, 59–67]. Our lattice action at non-zero imaginary-θ reads:

$$\mathcal{S}_{\rm L}(\theta_{\rm L}) = \mathcal{S}_{\rm W} + \theta_{\rm L} Q_{\rm clov}, \tag{1}$$

where S_w is the standard Wilson plaquette action,

$$\mathcal{S}_{\rm W} = -\frac{\beta}{2N}\sum_x \sum_{\nu>\mu} \mathrm{Tr}\left[\mathcal{P}_{\mu\nu}(x)\right] , \tag{2}$$

with β the bare gauge coupling, $\mathcal{P}_{\mu\nu}(x)$ the product of gauge links around an elementary plaquette,

$$\mathcal{P}_{\mu\nu}(x) \quad = \quad U_\mu(x)U_\nu(x+a\hat{\mu})U^\dagger_\mu(x+a\hat{\nu})U^\dagger_\nu(x), \tag{3}$$

based in the site x of the lattice and lying in the (μ,ν) plane, and $U_\mu(x) \in \mathrm{SU}(N)$ are gauge link variables.

For the lattice topological charge, we employed the standard clover discretization,

$$Q_{\rm clov} = \frac{1}{2^9\pi^2}\sum_{\mu\nu\rho\sigma=\pm1}^{\pm4} \varepsilon_{\mu\nu\rho\sigma}\mathrm{Tr}\left[\mathcal{P}_{\mu\nu}(x)\mathcal{P}_{\rho\sigma}(x)\right] . \tag{4}$$

$Q_{\rm clov}$ is not integer-valued on the lattice and is related to the continuum topological charge via a finite renormalization [68], $Q_{\rm clov} = Z_Q Q$, where $Z_Q(\beta) < 1$ tends to 1 only in the continuum limit ($\beta \to \infty$). As a result, the lattice parameter $\theta_{\rm L}$ is thus related to the physical one by: $\theta = \mathrm{i}Z_Q\theta_{\rm L}$.

Obtaining the renormalization constant Z_Q requires the calculation of the lattice topological charge. This can be computed by means of smoothing. To this end one can adopt any of the various algorithms that have been proposed in the literature, such as cooling [69–75], smearing [76, 77], or gradient flow [78–80], as they have been shown to be all numerically equivalent when matched to one another [75, 81, 82]. In this work, we determine the lattice topological charge and the renormalization factor Z_Q via cooling as follows [38]:

$$Z_Q = \frac{\langle Q_{\rm I} Q_{\rm clov}\rangle}{\langle Q_{\rm I}^2\rangle}, \qquad Q_{\rm I} = \mathrm{round}\left\{\alpha\, Q_{\rm clov}^{(\rm cool)}\right\}, \tag{5}$$

with $Q_{\rm I}$ the lattice integer-valued topological charge [33], $Q_{\rm clov}^{(\rm cool)}$ the clover-discretized charge computed after 20 cooling steps, and α the numerical value minimizing

$$\left\langle\left(\alpha Q_{\rm clov}^{(\rm cool)} - \mathrm{round}\left\{\alpha\, Q_{\rm clov}^{(\rm cool)}\right\}\right)^2\right\rangle, \qquad 1 < \alpha < 2. \tag{6}$$

We performed simulations for $N = 3$ and $N = 6$ on hypercubic lattices L^4 and several values of β. For the $N = 3$ runs, we adopted the standard 4:1 mixture of over-relaxation [83] and heat-bath [84, 85] algorithms. For $N = 6$ runs we instead adopted the Parallel Tempering on Boundary Conditions (PTBC) algorithm [86] to overcome the severe critical slowing down experienced at large-N and close to the continuum limit by topological modes [87–89], known as *topological freezing*. The PTBC algorithm has been extensively applied both in $2d$ models [53, 86, 90] and in $4d$ gauge theories, both with [91] and without [66, 67, 92–94] dynamical fermions. This algorithm consists in simulating several replicas of the lattice, all differing from each other by just for the boundary conditions imposed on a small sub-region of the lattice, known as the defect. Boundary conditions are taken to be periodic everywhere but on the defect where, on each replica, they are chosen to interpolate between periodic and open. The state of each replica is evolved with a standard local Monte Carlo updating algorithm except for swaps between gauge configurations of the different replicas, that are proposed and stochastically accepted/rejected via a standard Metropolis step. The calculation of observables is always performed on the replica with periodic boundary conditions. This algorithm enables us to enjoy the fast decorrelation of topological modes achieved with open boundaries (which is transferred towards the periodic replica by the swaps) and, at the same time, to avoid the systematic effects introduced with open boundary conditions.

We determine the SU(N) spectrum with the variational method. An appropriate variational basis of zero-momentum projected operators $\{O_i(t)\}$ was defined for each symmetry channel of interest. In particular, the operators were path ordered products of link variables along space-like paths of various shapes and sizes, and at different levels of blocking and smearing [76, 95–104]. Their correlator was computed on the generated ensembles,

$$C_{ij}(t) = \langle O_i(t) O_j(0) \rangle \tag{7}$$

and then a Generalized EigenValue Problem (GEVP), $C_{ij}(t)v_j = \lambda(t, t_0) C_{ij}(t_0) v_j$, was solved. This enabled us to find the optimal combination of operators for each symmetry channel, and to define the corresponding correlation function,

$$\overline{C}(t) = C_{ij}(t)\overline{v}_j, \tag{8}$$

with $\overline{v}$ the eigenvector related to the largest eigenvalue $\lambda(t, t_0)$. The GEVP was always solved for $t_0 = a$, and we checked in a few cases that $t_0 = 2a$ gave compatible results. The ground state mass was then obtained via a best fit of $A\,[\exp(-mt) + \exp(-m(La - t))]$ to the correlator, using m and A as fitting parameters, over a range of t where the effective mass, defined as follows,

$$am_{\rm eff}(t) = -\log\left[\frac{\overline{C}(t+a)}{\overline{C}(t)}\right], \tag{9}$$

exhibited a plateaux.

For the mass gap of the theory, we considered a variational basis made of 4-, 6- and 8-link operators in the A_1 representation of the octahedral group. For the torelon mass we used a variational basis made of products of fat-links winding around the time direction once. We then extracted the string tension using [105] (with L the lattice size in lattice units):

$$a^2\sigma = \frac{am_{\rm tor}}{L} + \frac{\pi}{3L^2}. \tag{10}$$

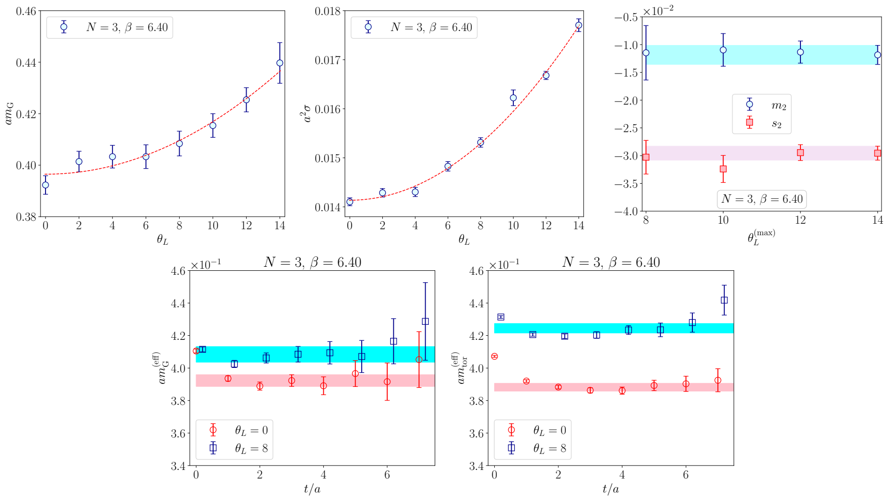

Figure 1: *Results for $N = 3$ with $\beta = 6.40$ (finest lattice spacing explored).*

3. Results

We determined the mass gap of the theory (i.e., the mass of the lightest glueball state) and the string tension in lattice units for several values of β and $\theta_{\rm L}$. The θ dependence was parameterized by Taylor expanding in up to the next-to-leading order, around $\theta = 0$,

$$am_{\rm G}(\theta) = am_{0^{++}}\left[1 + m_2\theta^2 + O(\theta^2)\right], \tag{11}$$

$$a^2\sigma(\theta) = a^2\sigma\left[1 + s_2\theta^2 + O(\theta^2)\right], \tag{12}$$

where the well-established fact that at $\theta = 0$ the mass of the 0^{++} glueball is the lightest one in pure-Yang–Mills theories [99, 103, 104, 106]) was used. Using analyticity, and the renormalization property of the lattice imaginary-θ parameter, one simply has:

$$am_{\rm G}(\theta_{\rm L}) = am_{0^{++}}\left[1 - m_2 Z_Q^2\theta_{\rm L}^2 + O(\theta_{\rm L}^2)\right], \tag{13}$$

$$a^2\sigma(\theta_{\rm L}) = a^2\sigma\left[1 - s_2 Z_Q^2\theta_{\rm L}^2 + O(\theta_{\rm L}^2)\right]. \tag{14}$$

We thus performed a best fit of our determinations of $m_{\rm G}(\theta_{\rm L})$ and $\sigma(\theta_{\rm L})$ as a function of $\theta_{\rm L}$ at fixed β and determined the quantities $m_2 Z_Q^2$ and $s_2 Z_Q^2$. Since the value of $Z_Q(\beta)$ was known for each β, we could obtain m_2 and s_2. Our results for m_2 and s_2 at $N = 3$ are displayed in Fig. 1. They are very stable as a function of the fitting range, signaling that we are insensitive to the effects of higher-order corrections. We also display a few examples of plateaux of effective masses.

In Fig. 2 we display the continuum extrapolation of our results for m_2 and s_2. We also extrapolated towards the continuum limit the dimensionless ratio $m_{0^{++}}/\sqrt{\sigma}$ in order to verify that our result is in agreement with the previous determination provided in Ref. [103].

These are our final determinations for $N = 3$, in the continuum limit,

$$\frac{m_{0^{++}}}{\sqrt{\sigma}} = 3.398(25), \qquad \text{(continuum limit, } N = 3\text{)}, \tag{15}$$

$$m_2 = -0.0083(23), \qquad \text{(continuum limit, } N = 3\text{)}, \tag{16}$$

$$s_2 = -0.0258(14), \qquad \text{(continuum limit, } N = 3\text{)}. \tag{17}$$

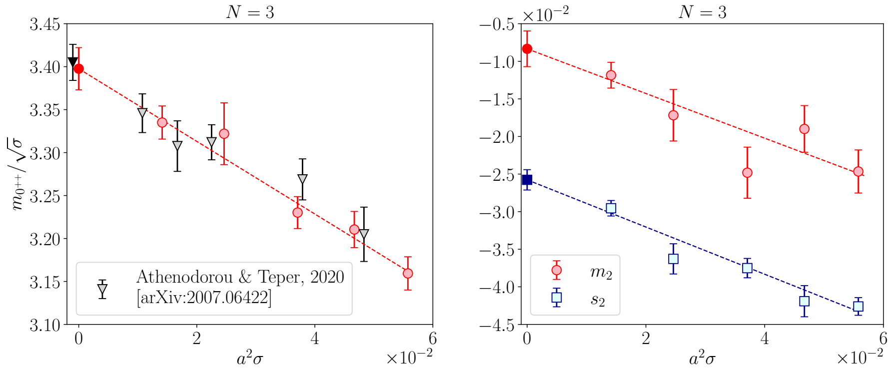

Figure 2: *Continuum limit of our $N = 3$ results for m_2 and s_2. We also computed the continuum limit of $m_{0^{++}}/\sqrt{\sigma}$, which is in perfect agreement with the previous result of [103].*

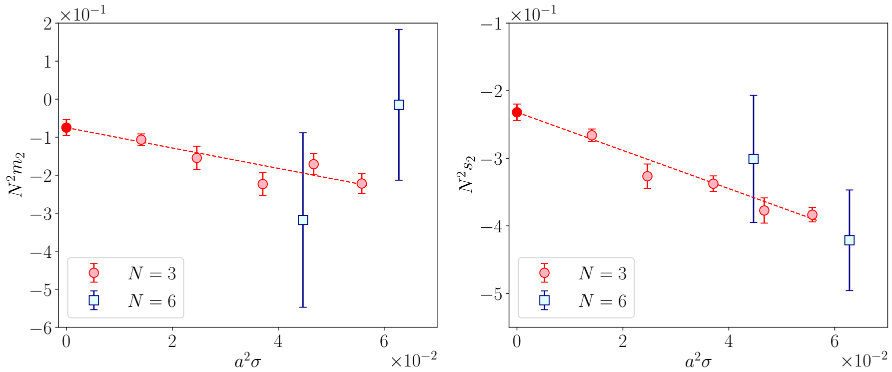

Figure 3: *Continuum scaling of $N^2 m_2$ and $N^2 s_2$ for $N = 3$ and $N = 6$.*

Concerning $N = 6$, we obtained results only for two fairly fine lattice spacings, thus we cannot perform a continuum limit of these data alone. However, our data allowed for a first quantitative check of the following expected large-N scaling:

$$m_2 = \frac{\overline{m}_2}{N^2} + O\left(\frac{1}{N^4}\right), \qquad s_2 = \frac{\overline{s}_2}{N^2} + O\left(\frac{1}{N^4}\right). \tag{18}$$

Our $N = 3$ and 6 results are perfectly compatible with this expected scaling, see Fig. 3. Thus, in the end we can quote the following estimates:

$$\overline{s}_2 \simeq -0.23(1)\ , \quad \overline{m}_2 \simeq -0.075(20)\ . \tag{19}$$

4. Conclusions

The present manuscript reports on the main finding of [58]. We have studied the θ-dependence of the SU(N) spectrum, focusing on the mass gap of the theory and on the string tension for $N = 3$ and $N = 6$.

For SU(3), in the continuum limit we found:

$$\left.\frac{m_{\mathrm{G}}}{\sqrt{\sigma}}\right|_{\theta=0} = \frac{m_{0^{++}}}{\sqrt{\sigma}} = 3.398(25)\ , \quad m_2 = -0.0083(23), \quad s_2 = -0.0258(14), \tag{20}$$

where

$$m_2 \equiv \frac{1}{2m_{0^{++}}} \times \left.\frac{\mathrm{d}m_{\mathrm{G}}(\theta)}{\mathrm{d}\theta^2}\right|_{\theta=0}, \qquad s_2 \equiv \frac{1}{2\sigma} \times \left.\frac{\mathrm{d}\sigma(\theta)}{\mathrm{d}\theta^2}\right|_{\theta=0}. \tag{21}$$

The results obtained at $N = 6$ also enabled us to check that the expected large-N scaling was realized and to estimate:

$$m_2(N) \simeq \frac{-0.075(20)}{N^2} + O\left(\frac{1}{N^4}\right), \qquad s_2(N) \simeq \frac{-0.23(1)}{N^2} + O\left(\frac{1}{N^4}\right). \tag{22}$$

Note that for $N = 3$, the value of m_2 is very close to $s_2/2$. As a result, the coefficient g_2 of the order $O(\theta^2)$ correction to the dimensionless ratio $m_{\mathrm{G}}/\sqrt{\sigma}$,

$$\left(\frac{m_{\mathrm{G}}}{\sqrt{\sigma}}\right)(\theta) = \frac{m_{0^{++}}}{\sqrt{\sigma}}\left(1 + g_2\theta^2 + O(\theta^4)\right), \tag{23}$$

is compatible with zero within two standard deviations,

$$g_2 = m_2 - \frac{s_2}{2} = 0.0046(24)\ . \tag{24}$$

We are not aware of any general theoretical argument that would dictate the θ-independence of this dimensionless ratio. Actually, we can provide a counter-example to this. In Refs. [64, 65, 67], the θ-dependence of the SU(N) deconfinement critical temperature T_c was investigated for $N \geq 3$ (for a first SU(2) study see [107]). It was concluded that if

$$T_c(\theta) = T_c[1 - R\theta^2 + O(\theta^4)]\ , \tag{25}$$

then

$$R(N = 3) = 0.0178(5)\ , \quad R(N) = \frac{0.159(4)}{N^2} + O\left(\frac{1}{N^4}\right) \quad (N > 3)\ . \tag{26}$$

Using our result for s_2, we would then find,

$$\frac{T_c(\theta)}{\sqrt{\sigma(\theta)}} = \frac{T_c}{\sqrt{\sigma}}[1 - t_2\theta^2 + O(\theta^4)]\ , \tag{27}$$

and the coefficient t_2 would then be non-vanishing,

$$t_2 = R + \frac{s_2}{2} = 0.0049(9)\ . \tag{28}$$

It is interesting to observe that the θ-dependence of m_{G} and σ in large-N Yang–Mills theories has been also addressed within holographic models in [108], providing the following prediction:

$$\frac{s_2}{m_2} = \frac{\bar{s}_2}{\bar{m}_2} = 4, \qquad \text{(holography)}, \tag{29}$$

which nicely agrees with our lattice result

$$\frac{s_2}{m_2} = \frac{\bar{s}_2}{\bar{m}_2} = 3.07(82), \qquad \text{(lattice)}. \tag{30}$$

On the other hand, Ref. [108] predicts that the ratio $T_c(\theta)/m_G(\theta)$ is θ-independent at $O(\theta^2)$, i.e., $R/m_2 = -1$, in contrast with our lattice result $R/m_2 = -2.14(57)$ indicating that $T_c(\theta)/m_G(\theta)$ has a non-trivial θ-dependence already at leading order in θ.

Finally, we recall the interesting role played by m_2, identified in [109, 110] in the estimation of the systematic error introduced in lattice spectra calculations performed at fixed topological sector. At a fixed value Q of the topological charge, the following approximate relation holds for the mass M of any bound state,

$$\frac{M^{(Q)} - M}{M} \approx \frac{M_2}{2\chi V}\,, \tag{31}$$

where $\chi = \langle Q^2 \rangle / V$ is the topological susceptibility and M_2 is the order $O(\theta)^2$ coefficient of $M(\theta) = M[1 + M_2\theta^2 + O(\theta^4)]$. For $N = 3$ the topological susceptibility is roughly $\chi \simeq (1\ \text{fm})^{-4}$. For a standard lattice volume of $V = (1.5\ \text{fm})^4$, one has the following bound on the systematic error on the numerical estimation of the lightest 0^{++} glueball:

$$\left.\frac{\Delta m_{0^{++}}}{m_{0^{++}}}\right|_{N=3} \approx \frac{m_2}{2\chi V} \approx -0.08\%. \tag{32}$$

This bound will become even more favorable at larger value of N, since χ does not change appreciably with N, while $m_2 \sim O(1/N^2)$.

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