Simulating a CP-violating topological term in gauge theories

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Abstract. We present recent results on the \(\theta\)-dependence of four-dimensional SU\((N)\) gauge theories, where \(\theta\) is the coefficient of the CP-violating topological term in the Lagrangian. In particular, we study the scaling behavior of these theories, by Monte Carlo simulations at imaginary \(\theta\). The numerical results provide good evidence of scaling in the continuum limit. The imaginary \(\theta\) dependence of the ground-state energy turns out to be well described by the first few terms of related expansions around \(\theta=0\), providing accurate estimates of the first few coefficients, up to \(O(\theta^6)\).

Four-dimensional SU\((N)\) gauge theories have a nontrivial dependence on the parameter \(\theta\) which appears in the Euclidean Lagrangian as

\[
\mathcal{L}_\theta = \frac{1}{4} F_{\mu\nu}^a(x) F^{a\mu\nu}(x) - i \theta q(x), \quad q(x) = g^2/(64\pi^2) \epsilon_{\mu\nu\rho\sigma} F_{\mu\nu}^a(x) F_{\rho\sigma}^a(x),
\]

where \(q(x)\) is the topological charge density. The ground-state energy density \(F(\theta)\) behaves as

\[
\mathcal{F}(\theta) \equiv F(\theta) - F(0) = (1/2) \chi \theta^2 s(\theta),
\]

where \(\chi\) is the topological susceptibility at \(\theta = 0\),

\[
\chi = \int d^4x \langle q(x) q(0) \rangle_{\theta=0} = \langle Q^2 \rangle_{\theta=0}/V,
\]

\(V\) is the spacetime volume and \(s(\theta)\) is a dimensionless even function of \(\theta\) such that \(s(0) = 1\). Assuming analyticity at \(\theta = 0\), \(s(\theta)\) can be expanded as: \(s(\theta) = 1 + b_2 \theta^2 + b_4 \theta^4 + \cdots\), where only even powers of \(\theta\) appear. Large-\(N\) scaling arguments applied to the Lagrangian (1) indicate that the relevant scaling variable in the large-\(N\) limit is \(\theta \equiv \theta/N\). This implies that in this limit \(\chi = O(1)\), while the coefficients \(b_{2i}\) are suppressed by powers of \(N\), i.e. \(b_{2i} = O(N^{-2i})\).

Due to the nonperturbative nature of the \(\theta\) dependence, quantitative assessments have largely focused on the lattice formulation of the theory, using Monte Carlo (MC) simulations. However, the complex nature of the \(\theta\) term in the Euclidean Lagrangian prohibits a direct MC simulation at \(\theta \neq 0\). Information on the \(\theta\) dependence of physically relevant quantities, such as the ground state energy and the spectrum, has been obtained by computing the coefficients of the corresponding expansions around \(\theta = 0\). The coefficients of \(s(\theta)\) can be determined from appropriate zero-momentum correlation functions of \(q(x)\) at \(\theta = 0\), which are related to the moments of the \(\theta = 0\) probability distribution \(P(Q)\) of the topological charge \(Q\). Indeed

\[
b_2 = -\frac{1}{12 \chi V} \left[ \langle Q^4 \rangle - 3 \langle Q^2 \rangle^2 \right]_{\theta=0}, \quad b_4 = -\frac{1}{360 \chi V} \left[ \langle Q^6 \rangle - 15 \langle Q^2 \rangle^2 \langle Q^4 \rangle + 30 \langle Q^2 \rangle^3 \right]_{\theta=0},
\]
etc. They parameterize the deviations of $P(Q)$ from a simple Gaussian behavior. It has been shown that correlations involving multiple insertions of the topological charge can be defined in a nonambiguous, regularization independent way, and therefore $b_{2i}$ are well defined renormalization group invariant quantities. The numerical evidence for a nontrivial $\theta$-dependence, obtained through MC simulations, appears quite robust. We refer the reader to Ref. [1] for a recent review. On the other hand, MC simulations at $\theta = 0$ have only made it possible to estimate the ground-state energy up to $O(\theta^4)$. The large-$N$ prediction $b_2 = O(N^{-2})$ has been already supported by numerical results; the calculation of the higher-order terms would provide a further check of the power-law suppression predicted by large-$N$ arguments.

In this paper we consider imaginary values of $\theta$, which make the Euclidean Lagrangian (1) real, thus making MC simulations possible. For further details and references, the reader may consult our Ref. [2]. Assuming analyticity at $\theta = 0$, the results provide quantitative information on the expansion around $\theta = 0$. Indeed, fits of the data to polynomials of imaginary $\theta$ may provide more accurate estimates of the coefficients, overcoming the rapid increase of statistical errors observed at $\theta = 0$. Perturbative renormalization-group (RG) arguments indicate that $\theta$ is a RG invariant parameter of the theory, thus the continuum limit should be approached while keeping $\theta$ fixed to any complex value. We find that this is indeed supported by the numerical data for the 4D SU(3) lattice gauge theory, at least for $|\theta| < \pi$, which are well described by the first few nontrivial terms of the expansion around $\theta = 0$.

Introducing the real parameter $\theta_i$, defined by $\theta \equiv -i\theta_i$, Eq. (2) leads to:

$$\frac{\langle Q \rangle_{\theta_i}}{V} = -\frac{\partial F(-i\theta_i)}{\partial \theta_i} = \chi \theta_i \left(1 - 2b_2 \theta_i^2 + 3b_4 \theta_i^4 + \cdots\right),$$

$$\frac{\langle Q^2 \rangle_{\theta_i}}{V} = -\frac{\partial^2 F(-i\theta_i)}{\partial \theta_i^2} = \chi \left(1 - 6b_2 \theta_i^2 + 15b_4 \theta_i^4 + \cdots\right).$$

The nonperturbative formulation of the above theory on the lattice requires a discretization of the action, $S_L - \theta_L Q_L$; for $S_L$ we use the plaquette gluon action, while for $Q_L$ we employ the “twisted double plaquette” operator $q_L (Q_L = \sum_x q_L(x))$. Notice that this is not the only possible choice for $q_L$; the only requirement is that it have the correct continuum limit when $a \rightarrow 0$ ($a$: lattice spacing). In the continuum limit $q_L(x)$, being a local operator, behaves as

$$q_L(x) \rightarrow a^4 Z_q q(x) + O(a^6),$$

where $Z_q$ is a finite function of the bare coupling $g_0$, going to one in the limit $\beta \equiv 2N/g_0^2 \rightarrow \infty$. Thus, we have the correspondence: $\theta_i = Z_q \theta_L$, apart from $O(a^2)$ corrections. The renormalization $Z_q$ may be evaluated by MC simulation at $\theta = 0$, computing

$$Z_q = \frac{\langle QQ_L \rangle_{\theta=0}}{\langle Q^2 \rangle_{\theta=0}},$$

where $Q$ is an estimator such as those obtained by the overlap method or the cooling method, which are not affected by renormalizations, nor by nonphysical contact terms. Thus, the ratios

$$\frac{\langle Q \rangle_{\theta_i}}{\langle Q \rangle_{\theta=0}} = \theta_i - 2b_2 \theta_i^3 + 3b_4 \theta_i^5 + \cdots, \quad \frac{\langle Q^2 \rangle_{\theta_i}}{\langle Q^2 \rangle_{\theta=0}} = 1 - 6b_2 \theta_i^2 + 15b_4 \theta_i^4 + \cdots.$$
are expected to have a well defined continuum limit as functions of $\theta_1$.

We have carried out MC simulations of the 4D SU(3) lattice gauge theory, at $\beta = 5.9, 6, 6.2,$ for lattice sizes $L = 16, 16, 20$, respectively; the simulations are carried out both at $\theta_L = 0$ and $\theta_L \neq 0$, within the region $|\theta_i| \leq \pi$. Since our numerical study requires high-statistics MC simulations, we choose the cooling method as estimator of the topological charge $Q$. The topological charge has been measured on cooled configurations (by locally minimizing the lattice action), using the twisted double plaquette operator. As is well known, this procedure leads to topological charge estimates obtained from MC simulations, we choose the cooling method as estimator of the topological charge $Q$. The MC data at different $\beta$ values follow the same curve, providing evidence of scaling. Scaling corrections, expected to be $O(a^2)$, are quite small, and tend to increase with increasing $\theta_t$. This good scaling behavior corroborates the existence of a nontrivial continuum limit for any value of $\theta_t$. Fitting our data to Eqs. (5,6,9) improves significantly the $\theta = 0$ results. In particular, a much smaller bound on $b_4$ is obtained: $|b_4| < 0.001$; also, we find: $b_2 = -0.026(3)$, which is clearly more precise than the estimate obtained from $\theta = 0$ runs only: $b_2 = -0.029(7)$.

Besides allowing more precise determinations of the $\theta$ expansion coefficients of the ground-state energy and other observables, using imaginary $\theta$ values might turn out useful in overcoming the dramatic critical slowing down of topological modes, by performing parallel tempering simulations with a set of $\theta$ values including $\theta = 0$; this is an exact MC algorithm for the model.

References
[1] E. Vicari and H. Panagopoulos, $\theta$ dependence of SU(N) gauge theories in the presence of a topological term, Phys. Rep. 470 (2009) 93 [arXiv:0803.1593 hep-th].
[2] H. Panagopoulos and E. Vicari, The 4D SU(3) gauge theory with an imaginary $\theta$ term, JHEP 11 (2011) 119 [arXiv:1109.6815].