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SU($N$) gauge theories in the presence of a topological term

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Abstract: We review recent results on the $\theta$ dependence of the ground-state energy and spectrum of four-dimensional SU($N$) gauge theories, where $\theta$ is the coefficient of the CP-violating topological term $\tilde{F}\tilde{F}$ in the Lagrangian. In particular, we discuss the results obtained by Monte Carlo simulations of the lattice formulation of QCD, which allow the investigation of $\theta$ dependence around $\theta = 0$ by determining the moments of the topological charge distribution, and their correlations with other observables. The results for $N = 3$ and larger values of $N$ support the scenario obtained by general large-$N$ scaling arguments.
1. \( \theta \) dependence of the ground-state energy

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

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

(1.1)

where \( q(x) = \frac{g^2}{64\pi^2} \epsilon_{\mu\nu\rho\sigma} F_{\mu\nu}^a(x) F_{\rho\sigma}^a(x) \) is the topological charge density. Semiclassical instanton solutions are one example of field configurations which have nontrivial topological properties. Moreover, the most plausible explanation of how the solution of the so-called U\((1)_A \) problem can be compatible with the \( 1/N \) expansion (performed keeping \( g^2N \) fixed [1]) requires a nontrivial \( \theta \) dependence of the ground-state energy density \( F(\theta) \) [2, 3],

\[
\exp[-VF(\theta)] = \int [dA] \exp \left( - \int d^4x \mathcal{L}_\theta \right)
\]

(1.2)

where \( V \) is the volume. Evidence for such a dependence has been obtained by exploiting the lattice formulation of the theory, using numerical Monte Carlo simulations, as will be described in Section 3. The complex nature of the \( \theta \) term in the Euclidean QCD Lagrangian makes the Monte Carlo studies of the \( \theta \) dependence quite hard,
since the lattice action corresponding to the Lagrangian (1.1) cannot be directly simulated for $\theta \neq 0$. Nevertheless, important information on the $\theta$ dependence of relevant physical quantities, such as the ground-state energy and the spectrum, can also be inferred from results at $\theta = 0$, by expanding them about $\theta = 0$ and computing the coefficients of the expansion [4, 5]. The $\theta$ dependence is particularly interesting in the large-$N$ limit where the issue may also be addressed by other approaches, such as AdS/CFT correspondence applied to nonsupersymmetric and nonconformal theories, see e.g. Ref. [6].

We introduce a scaling energy density

$$f(\theta) = \frac{\Delta F(\theta)}{\sigma^2},$$

where $\Delta F(\theta) \equiv F(\theta) - F(0)$ and $\sigma$ is the string tension at $\theta = 0$. By expanding $f(\theta)$ around $\theta = 0$, one can study its $\theta$ dependence in the region of small $\theta$ values. The function $f(\theta)$ is conveniently parametrized as

$$f(\theta) = \frac{1}{2} C \theta^2 s(\theta),$$

where $C$ is the ratio $\chi/\sigma^2$ and $\chi$ is the topological susceptibility at $\theta = 0$,

$$\chi = \int d^4x \langle q(x)q(0) \rangle = \frac{\langle Q^2 \rangle}{V}$$

where $Q = \int d^4x q(x)$. $s(\theta)$ is a dimensionless function of $\theta$ such that $s(0) = 1$.

The function $s(\theta)$ can be expanded around $\theta = 0$ as

$$s(\theta) = 1 + b_2 \theta^2 + b_4 \theta^4 + \cdots$$

The coefficients of the expansion of $f(\theta)$ are related to the zero-momentum $n$-point connected correlation functions of the topological charge density, and therefore to the moments of the probability distribution $P(Q)$ of the topological charge $Q$. If $s(\theta) = 1$, and therefore $b_{2n} = 0$, the corresponding distribution $P(Q)$ is Gaussian, i.e.

$$P(Q) = \frac{1}{\sqrt{2\pi \langle Q^2 \rangle}} \exp \left( -\frac{Q^2}{2\langle Q^2 \rangle} \right).$$

Therefore the coefficients $b_{2n}$ of the expansion of $s(\theta)$ parametrize the deviations from a simple Gaussian behavior. For example, he first non–trivial correction is given by

$$b_2 = -\frac{\chi_4}{12\chi},$$

$$\chi_4 = \frac{1}{V} \left[ \langle Q^4 \rangle_{\theta=0} - 3 \left( \langle Q^2 \rangle_{\theta=0} \right)^2 \right].$$

It has been recently shown [7] (see also [8]) that correlation functions involving multiple zero-momentum insertions of the topological charge density can be defined in a nonambiguous, regularization-independent way, and therefore the expansion coefficients $b_{2n}$ are well defined renormalization-group invariant quantities.
2. Behavior in the large-$N$ limit

Witten argued [9] that in the large-$N$ limit $F(\theta)$ is a multibranched function of the type

$$F(\theta) = N^2 \min_k H \left( \frac{\theta + 2\pi k}{N} \right)$$

(2.1)

which is periodic in $\theta$, but not smooth since at some value of $\theta$ there is a jump between two different branches. This issue was also discussed in Ref. [10]. More recently, the conjecture was refined [11] leading to a rather simple expression for $\Delta F(\theta)$ in the large-$N$ limit, that is

$$\Delta F(\theta) = A \min_k (\theta + 2\pi k)^2 + O(1/N).$$

(2.2)

In particular, for sufficiently small values of $\theta$, i.e. $|\theta| < \pi$,

$$\Delta F(\theta) = A \theta^2 + O(1/N).$$

(2.3)

Thus possible $O(\theta^4)$ terms are expected to be depressed by powers of $1/N$. This conjecture has been supported using arguments based on duality between large-$N$ gauge theories and string theory [11]. It has also been discussed in a field-theoretical framework in Ref. [12].

The large-$N$ behavior of the coefficients $b_{2n}$ of the expansion of $f(\theta)$ around $\theta = 0$ can be inferred by using general large-$N$ scaling arguments applied to the Lagrangian (1.1). They indicate the ratio $\bar{\theta} \equiv \theta/N$ as the relevant quantity in the large-$N$ limit of the ground-state energy, and more generally of the spectrum of the theory. Then we expect

$$f(\theta) = N^2 \bar{f}(\bar{\theta} \equiv \theta/N),$$

$$\bar{f}(\bar{\theta}) = \frac{1}{2} C_\infty \bar{\theta}^2 (1 + \bar{b}_2 \bar{\theta}^2 + \bar{b}_4 \bar{\theta}^4 + \cdots),$$

(2.5)

where $C_\infty$ is the large-$N$ limit of the ratio $C = \chi/\sigma^2$. Comparing with Eq. (1.4), one derives

$$C = C_\infty + c_2/N^2 + \ldots, \quad b_{2i} = \bar{b}_{2i}/N^{2i} + \ldots,$$

(2.6)

We recall that a nonzero value of $C_\infty$ is essential to provide an explanation to the $U(1)_A$ problem in the 't Hooft large-$N$ limit, and can be related to the $\eta'$ mass [2, 3] through the relation

$$\chi_\infty = \frac{f^2 m_{\eta'}^2}{4 N_f} + O(1/N).$$

(2.7)

The quantity $b_2$ also lends itself to a physical interpretation, being related to the $\eta' - \eta'$ elastic scattering amplitude [3].
3. Results for the first few terms of the expansion around \( \theta = 0 \) of the ground-state energy

The \( \theta \) dependence of SU(\( N \)) gauge theories has been investigated by Monte Carlo simulations of their Wilson lattice formulation. The lattice action corresponding to the Lagrangian (1.1) cannot be directly simulated for \( \theta \neq 0 \), by virtue of the complex nature of the \( \theta \) term. On the other hand, the coefficients \( b_{2n} \) in the expansion of the ground-state energy \( F(\theta) \) around \( \theta = 0 \) can be accessed by determining the moments of the topological charge distribution at \( \theta = 0 \). They are dimensionless renormalization-group invariant quantities, which should approach a constant in the continuum limit, with \( O(a^2) \) scaling corrections (\( a \) is the lattice spacing).

Computing quantities related to topology using lattice simulation techniques is not a simple task. In the case \( N = 3 \) several methods have been employed to determine the topological susceptibility, see e.g. Refs. [13]-[35], [4], [36]-[38]. Cooling, geometrical, heating techniques have been used to address the problems caused by power–divergent additive contributions and multiplicative renormalizations in definitions of the topological susceptibility based on discretized versions of the topological charge density operator \( q(x) \). These methods have their drawbacks, since their systematic errors are not under robust theoretical control.

A substantial progress has been achieved after the introduction of the Neuberger overlap formulation [39, 40] of fermions, which represented a breakthrough for the lattice formulation of QCD. Overlap lattice fermions satisfy the Ginsparg-Wilson relation [11] and therefore preserve an exact chiral symmetry [12]. As a by product, the index of the overlap Dirac operator [43] provides a well–defined estimator for the topological charge [11, 14, 8, 7], which can also be used in pure gauge theories. This method circumvents completely the problem of renormalization arising in bosonic approaches, even though at a much higher computational cost. Using these methods, the topological susceptibility of the pure SU(3) gauge theory has been investigated in Refs. [13]-[53], finally obtaining the accurate estimate [53] \( \chi r_0^4 = 0.059(3) \) (\( r_0 \) is the length scale defined in [54]). This value corresponds to \( C = \chi/\sigma^2 = 0.029(2) \) (using [53] \( \sigma^{1/2}r_0 = 1.193(10) \)).

It is important to note that the results obtained by the (less computer-power demanding) bosonic methods are substantially consistent, see e.g. Refs. [27, 32, 43, 4, 38], showing their effectiveness although they are supported by a weaker theoretical ground. For example, we mention the results: [27] \( C = 0.027(4) \), obtained using the heating method, [4] \( C = 0.0282(12) \), obtained using cooling, and the more recent result [38] \( C = 0.0259(11) \).

For larger values of \( N \), results have been obtained only by the cooling method so far [33, 1, 33], up to \( N = 8 \). They fit well the expected large-\( N \) behavior: \( C = C_\infty + c_2/N^2 \), providing an estimate of \( C_\infty \), and therefore of the topological susceptibility in the large-\( N \) limit: \( C_\infty = 0.0200(43) \) [33], \( C_\infty = 0.0221(14) \) [4], \( C_\infty = 0.0248(18) \)
(the latter was obtained using $N \leq 8$ and keeping $a$ fixed). These results are in substantial agreement with the large-$N$ relation (2.7). We stress that the good agreement for $N = 3$ of the cooling method with the more rigorous overlap result make us quite confident on the reliability of results for higher values of $N$, since there are no arguments to suggest that this agreement could be spoiled with increasing $N$ (actually there are reasons in favor of improved agreement [48, 56]). An independent determination of $C_{\infty}$ using other methods would be welcome.

Higher moments of the topological charge distribution provide estimates of the coefficients $b_{2n}$ of the expansion of the scaling energy density $f(\theta)$, cf. Eqs. (1.4) and (1.6). In particular $b_2$ can be estimated using formulae (1.8, 1.9). There are a number of results at $N = 3$, obtained by different approaches: Ref. [4] used the cooling method, Ref. [57] used the heating technique to estimate additive and multiplicative renormalizations in zero-momentum correlations of lattice discretizations of $q(x)$, and finally Ref. [58] used the most rigorous and CPU intensive overlap method. The results reported in Table 1 are in good agreement, suggesting that the systematic errors of the various methods are sufficiently small. We mention that the fourth moment of the topological charge distribution has been numerically investigated also in Ref. [38], without arriving at any definite conclusion.

The results of Table 1 provide robust evidence that $b_2$ is nonzero, and therefore that there are deviations from a Gaussian distribution of the topological charge. However, $b_2$ turns out to be quite small, indeed $|b_2| \ll 1$. Thus deviations from a simple Gaussian behavior are already small at $N = 3$.

<table>
<thead>
<tr>
<th>$N$</th>
<th>Ref. method</th>
<th>$b_2$</th>
</tr>
</thead>
<tbody>
<tr>
<td>3</td>
<td>cooling</td>
<td>$-0.023(7)$</td>
</tr>
<tr>
<td></td>
<td>heating</td>
<td>$-0.024(6)$</td>
</tr>
<tr>
<td></td>
<td>overlap</td>
<td>$-0.025(9)$</td>
</tr>
<tr>
<td>4</td>
<td>cooling</td>
<td>$-0.013(7)$</td>
</tr>
<tr>
<td>6</td>
<td>cooling</td>
<td>$-0.01(2)$</td>
</tr>
</tbody>
</table>

Table 1: Results for the coefficient $b_2$ of the expansion (1.6)

There are also estimates for larger values of $N$, see Table 1, but only using the cooling method. Again, given the agreement found at $N = 3$, higher $N$ results should be sufficiently reliable. They appear to decrease consistently with the expectation from the large-$N$ scaling arguments, i.e. $b_2 \approx \bar{b}_2/N^2$ with $\bar{b}_2 \approx -0.2$.

We also mention that the analytical properties at $\theta = 0$ have been recently discussed and numerically checked in Ref. [37].

1An apparently contradictory result has been reported in Refs. [59, 51, 53] for the expected large-volume probability distribution $P(Q)$, i.e. $P(Q) = (2\pi\langle Q^2 \rangle)^{-1/2}e^{-Q^2/2\langle Q^2 \rangle} \left[1 + O(1/V)\right]$. A purely gaussian behaviour would imply an exact quadratic form for $f(\theta)$, and in particular a vanishing $b_2$, thereby contradicting the assumption of a generic expansion of $f(\theta)$.
Overall, these results support the scenario obtained by general large-$N$ scaling arguments, which indicate $\tilde{\theta} \equiv \theta/N$ as the relevant Lagrangian parameter in the large-$N$ expansion. They also show that $N = 3$ is already in the regime of the large-$N$ behavior. For $N \geq 3$ the simple Gaussian form

$$F(\theta) \approx \frac{1}{2} \chi \theta^2$$

provides a good approximation of the dependence on $\theta$ for a relatively large range of values of $\theta$ around $\theta = 0$.

### 4. $\theta$ dependence at finite temperature

Another interesting issue concerns the behavior of topological properties at finite temperature, and in particular their change at the finite-temperature deconfining transition, which is first order for $N \geq 3$, see e.g. Ref. [61] and references therein. This issue has been investigated in a number of numerical works, see e.g. Refs. [21, 27, 30, 60, 62, 64], using different methods. They show that the topological properties, and in particular the topological susceptibility $\chi$, vary very little up to $T \lesssim T_c$. They change across the transition, where $\chi$ shows a significant decrease. Then, at high temperature $T \gg T_c$, where the instanton calculus is reliable, a rather different scenario emerges [63].

Concerning the large-$N$ behavior (investigated by performing simulations at various values of $N \geq 3$ [60, 64]), the results indicate that $\chi$ has a nonvanishing large-$N$ limit for $T < T_c$, as at $T = 0$, and that the topological properties, and therefore $F(\theta)$, remain substantially unchanged in the low-temperature phase, up to $T_c$. On the other hand, above the deconfinement phase transition, for $T > T_c$, $\chi$ shows a large suppression, hinting at a vanishing large-$N$ limit for $T > T_c$. These results support the hypothesis put forward in Ref. [64]: At large $N$ the topological properties in the high-temperature phase, for $T > T_c$, are essentially determined by instantons that are exponentially suppressed, i.e. behave as $e^{-N}$, and therefore the topological susceptibility gets rapidly suppressed in the large-$N$ limit.

### 5. $\theta$ dependence of the spectrum

Another interesting issue concerns the $\theta$ dependence of the spectrum of the theory. The analysis of the $\theta$ dependence of the glueball spectrum using AdS/CFT suggests that the only effect of the $\theta$ term in the leading large-$N$ limit on the lowest spin-zero glueball state is that this state becomes a mixed state of $0^{++}$ and $0^{--}$ glueballs, as a consequence of the fact that the $\theta$ term breaks parity, but its mass does not change [63].
Ref. [5] presented an exploratory numerical study of the \( \theta \) dependence in the spectrum of SU(\( N \)) gauge theories. Again numerical simulations of the Wilson lattice formulation were employed to investigate the \( \theta \) dependence of the string tension \( \sigma(\theta) \) and the lowest glueball mass \( M(\theta) \). Around \( \theta = 0 \) one can write

\[
\begin{align*}
\sigma(\theta) &= \sigma \left( 1 + s_2 \theta^2 + \ldots \right), \\
M(\theta) &= M \left( 1 + g_2 \theta^2 + \ldots \right)
\end{align*}
\]

where \( \sigma \) and \( M \) are respectively the string tension and the \( 0^{++} \) glueball mass at \( \theta = 0 \). Then the coefficients of these expansions can be computed from appropriate correlators at \( \theta = 0 \). In particular, \( s_2 \) can be determined [5] from the large-\( t \) behavior of connected correlation functions of two Polyakov lines at distance \( t \) and the square topological charge, such as

\[
\langle A_P(t) Q^2 \rangle_{\theta=0} - \langle A_P(t) \rangle_{\theta=0} \langle Q^2 \rangle_{\theta=0}
\]

where

\[
A_P(t) = \sum_{x_1,x_2} \text{Tr} \, P^\dagger(0;0) \, \text{Tr} \, P(x_1,x_2;t),
\]

\( P(x_1,x_2;t) \) is the Polyakov line along the \( x_3 \) direction of size \( L \), and \( Q \) is the topological charge. Analogously, the \( O(\theta^2) \) term of the glueball mass can be obtained from appropriate connected correlation functions of plaquette operators and \( Q^2 \). The \( O(\theta^2) \) coefficients \( s_2 \) and \( g_2 \) are dimensionless scaling quantities, which should approach a constant in the continuum limit, with \( O(a^2) \) scaling corrections.

Ref. [5] obtained the first estimates of \( s_2 \) and \( g_2 \) using the cooling method to determine the topological charge, and for \( N = 3, 4, 6 \) to also check their large-\( N \) behavior. The \( O(\theta^2) \) terms in the expansion around \( \theta = 0 \) of the spectrum of SU(\( N \)) gauge theories are small for all \( N \geq 3 \), especially when dimensionless ratios are considered, such as \( M/\sqrt{\sigma} \) and, for \( N > 3 \), the ratios of independent \( k \) strings. For example we mention the estimates \( s_2 = -0.08(1) \) and \( g_2 = -0.06(2) \) for \( N = 3 \). One may also consider the \( \theta \) dependence of the scaling ratio

\[
\frac{M(\theta)}{\sqrt{\sigma}(\theta)} = \frac{M}{\sqrt{\sigma}} \left( 1 + c_2 \theta^2 + \ldots \right),
\]

where \( c_2 = g_2 - s_2/2 \), thus \( c_2 = -0.02(2) \) for \( N = 3 \). Moreover, the \( O(\theta^2) \) corrections appear to decrease with increasing \( N \), and the coefficients do not show evidence of convergence to a nonzero value. This is suggestive of a scenario in which the \( \theta \) dependence of the spectrum disappears in the large-\( N \) limit, at least for sufficiently small values of \( \theta \) around \( \theta = 0 \). In the case of the spectrum, the general large-\( N \) scaling arguments of Sec. 2, which indicate \( \bar{\theta} \equiv \theta/N \) as the relevant Lagrangian parameter in the large-\( N \) limit, imply that \( O(\theta^2) \) coefficients should decrease as
The results of Ref. [5] appear substantially consistent: In the case of the string tension they suggest $s_2 \approx -0.9/N^2$.

Of course, further investigation is required to put this scenario on a firmer ground, using for example other definitions of topological charge.

6. The case of the two-dimensional CP$^{N-1}$ model

Issues concerning the $\theta$ dependence can also be discussed in two-dimensional CP$^{N-1}$ models [66, 67].

$$\mathcal{L} = \frac{N}{2g} D_\mu \bar{z} D_\mu z$$

(6.1)

where $z$ is a $N$-component complex scalar field subject to the constraint $\bar{z}z = 1$, $A_\mu = i\bar{z}\partial_\mu z$ is a composite gauge field, and $D_\mu = \partial_\mu + iA_\mu$ is a covariant derivative. They provide an interesting theoretical laboratory. Indeed they present several features that hold in QCD: Asymptotic freedom, gauge invariance, existence of a confining potential between non gauge invariant states (that is eventually screened by the dynamical constituents), and non-trivial topological structure (instantons, $\theta$ vacua). Moreover, unlike four-dimensional SU($N$) gauge theories, a systematic $1/N$ expansion can be performed around the large-$N$ saddle-point solution [66, 67, 68].

Analogously to four-dimensional SU($N$) gauge theories, one may add a $\theta$ term to the Lagrangian, writing

$$\mathcal{L}_\theta = \frac{N}{2g} D_\mu \bar{z} D_\mu z + i\theta \frac{1}{2\pi} \epsilon_{\mu\nu} \partial_\mu A_\nu,$$

(6.2)

where $q(x) = \frac{1}{2\pi} \epsilon_{\mu\nu} \partial_\mu A_\nu$ is the the topological charge density. Then one may study the $\theta$ dependence of the ground state and other observables. In the following we discuss this issue within the $1/N$ expansion, performed keeping $g$ fixed. Simple large-$N$ scaling arguments applied to the Lagrangian (6.1) indicate that the relevant $\theta$ parameter in the large-$N$ limit should be $\bar{\theta} \equiv \theta/N$.

Analogously to SU($N$) gauge theories, the ground state energy $F(\theta)$ depends on $\theta$. One may define a scaling ground state energy $f(\theta)$ and expand it around $\theta = 0$,

$$f(\theta) \equiv M^{-2}[F(\theta) - F(0)] = \frac{1}{2} C \bar{\theta}^2 \left(1 + \sum_{n=1} b_{2n} \bar{\theta}^{2n}\right)$$

(6.3)

where $F(\theta)$ is defined as in Eq. (1.2), $M$ is the mass scale at $\theta = 0$ defined from the second moment of the two-point function of the operator $P_{ij}(x) \equiv \bar{z}_i(x)z_j(x)$, $C$ is the scaling ratio $\chi/M^2$ at $\theta = 0$, where $\chi$ is the topological susceptibility. The correlation function of the topological charge density, and in particular the topological susceptibility, has been computed within the $1/N$ expansion [69, 70, 71].

We have

$$C = \chi/M^2 = \frac{1}{2\pi N} + O(1/N^2)$$

(6.4)
The coefficients $b_{2n}$ are obtained from appropriate $2n$-point correlation functions of the topological charge density operators at $\theta = 0$. The analysis of the $1/N$-expansion Feynman diagrams [68] of the connected correlations necessary to compute $b_{2n}$ shows that they are suppressed in the large-$N$ limit, as [3]

$$b_{2n} = O(1/N^{2n}).$$

This implies that the ground-state energy can be rewritten as

$$f(\theta) = N \bar{f}(\bar{\theta} \equiv \theta/N),$$

$$\bar{f}(\bar{\theta}) = \frac{1}{2} \bar{C} \bar{\theta}^2 (1 + \sum_{n=1} b_{2n} \bar{\theta}^{2n}),$$

where $\bar{C} \equiv NC$ and $\bar{b}_{2n} = N^{2n}b_{2n}$ are $O(N^0)$. Note the analogy with the expected $\theta$ dependence of the ground-state energy in SU($N$) gauge theories, cf. Eq. (2.4). Rather cumbersome calculations lead to the results [5] $\bar{b}_2 = -\frac{27}{5}$, and $\bar{b}_4 = -\frac{1830}{7}$.

Within the $1/N$ expansion one may also study the dependence of the mass $M$ on the parameter $\theta$. We write

$$M(\theta) = M \left(1 + m_2 \theta^2 + \ldots\right)$$

The analysis of its diagrams in the corresponding $1/N$ expansion indicates that $m_2$ is suppressed as

$$m_2 = O(1/N^2)$$

Once again, the relevant parameter is seen to be $\bar{\theta} \equiv \theta/N$.

7. Critical slowing down of topological modes

Monte Carlo simulations of critical phenomena in statistical mechanics and of quantum field theories, such as QCD, in the continuum limit are hampered by the problem of critical slowing down (CSD) [72]. The autocorrelation time $\tau$, which is related to the number of iterations needed to generate a new independent configuration, grows with increasing length scale $\xi$. In simulations of lattice QCD where the upgrading methods are essentially local, it has been observed, see e.g. Refs. [73, 74, 75, 4, 76] that the topological modes show autocorrelation times that are typically much larger than those of other observables not related to topology, such as Wilson loops and their correlators. Actually, the heating method [24], used to estimate the topological susceptibility, essentially relies on this phenomenon.

Recent Monte Carlo simulations [1, 73] of the four-dimensional SU($N$) lattice gauge theories (for $N = 3, 4, 6$) provided evidence of a severe CSD for the topological modes, using a rather standard local overrelaxed upgrading algorithm. Indeed, the autocorrelation time $\tau_{\text{top}}$ of the topological charge grows very rapidly with the
length scale $\xi \equiv \sigma^{-1/2}$, where $\sigma$ is the string tension, showing an apparent exponential behavior $\tau_{\text{top}} \sim \exp(c\xi)$ in the range of values of $\xi$ where data are available. Such a phenomenon worsens with increasing $N$, indeed the constant $c$ appears to increase as $c \propto N$. Of course, this behaviour does not depend on the particular estimator of the topological charge. This peculiar effect has not been observed in plaquette-plaquette or Polyakov line correlations, suggesting an approximate decoupling between topological modes and nontopological ones, such as those determining the confining properties.

These results suggest that the dynamics of the topological modes in Monte Carlo simulations is rather different from that of quasi-Gaussian modes. CSD of quasi-Gaussian modes for traditional local algorithms, such as standard Metropolis or heat bath, is related to an approximate random-walk spread of information around the lattice. Thus, the corresponding autocorrelation time $\tau$ is expected to behave as $\tau \sim \xi^2$ (an independent configuration is obtained when the information travels a distance of the order of the correlation length $\xi$, and the information is transmitted from a given site/link to the nearest neighbors). This guess is correct for Gaussian (free field) models; in general one expects that $\tau \sim \xi^z$ where $z$ is a dynamical critical exponent, and $z \approx 2$ for quasi-Gaussian modes. On the other hand, in the presence of relevant topological modes, the random-walk picture may fail, and therefore we may have qualitatively different types of CSD. These modes may give rise to sizeable free-energy barriers separating different regions of the configuration space. The evolution in the configuration space may then present a long-time relaxation due to transitions between different topological charge sectors, and the corresponding autocorrelation time should behave as $\tau_{\text{top}} \sim \exp F_b$ where $F_b$ is the typical free-energy barrier among different topological sectors. However, this picture remains rather qualitative, because it does not tell us how the typical free-energy barriers scale with the correlation length. For example, we may still have a power-law behavior if $F_b \sim \ln \xi$, or an exponential behavior if $F_b \sim \xi^\theta$. It is worth mentioning that in physical systems, such as random-field Ising systems [77] and glass models [78], the presence of significant free-energy barriers in the configuration space causes a very slow dynamics, and an effective separation of short-time relaxation within the free-energy basins from long-time relaxation related to the transitions between basins. In the case of random-field Ising systems the free-energy barrier picture supplemented with scaling arguments leads to the prediction that $\tau \sim \exp(c\xi^\theta)$ where $\theta$ is a universal critical exponent [77].

The severe CSD experienced by the topological modes under local updating algorithms should be a general feature of Monte Carlo simulations of lattice models with nontrivial topological properties, since the mechanism behind this phenomenon should be similar. This has been also observed in two-dimensional CP$^{N-1}$ models [74, 80]. The numerical study of Ref. [73] for various values of $N$ show that an exponential Ansatz, i.e. $\tau_{\text{top}} \sim \exp(c\xi^\theta)$ with $\theta \approx 1/2$, and $c \propto N$, provides a
good effective description in the range of the correlation length $\xi$ where data are available (however, the statistical analysis of the data did not allow one to exclude an asymptotic power-law behavior $\tau \sim \xi^z$ with $z \gtrsim N/2$ setting in at relatively large $\xi$).

The issue of CSD of topological modes is particularly important for lattice QCD, because it may pose a serious limitation for numerical studies of physical issues related to topological properties, such as the mass and the matrix elements of the $\eta'$ meson, and in general the physics related to the broken $U(1)_A$ symmetry. Indeed, it may substantially worsen the cost estimates of the dynamical fermion simulations for lattice QCD, see, e.g., Ref. [81].

Finally, we note that although the effects of the topological CSD have not been directly observed in plaquette-plaquette or Polyakov line correlations, such a CSD will eventually affect them. The point is that the results of Ref. [5], summarized in Sec. 5, show that the correlators of plaquette operators and topological charge do not vanish at finite $N$, although they are quite small, and therefore there is not a complete decoupling between topological and nontopological modes. Therefore the strong critical slowing down that is clearly observed in the topological sector will eventually affect also the measurements of nontopological quantities, such as those related to the string and glueball spectrum.
References


