Theta dependence of the vacuum energy in the SU(3) gauge theory from the lattice

Leonardo Giusti\textsuperscript{a,}\textsuperscript{*}, Silvano Petrarca\textsuperscript{b,}\textsuperscript{c}, Bruno Taglienti\textsuperscript{c}

\textsuperscript{a} CERN, Department of Physics, TH Division, CH-1211 Geneva 23, Switzerland.
\textsuperscript{b} Dipartimento di Fisica, Università di Roma “La Sapienza”, P.le A. Moro 2, I-00185 Rome, Italy.
\textsuperscript{c} INFN, Sezione di Roma, P.le A. Moro 2, I-00185 Rome, Italy.

We report on a precise computation of the topological charge distribution in the SU(3) Yang–Mills theory. It is carried out on the lattice with high statistics Monte Carlo simulations employing the definition of the topological charge suggested by Neuberger’s fermions. We observe significant deviations from a Gaussian distribution. Our results disfavor the \( \theta \) behaviour of the vacuum energy predicted by instanton models, while they are compatible with the expectation from the large \( N_c \) expansion.

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Introduction. — The \( \theta \) dependence of the vacuum energy \([1, 2, 3, 4]\), or equivalently the functional form of the topological charge distribution, is a distinctive feature of the ensemble of gauge configurations that dominate the path integral of a Yang–Mills theory. In the Euclidean space-time the ground-state energy \( F(\theta) \) is defined as

\[
e^{-F(\theta)} = \langle e^{i\theta Q} \rangle, \tag{1}\]

where, as usual, \( \langle \ldots \rangle \) indicates the path-integral average (our normalization is \( F(0) = 0 \)). In the large volume regime \( F(\theta) \) is proportional to the size \( V \) of the system, a direct consequence of the fact that the topological charge operator \( Q \) is the four-dimensional integral of a local density. The function \( F(\theta) \) is related to the probability of finding a gauge field configuration with topological charge \( Q = \nu \) by the Fourier transform

\[
P_\nu = \int_{-\pi}^{\pi} \frac{d\theta}{2\pi} e^{-i\nu \theta} e^{-F(\theta)} . \tag{2}\]

Large \( N_c \) arguments \([3]\), with \( N_c \) being the number of colors, suggest that the fluctuations of the topological charge are of quantum non-perturbative nature \([3, 4]\). The \( \theta \) dependence of the vacuum energy is expected at leading order in \( 1/N_c \), and the normalized cumulants

\[
C_n = (-1)^{n+1} \frac{1}{V} \left[ \frac{d^n}{d\theta^n} F(\theta) \right] \bigg|_{\theta=0} n = 1, 2, \ldots, \tag{3}\]

which should scale asymptotically as \( N_c^{3-2n} \) \([3, 4]\), have to be determined with a non-perturbative computation. On the other hand several models, such as the dilute gas or liquid of instantons, assume that the path integral is dominated by semiclassical configurations \([8, 9, 10, 11]\). They predict a \( \theta \) behaviour of the form

\[
F^{\text{inst}}(\theta) = -VA\{\cos(\theta) - 1\} , \tag{4}\]

with \( A \) being exponentially suppressed at large \( N_c \).

The \( \theta \) dependence of the vacuum energy plays a crucial rôle also in the solution of the so-called \( U(1)_A \) problem in QCD. The Witten–Veneziano mechanism relates the cumulants of the topological charge distribution in the Yang–Mills theory with the leading anomalous contribution to the mass and scattering amplitudes of the \( \eta' \) meson in QCD \([12, 13, 14, 15, 16]\). The known value of \( C_1 \) in the SU(3) theory supports indeed the fact that the bulk of the \( \eta' \) mass is due to the anomaly \([17]\).

Recent theoretical developments in lattice gauge theory made it possible to find an unambiguous definition of the topological charge distribution with a finite and universal continuum limit \([15, 18, 19, 20, 21, 22]\). The aim of this work is a precise computation of the distribution of the topological charge in the SU(3) Yang–Mills theory. We observe significant deviations from a Gaussian behaviour: they disfavor the \( \theta \) dependence given in Eq. \((3)\), while they are compatible with expectations from the large \( N_c \) expansion.

In the past the distribution of the topological charge was already studied (see Ref. \([17]\) and references therein). These computations, however, were not precise enough to observe deviations from the leading Gaussian behaviour. In this respect we have exploited the efficiency of the algorithm for the determination of the charge developed in Ref. \([23]\). Properties of the charge distribution have been investigated also with fermionic and bosonic methods (see Refs. \([24, 25]\) and references therein). These results, however, are affected by model-dependent systematic errors that are not quantifiable, and their interpretation rests on a weak theoretical ground.

Topological charge definition. — The Neuberger–Dirac operator \( D \) is defined as

\[
D = \frac{1}{a} \left[ 1 + \gamma_5 \text{sign}(H) \right] , \tag{5}\]

\[
H = \gamma_5 (aD_w - 1 - s) , \quad \bar{a} = \frac{a}{1 + s} , \tag{6}\]

where \( D_w \) is the standard Wilson–Dirac operator and \( s \) is an adjustable parameter in the range \( |s| < 1 \) (for notations not explained here see Ref. \([23]\)). It satisfies the

\[\text{Eq. (4)}\] with \( A \) being exponentially suppressed at large \( N_c \).

\[\text{F}(\theta) = \langle e^{i\theta Q} \rangle, \tag{1}\]
functions of are thus defined as the integrated connected correlation small corrections proportional to inserting Eq. (9) in Eq. (2), and neglecting exponentially ligible as soon as lightest glueball mass [28], and they become rapidly neg-

The parameters are \( \sigma^2 = V C_1 \) and \( \tau = C_2/C_1 \), and the Hermite polynomial \( \text{He}_4 \) can be found in Ref. [31]. The semiclassical models provide a sharp prediction of the topological charge distribution. By inserting Eq. (4) in Eq. (2), and taking into account that \( \nu \) is an integer, we obtain

\[
P_{\nu}^{\text{Inst}} = e^{-VAI_{\nu}(VA)},
\]

where \( J_{\nu} \) are the modified Bessel functions of the first kind [31]. By construction all normalized cumulants are equal to \( A \).

**Lattice computation.**— The numerical computation is performed by standard Monte Carlo techniques. The ensembles of gauge configurations are generated with the Wilson action and periodic boundary conditions. Each update cycle consists in 1 heat-bath and several over-relaxations of all link variables (more details can be found in Ref. [20]). The charge density is defined as in Eq. (7) with \( s = 0.4 \), and the corresponding topologi-

The large volume limit.— Being \( \nu \) integer-valued, \( F(\theta) \) is a periodic function with period \( 2\pi \). In the interval \( -\pi < \theta < \pi \) it has its absolute minimum at \( \theta = 0 \), and it may then be expanded as

\[
F(\theta) = V \sum_{n=1}^{\infty} (-1)^{n+1} \frac{2n}{(2n)!} C_n.
\]

Leading finite-size effects in the \( C_n \) are exponentially suppressed at asymptotically large volumes. They are proportional to \( e^{-M_n L} \), with \( M_n \sim 1.6 \text{ GeV} \) being the lightest glueball mass [23], and they become rapidly neg-

\[
a^4 q(x) = -\frac{a}{2} \text{Tr} \left[ \gamma_5 D(x, x) \right],
\]

where the trace runs over spin and color indices. With this definition the topological charge in a given back-

\[
C_n = \frac{a^4}{V} \sum_{x_1, \ldots, x_{2n}} (q(x_1) \cdots q(x_{2n}))^{\text{con}}.
\]

They have an unambiguous finite continuum limit which is independent of the details of the regularization [15] [21] [22]. At finite lattice spacing they are affected by discretization errors which start at \( O(a^2) \).

1 Correlation functions of an odd number of topological charges vanish thanks to the invariance of the theory under parity.

2 The Edgeworth expansion is usually adopted in the context of the central limit theorem [33]. In our case the volume \( V \), or \( (N_s^2 V) \) at large \( N_c \), plays the rôle of the number of independent degrees of freedom.
of the first two cumulants

\begin{equation}
\overline{Q^2} = \frac{1}{N} \sum_{i=1}^{N} \nu_i^2 ,
\end{equation}

\begin{equation}
\overline{Q^4,\text{con}} = \frac{1}{N} \sum_{i=1}^{N} \nu_i^2 - 3 \left( \frac{1}{N} \sum_{i=1}^{N} \nu_i^2 \right)^2 ,
\end{equation}

with \( \nu_i \) being the value of the topological charge for a given gauge configuration and \( N \) the total number of configurations, have variances which, up to sub-leading corrections, are \((2\sigma^4 + \sigma^2 \tau)/N\) and \((24\sigma^8 + 72\sigma^6 \tau)/N\) respectively. The number of configurations on our main set of lattices, the A series, has been fixed to have a precision of 15 – 20% on the second cumulant \( C_2 \). For the lattice \( B_1 \) the number of configurations is chosen so to have a signal for \( \langle Q^4 \rangle_{\text{con}} \) and therefore a rough estimate of finite-size effects\(^3\). Lattice \( C_1 \) has been simulated to quantify finite-size effects in \( \langle Q^2 \rangle \) with confidence.

For each lattice we have compared the histogram of the topological charge distribution with three functional forms: a simple Gaussian centered at the origin, the Edgeworth expansion in Eq. (10) (Edge), and the prediction from instanton models in Eq. (11) (Inst). The free parameter(s) of each function has(ve) been fixed by maximizing the likelihood. For the symmetrized histograms the values of \( \chi^2 \) per degree of freedom at the minimum are reported in Table 11 and for the lattice \( A_2 \) the data points and the three curves are shown in Fig. 1. The Edgeworth expansion reproduces well the behaviour of the numerical data at these volumes and lattice spacings within our statistical errors\(^4\). On the A lattices the Gaussian distribution is incompatible with the data, while at the two larger volumes the \( \chi^2_{\text{dof}} \) is still rather good. The functional form suggested by instanton models is excluded on the lattices \( A_1–A_3 \) and \( B_1 \), and is off by more than two sigmas on the lattice \( C_1 \). On the A lattices a fit limited to \( |\nu| \leq 1 \) leads to the same conclusions. This is one of the main results of this paper.

To quantify the magnitude of discretization and finite-size effects we have computed the first two cumulants of the topological charge distribution with the estimators given in Eqs. (12) and (13). The numerical results are reported in Table 11. The contributions from the poorly sampled tail of the distributions, i.e. bins of the symmetrized histogram populated by less than 10 events, have been estimated from the large volume expression in Eq. (10) as suggested in Ref. 29. Within our statistical errors we do not observe a signal for the higher cumulants, and correlation functions of an odd number of topological charges are always compatible with zero.

For the data samples that can be directly compared, the values of \( \langle Q^2 \rangle \) are in very good agreement with the results in Ref. 17. We confirm that discretization effects on \( r_0^4 C_1 \), where \( r_0 \) is a low-energy reference scale well measured in the pure gauge theory \( 32 \), are moderate (of the order of 10% at our coarser lattice spacing), and finite size effects are below 5% at our smaller volume. Even though our errors for \( \langle Q^2 \rangle \) are much smaller with respect to those in Ref. 17, a significative improvement of the determination of \( C_1 \) in the continuum limit requires further simulations and is left to a future publication.

The second cumulant is best expressed by the adimensional ratio \( \langle Q^4 \rangle_{\text{con}}/\langle Q^2 \rangle \) which has a well defined continuum and infinite-volume limit. The numerical results for the lattices \( A_1–A_3 \) and \( B_1 \) are reported in Table 11 and they are plotted in Fig. 2 as a function of \((a/r_0)^2\). All values are incompatible with 1, the predicted value from Eq. (4). The results from \( A_1, A_2 \) and \( A_3 \) agree within

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\(^3\) Given the scaling of the statistical error with \( V \) and \( n \), it is very inefficient to compute higher cumulants at large volumes with the standard sampling procedure. Once \( \sigma^2 \) is known, however, one could devise an adaptive importance sampling algorithm which integrates this information so to have a reduced \( \sigma^2_{\text{eff}} \).

\(^4\) We also fitted the data with the functional form in Eq. (2) and two non-vanishing cumulants. The conclusions are analogous.
A direct estimate of these effects on the path integral. The large $N_c$ expansion does not provide a sharp prediction for the value of $\langle Q^4 \rangle_{\text{con}} / \langle Q^2 \rangle$. Its small value, however, is compatible with being a quantity suppressed in the large $N_c$ limit. The value of $\langle Q^4 \rangle_{\text{con}}$ is related via the Witten–Veneziano mechanism to the leading anomalous contribution to the $\eta'\to\eta'$ elastic scattering amplitude in QCD.

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### Table II: Results for the first two cumulants and their ratio.

| Lat | $\langle Q^2 \rangle$ | $\langle Q^4 \rangle_{\text{con}}$ | $\langle Q^4 \rangle_{\text{con}} / \langle Q^2 \rangle$ |
|-----|----------------------|----------------------------------|----------------------------------|
| A₁  | 1.637(13)            | 0.60(9)                          | 0.37(6)                          |
| A₂  | 1.566(13)            | 0.47(9)                          | 0.30(6)                          |
| A₃  | 1.432(12)            | 0.43(7)                          | 0.30(5)                          |
| B₁  | 3.09(3)              | 0.8(3)                           | 0.27(10)                         |
| C₁  | 5.44(8)              | -                                | -                                |

### Figures

- **Fig. 2**: Ratio of the first two cumulants vs the lattice spacing.

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