θ dependence of the vacuum energy in SU(3) gauge theory from the latticeLeonardo Giusti,^{1,*} Silvano Petrarca,^{2,3} and Bruno Taglienti³¹*CERN, Department of Physics, TH Division, CH-1211 Geneva 23, Switzerland*²*Dipartimento di Fisica, Università di Roma "La Sapienza", P.le A. Moro 2, I-00185 Rome, Italy*³*INFN, Sezione di Roma, P.le A. Moro 2, I-00185 Rome, Italy*

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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 by employing the definition of the topological charge suggested by Neuberger's fermions. We observe significant deviations from a Gaussian distribution. Our results disfavor the θ behavior of the vacuum energy predicted by dilute instanton models, while they are compatible with the expectation from the large N_c expansion.

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I. INTRODUCTION

The θ dependence of the vacuum energy [1–4], 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

$$e^{-F(\theta)} = \langle e^{i\theta Q} \rangle, \quad (1)$$

where, as usual, $\langle \dots \rangle$ 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

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

Large N_c arguments [5], with N_c being the number of colors, suggest that the fluctuations of the topological charge are of quantum nonperturbative nature [6,7]. The θ dependence of the vacuum energy is expected at leading order in $1/N_c$, and the normalized cumulants

$$C_n = (-1)^{n+1} \frac{1}{V} \frac{d^{2n}}{d\theta^{2n}} F(\theta) \Big|_{\theta=0} \quad n = 1, 2, \dots, \quad (3)$$

which should scale asymptotically as N_c^{2-2n} [6,7], have to be determined with a nonperturbative 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 [8–10]. They predict a θ behavior of the form

$$F^{\text{Inst}}(\theta) = -VA\{\cos(\theta) - 1\}, \quad (4)$$

with A being exponentially suppressed at large N_c .

The θ dependence of the vacuum energy plays a crucial role 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 η' meson in QCD [11–15]. The known value of C_1 in the SU(3) theory supports indeed the fact that the bulk of the η' mass is due to the anomaly [16].

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 [14,17–21]. 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 behavior: they disfavor the θ dependence given in Eq. (4), 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. [16] and references therein). These computations, however, were not precise enough to observe deviations from the leading Gaussian behavior. In this respect we have exploited the efficiency of the algorithm for the determination of the charge developed in Ref. [22]. Properties of the charge distribution, and, in particular, deviations from a Gaussian behavior, have been investigated also with bosonic methods [23,24] (see also Ref. [25]). These results, however, are affected by model-dependent systematic errors that are not quantifiable, and their interpretation rests on a weak theoretical ground.

II. TOPOLOGICAL CHARGE DEFINITION

The Neuberger-Dirac operator D is defined as

$$D = \frac{1}{\bar{a}} [1 + \gamma_5 \text{sign}(H)], \quad (5)$$

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

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. [22]). It satisfies the Ginsparg-Wilson relation [26], and therefore the associated fermion action preserves an exact chiral symmetry at finite lattice spacing [18]. The corresponding Jacobian is nontrivial, and the chiral anomaly is recovered *à la* Fujikawa [18,27] with the topological charge density operator defined as [19]

$$a^4 q(x) = -\frac{\bar{a}}{2} \text{Tr}[\gamma_5 D(x, x)], \quad (7)$$

where the trace runs over spin and color indices. With this definition the topological charge in a given background is given by $Q \equiv \sum_x q(x) = n_+ - n_-$, with n_+ (n_-) being the number of zero modes of D with positive (negative) chirality. The normalized cumulants C_n are thus defined as the integrated connected correlation functions of n charge densities¹

$$C_n = \frac{a^{8n}}{V} \sum_{x_1, \dots, x_{2n}} \langle q(x_1) \dots q(x_{2n}) \rangle^{\text{con}}. \quad (8)$$

They have an unambiguous finite continuum limit which is independent of the details of the regularization [14,20,21]. At finite lattice spacing they are affected by discretization errors which start at $O(a^2)$.

III. THE LARGE VOLUME LIMIT

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

$$F(\theta) = V \sum_{n=1}^{\infty} (-1)^{n+1} \frac{\theta^{2n}}{(2n)!} C_n. \quad (9)$$

Leading finite-size effects in the C_n are exponentially suppressed at asymptotically large volumes. They are proportional to $e^{-M_g L}$, with $M_g \sim 1.6$ GeV being the lightest glueball mass [28], and they become rapidly negligible as soon as L is larger than 1 fm or so [29]. By inserting Eq. (9) in Eq. (2), and neglecting exponentially small corrections proportional to $e^{-2\pi^2 \sigma^2}$, where $\sigma^2 = VC_1$, we can express the topological charge distribution P_ν at large volumes by a saddle point expansion (usually named the Edgeworth expansion in statistics²). This is an asymptotic series in powers of $1/V$ (or $1/(N_c^2 V)$ according to large N_c)

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

²The Edgeworth expansion is usually adopted in the context of the central limit theorem [30,31]. In our case the volume V , or $(N_c^2 V)$ at large N_c , plays the rôle of the number of independent degrees of freedom.

which, up to higher order corrections, reads

$$P_\nu = \frac{e^{-(\nu^2/2\sigma^2)}}{\sqrt{2\pi\sigma^2}} \left[1 + \frac{1}{4!} \frac{\tau}{\sigma^2} \text{He}_4(\nu/\sigma) \right]. \quad (10)$$

The parameters are σ^2 and $\tau = C_2/C_1$, and the Hermite polynomial He_4 can be found in Ref. [32].

The semiclassical models provide a sharp prediction of the topological charge distribution. By inserting Eq. (4) in Eq. (2), and taking into account that ν is an integer, we obtain

$$P_\nu^{\text{Inst}} = e^{-\nu A} I_\nu(VA), \quad (11)$$

where I_ν are the modified Bessel functions of the first kind [32]. By construction all normalized cumulants are equal to A .

IV. 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. [29]). The charge density is defined as in Eq. (7) with $s = 0.4$, and the corresponding topological charge has been computed by counting the number of zero modes of the Neuberger-Dirac operator with the algorithm proposed in Ref. [22].

The list of lattices, the value of the bare coupling constant $\beta = 6/g_0^2$, the linear size L/a in each direction, and the number of independent configurations are reported in Table I. Lattice spacings and volumes have been chosen to have normalized cumulants with small discretization and finite-size errors. To estimate discretization effects we have simulated three lattices, A_1 – A_3 , with the same physical volume but different lattice spacings. Two additional lattices, B_1 and C_1 , have been generated to quantify the magnitude of finite-size effects: they have the same bare coupling of A_1 but larger volumes. The autocorrelation function of the topological charge has been computed at the three values of β by monitoring its value for several thousands of consecutive update cycles of the A lattices.

TABLE I. Simulation parameters, number N of configurations generated, and values of χ_{dof}^2 for the fit of the data to a Gaussian (Norm), to the instanton prediction in Eq. (11) (Inst) and to the Edgeworth expansion in Eq. (10) (Edge).

Lattice	β	L/a	r_0/a	L [fm]	N	$\chi_{\text{dof}}^{2,\text{Norm}}$	$\chi_{\text{dof}}^{2,\text{Inst}}$	$\chi_{\text{dof}}^{2,\text{Edge}}$
A_1	6.0	12	5.368	1.12	34 800	15	27	1.5
A_2	6.0938	14	6.263	1.12	30 000	12	34	1.4
A_3	6.2623	18	8.052	1.12	30 000	13	41	1.1
B_1	6.0	14	5.368	1.30	30 000	1.3	6.7	0.14
C_1	6.0	16	5.368	1.49	10 000	0.67	2.4	0.79

FIG. 1 (color online). Number of configurations vs the topological charge for the lattice A_2 . To guide the eye, lines connect the values of the fitted distributions: the simple Gaussian (Norm), the instanton prediction in Eq. (11) (Inst), and the Edgeworth expansion in Eq. (10) (Edge). The plots on right are a blowup of the top and the bottom of the distribution.

The corresponding autocorrelation time is between 20 and 40 cycles. Since the cost of a Monte Carlo update is negligible with respect to the computation of the index of the Neuberger-Dirac operator, we separated subsequent measurements on all lattices by a number of update cycles between 1 and 2 orders of magnitude larger than the above estimates. Statistical errors are then computed with the jackknife method by considering the measurements as independent. A preliminary analysis of a subset of our results was presented at the conference “Lattice 2006” [33].

The Monte Carlo technique adopted here generates the gauge configurations with a probability density proportional to $e^{-S_{\text{YM}}}$, with S_{YM} being the chosen discretization of the Yang-Mills action. This algorithm performs an importance sampling of the topological charge with the probability distribution given in Eq. (2). A statistical signal for the n th cumulant is then obtained only if the number of configurations is high enough for the sample to be sensitive to terms suppressed as V^{n-1} in the Edgeworth expansion. For instance, the estimators of the first two cumulants

$$\bar{Q}^2 = \frac{1}{N} \sum_{i=1}^N \nu_i^2, \quad (12)$$

$$\bar{Q}^{4,\text{con}} = \frac{1}{N} \sum_{i=1}^N \nu_i^4 - 3 \left(\frac{1}{N} \sum_{i=1}^N \nu_i^2 \right)^2, \quad (13)$$

with ν_i being the value of the topological charge for a given gauge configuration and N the total number of configura-

tions, have variances which, up to subleading 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), and the prediction from instanton models in Eq. (11). The free parameter(s) of each function has(have) been fixed by maximizing the likelihood. For the symmetrized histograms the values of χ^2 per degree of freedom at the minimum are reported in Table I, and for the lattice A_2 the data points and the three curves are shown in Fig. 1. The Edgeworth expansion reproduces well the behavior 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 χ^2_{dof} is

³Given 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 σ^2 is known, however, one could devise an adaptive importance sampling algorithm which integrates this information so to have a reduced σ_{eff}^2 .

⁴We also fitted the data with the functional form in Eq. (2) and two nonvanishing cumulants. The conclusions are analogous.

TABLE II. Results for the first two cumulants and their ratio.

Lattice	$\langle Q^2 \rangle$	$\langle Q^4 \rangle^{\text{con}}$	$\langle Q^4 \rangle^{\text{con}} / \langle Q^2 \rangle$
A_1	1.637(13)	0.60(9)	0.37(6)
A_2	1.566(13)	0.47(9)	0.30(6)
A_3	1.423(12)	0.43(7)	0.30(5)
B_1	3.09(3)	0.8(3)	0.27(10)
C_1	5.44(8)		

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 II. 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. [16]. 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 [34], 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. [16], 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 II, 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 errors. No statistical-significant evidence of discretization effects is thus observed. The theoretical arguments given in the third section suggest small finite-size effects at these volumes. A direct estimate of these effects on $\langle Q^4 \rangle^{\text{con}}$ would require more precise data for the lattice C_1 . The compatibility of the results on lattices A_1 and B_1 , however, is consistent with the theoretical expectations. Our best estimate for the ratio of the first two cumulants is $\langle Q^4 \rangle^{\text{con}} / \langle Q^2 \rangle = 0.30(11)$. The central value is taken from the lattice A_3 , the one with the finer lattice spacing, and the error is the sum in quadrature of the statistical error and of the difference between the central values computed on the lattice A_1 and B_1 .

V. FINAL REMARKS

From the previous analysis we conclude that our results disfavor the θ behavior of the vacuum energy predicted by dilute instanton models. Our best estimate of the ratio $\langle Q^4 \rangle^{\text{con}} / \langle Q^2 \rangle = 0.30(11)$ is incompatible with 1, which is the value predicted from Eq. (4). This suggests that the quantum fluctuations of the topological charge are of quantum nonperturbative nature in the ensemble of gauge configurations that dominate 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 $\eta' - \eta'$ elastic scattering amplitude in QCD.

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FIG. 2 (color online). Ratio of the first two cumulants vs the lattice spacing.

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