Analyticity in θ on the lattice and the large volume limit of the topological susceptibility

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Nonanalyticity of QCD with a θ term at $\theta = 0$ may signal a spontaneous breaking of both parity and time reversal invariance. We address this issue by investigating the large volume limit of the topological susceptibility χ in pure SU(3) gauge theory. We obtain an upper bound for the symmetry breaking order parameter $\langle Q \rangle$ and, as a by-product, the value $\chi = [173.4(\pm 0.5)(\pm 1.2)(^{+1.1}_{-0.2})$ MeV$]^4$ at $\beta = 6$ ($a \approx 0.1$ Fermi). The errors are the statistical error from our data, the one derived from the value used for Λ_L and an estimate of the systematic error, respectively.

I. INTRODUCTION

The QCD Lagrangian $\mathcal{L}_{QCD}$ is parity invariant. On the other hand, the possible spontaneous breaking of parity is experimentally ruled out to a high precision. There is a debate as to whether the absence of spontaneous breaking can be analytically proved in QCD. By studying the Euclidean formulation of the theory, Vafa and Witten [1] argued that such breaking is not possible. Their argument is the following: Spontaneous breaking of parity occurs when there exists some parity violating operator $\mathcal{O}$ whose vacuum expectation value remains nonvanishing after sending $\theta \to 0$ in the extended theory $\mathcal{L}_{QCD} + \theta\mathcal{O}$. However, in the Euclidean formulation of the theory, any parity-odd operator must pick up an imaginary i factor.[1] Therefore the $\theta\mathcal{O}$ term contributes a phase to the Euclidean partition function and, hence, the free energy has its minimum at $\theta = 0$ and $\langle \mathcal{O} \rangle$ vanishes.

As pointed out by several authors [4–6], the above argument is insufficient to exclude the scenario of spontaneous parity breaking. It is necessary to prove as well that the free energy and its derivatives at its minimum are continuous functions of θ.

If the parity violating probe is the topological charge density $Q(x)$, then it is possible to show [6] that the partition function $Z(\theta)$ is finite throughout the whole complex plane of θ and arguments can be given against the appearance of dangerous Lee-Yang zeros [7].

We want to study on the lattice the question about the continuity of the derivatives of the free energy for the case of the parity-odd (and time inversion-odd) operator $Q(x)$ and give an upper bound to the order parameter $\langle Q \rangle$ where $Q \equiv \int d^4x Q(x)$ is the total topological charge.

We assume that the free energy $E(\theta)$ of the pure gauge theory at its minimum (at $\theta = 0$, after Vafa and Witten theorem) has a discontinuous derivative. If we call

$dE(\theta)/d\theta|_{\theta \to \pm 0} = \pm \alpha$ then the vacuum expectation value $\langle Q \rangle = \pm V\alpha$ where V is the spacetime volume and α is a positive real number which specifies the density of spontaneously generated net topological charge. The alternating sign indicates the choice of the vacuum. By inserting a complete set of intermediate states $\mathbb{1} = |0\rangle\langle 0| + |g\rangle\langle g| + \cdots$ ($|g\rangle$ represents pure gluonic states) between the two topological charge operators in $\langle Q^2 \rangle$ we obtain

$$\frac{\langle Q^2 \rangle}{V} = \alpha^2 V + \chi, \tag{1.1}$$

where χ is the usual topological susceptibility defined in [8]. Notice that if $\alpha \neq 0$ then the above expectation value depends linearly on the volume. In the present paper we investigate this volume dependence on the lattice for the pure SU(3) Yang-Mills theory in order to set a bound on the value of the slope α.
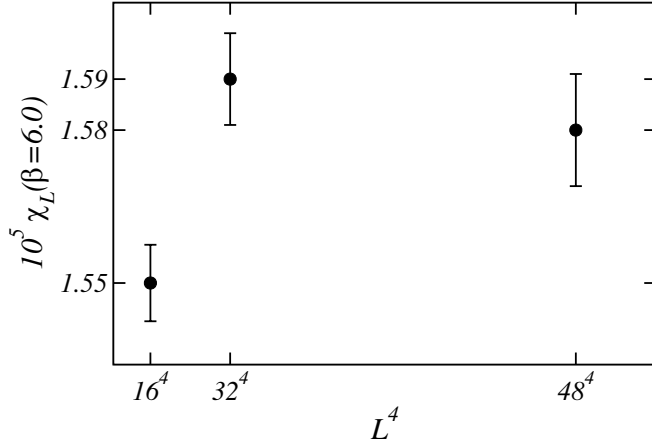
II. THE CALCULATION OF χ

The quenched theory was simulated by using the standard plaquette action [9] on the lattice at the inverse bare coupling $\beta = 6.0$ on three volumes: 16^4, 32^4 and 48^4. In all cases a heat-bath algorithm combined with over-relaxation was used for updating configurations and care was taken (by checking the autocorrelation function) to decorrelate successive measurements in order to render them independent.

The total topological charge was measured with the once-smeared operator [10] $Q_L^{(1)} = \sum_x Q_L^{(1)}(x)$. The lattice equivalent of Eq. (1.1) is $\chi_L \equiv \langle (Q_L^{(1)})^2 \rangle / L^4$. L^4 is the dimensionless volume of the lattice, $L^4 = V/a^4$, where a is the lattice spacing.

In Fig. 1 and Table I we show the result for χ_L for the three volumes. Our investigation requires a precise determination of the topological susceptibility, hence we used huge statistics. The simulations were performed with the APEmille facility in Pisa.

In general, the lattice topological susceptibility χ_L is related to the physical one χ by a multiplicative and an

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[1]This is not true in general at finite temperature [2] and the possibility of the existence of a stable parity breaking phase at nonzero temperature is still open [3].

FIG. 1. χ_L versus the lattice size for $\beta = 6.0$.

additive renormalization [11]. The equation that expresses this relationship is

$$\chi_L = \frac{\langle (Q_L^{(1)})^2 \rangle}{L^4} = Z^2 a^8 \alpha^2 L^4 + Z^2 a^4 \chi + M$$
$$\equiv Z^2 a^4 \chi_P + M; \qquad (2.1)$$

for convenience we call $a^4 \chi_P \equiv a^8 \alpha^2 L^4 + a^4 \chi$.

We renormalize the topological charge operator $Q_L^{(1)}$ by imposing that it takes integer eigenvalues in the continuum limit. To obtain this result we must introduce a renormalization constant [12,13] which is finite in virtue of the renormalization group invariance of Q in the quenched theory. This is the origin of the factor Z in expression (2.1).

The operator expansion of the product $[Q_L^{(1)}(x)Q_L^{(1)}(0)]$ contains a contact term [14]. Part of this term must be subtracted and this is M in expression (2.1). We fix this additive subtraction by imposing that the topological susceptibility must vanish in the absence of instantons [15]. By construction M is independent of the background topological sector.

These definitions are valid when $\alpha = 0$ and apply equally well to the case where $\alpha \neq 0$.

To extract information about the parameter α in Eq. (2.1) we have to know Z and M. We have calculated these renormalization constants paying attention to their possible volume dependence.

III. CALCULATION OF Z AND M

We determined the renormalization constants Z and M by the nonperturbative method introduced in [16,17].

Following the meaning of Z, we calculate it by computing the average topological charge within a fixed topological sector. If we choose a topological sector of charge n (any nonzero integer) then

$$Z = \frac{\langle Q_L^{(1)} \rangle |_{Q=n}}{n}, \qquad (3.1)$$

where the division by n entails the requirement that Q takes integer values as described above. The brackets $\langle \cdot \rangle |_{Q=n}$ mean thermalization within the topological sector of charge n.

We start our algorithm with a classical configuration with topological charge 1 ($n = 1$) and action $8\pi^2$ in appropriate units. Then we apply 80 heat-bath updating steps and measure $Q_L^{(1)}$ every four steps. This set of 20 measurements is called "trajectory." After each measurement we cool the configuration to verify that the topological sector is not changed. We repeat this procedure to obtain a number of trajectories. For each trajectory we always discard the first measurements because the configuration is not yet thermalized. Averaging over the thermalized steps (as long as the corresponding cooled configuration shows the correct background topological charge, $n = 1$ within a deviation δ) yields $\langle Q_L^{(1)} \rangle |_{Q=1}$. We estimate the systematic error that stems from the choice of δ as in [15].

We followed the above procedure on three lattice sizes to study any possible volume dependence of Z. In Table II the number of trajectories and volume sizes are displayed.

In Fig. 2 we show the results for Z extrapolated to the form $A + B/L^2$. They look very stable, mainly at the lattice sizes of our interest ($L = 16$, 32, and 48). The errors were calculated including the cross correlation, $\langle AB \rangle - \langle A \rangle \langle B \rangle \approx -6 \times 10^{-5}$. The χ^2/d.o.f. test leads to 0.02.

As for the additive renormalization constant M the procedure is quite analogous. This time we calculate $M = \chi_L |_{Q=0} \equiv \langle (Q_L^{(1)})^2 \rangle / L^4 |_{Q=0}$. Single trajectories consist again of 80 heat-bath steps with measurements every four steps and cooling tests after each measurement. Thermalization (with short distance fluctuations) require us to discard the initial steps. In Table II the number of trajectories for each lattice size is shown.

In Fig. 3 the results for M extrapolated with a fit to the form $A + B/L^2$ are shown. The nontrivial dependence on

TABLE I. Value of χ_L and statistics for each lattice size.

L^4	Statistics	$10^5 \chi_L$
16^4	120 000	1.550(7)
32^4	60 000	1.590(9)
48^4	50 000	1.580(11)

TABLE II. Number of trajectories utilized in the calculation of Z and M.

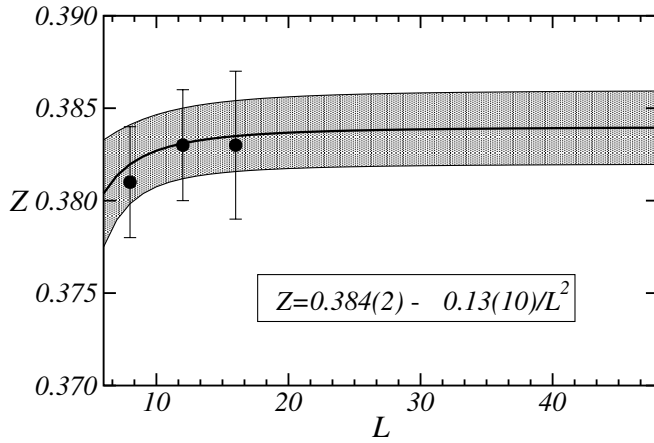| L^4	Z	M
8^4	147 000	129 000
12^4	60 000	74 000
16^4	50 000	57 000

FIG. 2. Z versus L for the 1-smeared topological charge operator $Q_L^{(1)}$ at $\beta = 6.0$. The line is the result of the fit (displayed in the legend) and the grey band is its 1-σ error.

L is evident. Hitherto this dependence had not been detected because the statistics (number of trajectories) was much lower than in the present paper.

Again the $\chi^2/$d.o.f. test is rather small: 0.05. Also a nonzero cross correlation is present, $\langle AB \rangle - \langle A \rangle \times \langle B \rangle \approx -1.5 \times 10^{-15}$ and the grey band of errors in Fig. 3 was calculated by making use of it.

In Table III the results extrapolated for Z and M on the lattice sizes used for the calculation of χ_P in Sec. II are shown.

It is interesting to check the results of M by calculating it on different background topological sectors. In fact this renormalization constant can also be calculated as $M = \chi_L|_{Q=n} - Z^2 n^2 / V$, where n can be any integer and Z is the previously determined renormalization constant. The results for M obtained by using different topological sectors n agree within errors [16,18]. Notice that this fact bears out the independence of M on the topological charge sector.

In Figs. 2 and 3 we have included the systematic error that is generated during the cooling test. This error shows
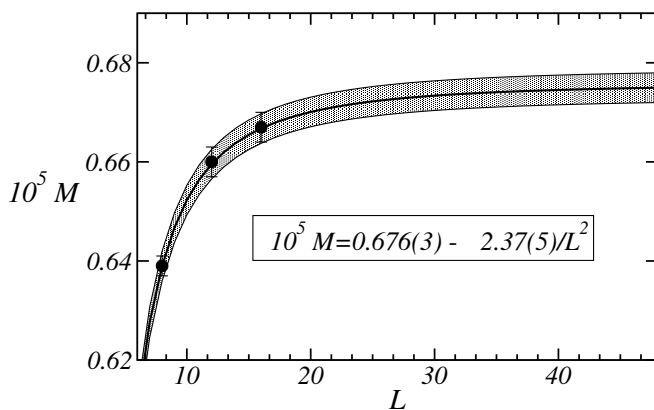

FIG. 3. M versus L for the 1-smeared topological charge operator $Q_L^{(1)}$ at $\beta = 6.0$. The line is the result of the fit (displayed in the legend) and the grey band is its 1-σ error.

TABLE III. Extrapolated values for Z and M.

L^4	Z	$10^5 M$
16^4	0.383(2)	0.667(3)
32^4	0.384(2)	0.674(3)
48^4	0.384(2)	0.675(3)

up because if some new instanton had appeared during the updating process along the trajectory then this trajectory must be discarded. However, in some cases the cooling relaxation eliminates this unwanted instanton and in this (rare[2]) event the configuration is wrongly taken as lying in the correct topological sector. This error tends to modify the values of M and Z. When $\langle Q^2 \rangle$ is calculated on the $n = 0$ topological sector, any jump from the $n = 0$ sector enlarges the value of M. On the other hand, in the calculation of Z on the $n = 1$ sector, due to the symmetry of the topological charge distribution around $n = 0$, the configuration prefers to move to the $n = 0$ sector and this effect lowers the result for Z. Therefore this uncertainty turns out to be asymmetric around the central value.

To estimate the influence of this error on the value of M we measure also the plaquette. After several heating steps the plaquette thermalizes and a plateau in its signal appears. The difference between the value of $\chi_L|_{Q=0}$ at the step where this plateau sets in and the value at the last step in the trajectory is taken as an estimate of this error. An analogous procedure was followed in the calculation of Z. This error was added to the one corresponding to the choice of δ (see above) to form the total systematic error of our calculation.

We are planning to study this systematic error more carefully by using the overlap algorithm [20–23] in place of cooling to evaluate the background topological charge Q.

IV. BOUND ON α AND CALCULATION OF χ

With the data of Tables I and III and Eq. (2.1), we obtain the values of $a^4 \chi_P$ that are shown in Fig. 4. A fit (with the $\chi^2/$d.o.f. estimator) to the functional form $a^4 \chi_P = \alpha^2 a^8 L^4 + a^4 \chi$ yields $\alpha^2 a^8 = 1.5(\pm 2.4)(^{+0.0}_{-2.0}) 10^{-13}$ and $a^4 \chi = 6.09(\pm 0.07)(^{+0.16}_{-0.03}) 10^{-5}$; the first errors being statistical and the second ones being systematic from cooling.

By using the values for $a(\beta) \Lambda_L$ and T_c/Λ_L tabulated in [24] and the ratio for $T_c/\sqrt{\sigma}$ from [25], we get $\Lambda_L = 7.90(6)$ MeV and $a(\beta = 6.0) = 0.1004(7)$ Fermi. This leads to the 1-σ bound on the parity violating order parameter

$$\alpha \lesssim \left(\frac{1}{4 \text{ Fermi}} \right)^4. \tag{4.1}$$

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[2]This event barely occurs because the autocorrelation time for the topological charge is much larger than for other operators both in the heating process [19] and in the cooling.
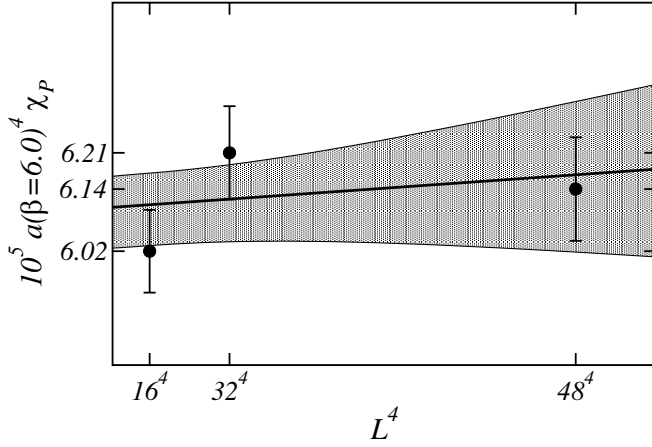
FIG. 4. $a^4\chi_P$ versus the lattice size for $\beta = 6.0$. The straight line is the result of the fit described in the text and the grey band is its 1-σ statistical error.

Much as an explicit θ term in the Lagrangian violates both parity and time reversal and allows for a nonzero value of the electric dipole moment d_e of fermions, the spontaneous breaking of parity driven by the topological charge operator brings about a nonvanishing d_e. This d_e is proportional to α times some volume which in the case of the neutron can be estimated as the volume occupied by this particle, roughly $1/m_N^4$. Moreover, the whole effect would disappear if the Lagrangian was chiral because then the extended theory $\mathcal{L}_{QCD} + \theta Q(x)$ would be equivalent to $\mathcal{L}_{QCD}$ with $\theta = 0$. This implies that the derivative of the free energy with respect to θ would vanish and spontaneous breaking of parity could not occur. To lowest order, this means that the result for d_e must be proportional to the squared pion mass. Barring large numerical factors, using the neutron mass m_N as the typical scale of the problem and assuming that the bound in expression (4.1) applies to the full theory too, we estimate the spontaneously generated electric dipole moment of the neutron as

$$d_e \approx e \, \frac{\alpha}{m_N^4} \, \frac{m_\pi^2}{m_N^3} < 3.5 \times 10^{-21} e \cdot cm, \qquad (4.2)$$

to be compared with the experimental limit, $6.3 \times 10^{-26} e \cdot$ cm [26]. The result (4.2) must not be confused with the electric dipole moment calculated for the neutron in the presence of an explicit nonzero physical value of θ [27,28]. In our case the physical θ is zero.

We explicitly notice that our bound on the parameter α was obtained at fixed β (fixed a) and it is not affected by the continuum limit.

Our method also allows one to extract the topological susceptibility with great precision. From the value for $a^4\chi$ obtained in the fit we get $\chi = [173.4(\pm 0.5)(\pm 1.2) \times (^{+1.1}_{-0.2})]$ MeV]^4 where the first error is our statistical, the second is the propagation of the error on Λ_L and the third

one is the systematic from cooling. The two first errors must be added in quadrature. This is the value of χ obtained at $\beta = 6$. An extrapolation $a \to 0$ should be made with comparable precision. Usually the error derived from this extrapolation is negligible as compared with the statistical one. However, our value of the topological susceptibility has been obtained after a very high statistics simulation and this causes the systematic effects to become important.

The result for the topological susceptibility can be compared with $[174(7)$ MeV]^4 obtained in [15] from a Monte Carlo simulation on a 16^4 lattice. It can also be compared with the analytical prediction [29] $\chi \approx (180$ MeV)^4 obtained within a $1/N_c$ expansion.

V. CONCLUSIONS

We have studied the consequences of the spontaneous breaking of parity and time inversion symmetries on the topological charge operator in pure Yang-Mills theory with gauge group SU(3). We assumed that in the infinite volume limit the free energy $E(\theta)$ of the extended theory $\mathcal{L}_{QCD} + \theta\mathcal{O}$ has a cusp at its minimum, $\theta = 0$, that signals a nonzero value of the topological charge in the vacuum, $d\langle Q\rangle/dV = \pm\alpha$.

By calculating the value of the topological susceptibility on the lattice to high precision we have obtained a bound on α: Within 1-σ error, there is no spontaneously generated net topological charge in a volume of $(4\,Fermi)^4$. The bound on α becomes an upper bound for the neutron electric dipole moment which however is 4 to 5 orders of magnitude less precise than the corresponding experimental limit.

As a by-product of our Monte Carlo simulation, we have also obtained a precise result for the topological susceptibility, $\chi = [173.4(\pm 0.5)(\pm 1.2)(^{+1.1}_{-0.2})$ MeV]^4 (the errors are, respectively, statistical from our Monte Carlo simulation, statistical from the value used for Λ_L and systematic from the cooling used during the evaluation of the renormalization constants). The precision in the statistics forced us to study this systematic error which otherwise can be neglected. The continuum limit should be made with comparable precision.

We have done the calculation by using the so-called "field theoretical method" where the renormalization constants relating the lattice and the physical susceptibilities are explicitly computed. This method proves to be fast and efficient enough to allow one to obtain a huge number of measurements on rather large lattices (see Table I). The APEmille facility in Pisa was used for the runs.

The renormalization constants in Eq. (2.1), Z and M, have been calculated with high statistics at various volumes. The value of Z looks rather stable with the volume, while the value of M displays a clean volume dependence (see Fig. 3).

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