Critical comparison of different definitions of topological charge on the lattice

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A detailed comparison is made between the field-theoretic and geometric definitions of topological charge density on the lattice. Their renormalizations with respect to the continuum are analyzed. The definition of the topological susceptibility χ, as used in chiral Ward identities, is reviewed. After performing the subtractions required by it, the different lattice methods yield results in agreement with each other. The methods based on cooling and on counting fermionic zero modes are also discussed. [S0556-2821(98)10921-9]

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I. INTRODUCTION

The definition of topological charge density and of topological susceptibility on the lattice has by now a long story with contrasting results [1,2]. This paper intends to be a contribution to clarify the issue.

Lattice is a regulator of the theory. It should reproduce continuum physics in the limit in which the cutoff is removed, i.e., in the limit in which the lattice spacing a tends to zero. Like any other regularization scheme, however, appropriate renormalizations have to be performed to determine physical quantities. Within the rules of renormalization theory, the topological charge density and its correlation functions can be defined on the lattice with the same rigor as for any other operator of the theory.

In QCD,

$$Q(x)=\frac{g^2}{64\pi^2}\epsilon_{\mu\nu\rho\sigma}F^a_{\mu\nu}(x)F^a_{\rho\sigma}(x). \tag{1}$$

$Q(x)$ has a fundamental physical role, being the anomaly of the $U_A(1)$ singlet axial vector current

$$\begin{aligned}\partial_\mu J^5_\mu(x)&=-2N_f Q(x),\\ J^5_\mu(x)&=\sum_{i=1}^{N_f}\overline{\psi}_i(x)\gamma_\mu\gamma_5\psi_i(x).\end{aligned} \tag{2}$$

N_f is the number of light flavors. Equation (2) provides a solution to the $U_A(1)$ problem of Gell-Mann's quark model in which J^5_μ is conserved and the corresponding $U_A(1)$ is a symmetry, whereas in hadron physics neither parity doublets are observed, which would correspond to a Wigner realization, nor is the inequality $m_{\eta'}\leqslant\sqrt{3}m_\pi$ satisfied, which would correspond to a spontaneous breaking in the manner of Goldstone.

Equation (2) could explain the higher value of $m_{\eta'}$ as suggested by an approach based on $1/N_c$ expansion of the theory. At the leading order the anomaly being $O(1/N_c)$, is absent and $U_A(1)$ is a Goldstone symmetry like axial $SU_A(3)$. The idea behind this expansion is that already at this order the theory describes the main physical features of hadrons (e.g., confinement) [3]. In the $1/N_c$ expansion, the anomaly acts as a perturbation, displacing the pole of the $U_A(1)$ Goldstone boson to the actual mass of the η'. The prediction is [4,5]

$$\chi=\frac{f_\pi^2}{2N_f}\,(m^2_\eta+m^2_{\eta'}-2m^2_K), \tag{3}$$

where

$$\chi=\int \mathrm{d}^4x\langle 0|T(Q(x)Q(0))|0\rangle \tag{4}$$

is the topological susceptibility of the vacuum in the unperturbed ($N_c=\infty$) theory. This means, among other facts, a quenched approximation, fermion loops being $O(g^2N_f)$ $\sim O(N_f/N_c)$.

In fact, as we shall discuss in detail below, χ in Eq. (4) is not defined if the prescription is not specified for the singularity of the product $Q(x)Q(0)$ as $x\to 0$. In Refs. [4,5] the prescription which leads to Eq. (3) is the following:

$$\chi=\int \mathrm{d}^4(x-y)\,\partial^x_\mu\partial^y_\nu\langle 0|T(K_\mu(x)K_\nu(y))|0\rangle, \tag{5}$$

where $K_\mu(x)$ is the Chern current

$$K_\mu=\frac{g^2}{16\pi^2}\epsilon_{\mu\nu\rho\sigma}A^a_\nu\left(\partial_\rho A^a_\sigma-\frac{1}{3}\,gf^{abc}A^b_\rho A^c_\sigma\right) \tag{6}$$

related to $Q(x)$ by the equation

$$\partial_\mu K_\mu(x)=Q(x). \tag{7}$$

The prescription [Eq. (5)] eliminates all the δ-like singularities in the product $K_\mu(x)K_\nu(y)$ as $x\to y$. In any regularization scheme the Eq. (5) only leaves a multiplicative renormalization Z^2 for χ, Z being the possible renormalization of $Q(x)$. Equation (7) implies that the total topological charge

$$Q\equiv\int d^4x\ Q(x) \tag{8}$$

has integer values.

The regularized version of $Q(x)$, $Q_L(x)$, does not, in general obey Eq. (7) [6]. According to the general rules of renormalization theory (in pure gauge theory),

$$Q_L(x)=ZQ(x). \tag{9}$$

In general $Z\neq 1$, unless Eq. (7) is preserved by regularization. To determine Z, it is sufficient to measure $\langle Q_L\rangle = a^4 Z\langle Q\rangle$ on a state belonging to a definite eigenvalue of Q (see Sec. II).

The product $Q_L(x)Q_L(y)$ will not satisfy Eq. (5), in general at the singularity $x\to y$. In the limit $a\to 0$ it will differ from it by additive terms $\delta\chi$, which can be classified by use of the Wilson operator product expansion [7]. Defining (V is the 4-volume)

$$\chi_L \equiv \frac{1}{V}\sum_{xy} Q_L(x)Q_L(y), \tag{10}$$

we will have

$$\chi_L=\frac{1}{V}Z^2Q^2a^4+\delta\chi, \tag{11}$$

where the first term corresponds to Eq. (5). Taking the vacuum expectation value of Eq. (11) gives

$$\chi_L=a^4Z^2\chi+\chi_0, \tag{12}$$

with

$$\chi_0=\langle 0|\delta\chi|0\rangle. \tag{13}$$

Taking the expectation value of Eq. (11) on eigenstates $|q_n\rangle$ of Q gives

$$\langle q_n|\chi_L|q_n\rangle=\frac{1}{V}Z^2q_n^2a^4+\langle q_n|\delta\chi|q_n\rangle. \tag{14}$$

It is a generally accepted wisdom that renormalization effects produced by short-range quantum fluctuations are practically independent of the semiclassical instanton background which determines q_n. The independence on q_n of $\langle q_n|\delta\chi|q_n\rangle$ can be checked numerically by Eq. (14) and proves to be true within errors [8]. Then $\langle q_n|\delta\chi|q_n\rangle=\chi_0$, and χ_0 can be determined from Eq. (14) as $\langle q_n=0|\chi_L|q_n=0\rangle$, i.e., as the expectation value of χ_L on the trivial topological sector.

From Eq. (12),

$$\chi=\frac{\chi_{\text{reg}}-\chi_0}{Z^2}. \tag{15}$$

It is with this prescription that χ is expected to be

$$\chi=(180\ \ \text{MeV})^4 \tag{16}$$

in the quenched approximation within an $O(1/N_c)$ systematic error.

In this paper we will show that, if the prescription [Eq. (5)] is properly implemented, all methods which have been proposed to determine χ on the lattice give the same result. We shall do this by comparing the geometric method [9,10] to define $Q(x)$ to the field-theoretic one [6,7] for $SU(2)$ gauge theory. The same procedure, applied to $SU(3)$, indeed confirms [11] the expectation [Eq. (16)].

II. DEFINING $Q(x)$ ON THE LATTICE

In analogy to any lattice operator, $Q_L(x)$ will be defined by the requirement that, in the formal (naïve) limit $a\to 0$,

$$Q_L(x)\overset{a\to 0}{\sim} a^4Q(x)+O(a^6). \tag{17}$$

A prototype definition is

$$Q_L(x)=\frac{-1}{2^9\pi^2}\sum_{\mu\nu\rho\sigma=\pm 1}^{\pm 4}\tilde{\epsilon}_{\mu\nu\rho\sigma}\ \text{Tr}[\Pi_{\mu\nu}(x)\Pi_{\rho\sigma}(x)]. \tag{18}$$

$\tilde{\epsilon}_{\mu\nu\rho\sigma}$ is the standard Levi-Civita tensor for positive directions, while for negative ones the relation $\tilde{\epsilon}_{\mu\nu\rho\sigma}=-\tilde{\epsilon}_{-\mu\nu\rho\sigma}$ holds.

$O(a^6)$ irrelevant terms in Eq. (17) will disappear in the scaling regime. However, their presence may be used to improve the operator [12]. In what follows $Q_L^{(i)}$ ($i=0$, 1, and 2) will denote the operator defined by Eq. (18) and the once and twice improved versions of it, respectively. Improvement is the recursive smearing of the links developed in Ref. [12]. Also, the geometric definition $Q_L^{\text{geom}}(x)$ satisfies Eq. (17) [9].

Like any other regularized operator, $Q_L(x)$ will mix in the continuum limit, when irrelevant terms become unimportant, with all the operators having the same quantum numbers and lower or equal dimension. The only pseudoscalar of dimension $\leqslant 4$ is $Q(x)$ itself:

$$Q_L(x)=ZQ(x). \tag{19}$$

The naïve expectation for Z would be $Z=1$ since Q, as an integer, should not renormalize. As first realized in Ref. [6], this is not true on the lattice where $Q_L(x)$ is not a divergence. Z can be computed in perturbation theory, as it was done in the early works on the subject [6]. A better way is to measure $\langle Q_L\rangle$, the total topological charge on the lattice, on a state on which Q has a known value, e.g., on a one-instanton state where $Q=1$. This can be done by a heating technique [8] where a background instanton is put by hand on the lattice, and quantum fluctuations at a given value of $\beta=2N_c/g^2$ are added to it. In the continuum, the instanton configuration is stable, being a minimum of the action, and therefore perturbing it by small fluctuations does not change the value of Q. On the lattice, instantons are not stable, so that Q could change during this heating procedure. The way to avoid this inconvenience is to create a sample of configurations by the usual Monte Carlo updating, starting from the original instanton. Each of them is checked in its instanton content by a rapid cooling: configurations where the original topological charge seems to be changed are discarded. This can be done after any number of heating steps, and the result

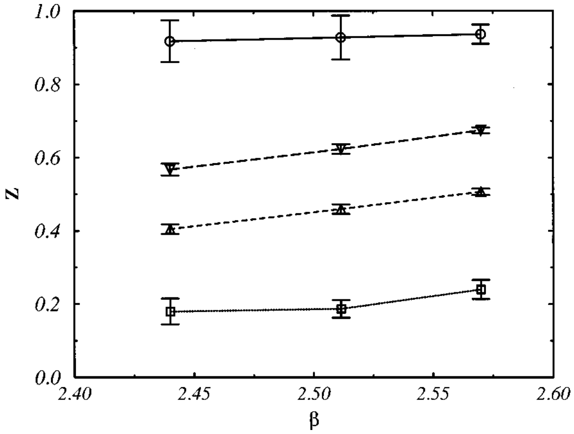

FIG. 1. Values of Z as obtained by the heating method for the geometric and 0-, 1-, and 2-smeared field-theoretic topological charges (circles, squares, up-triangles, and down-triangles, respectively).

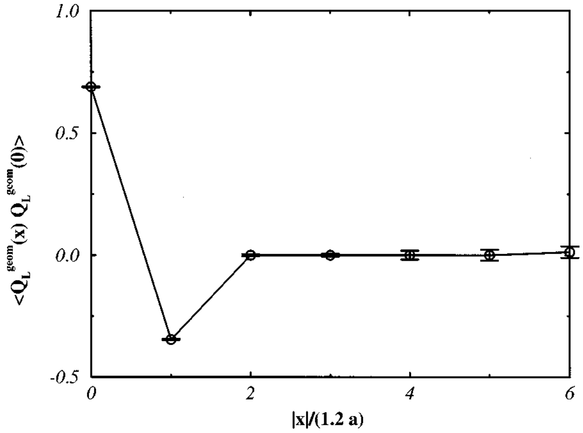

FIG. 3. The same as in Fig. 2 for the geometrical topological charge.

must be independent of this number. The result is a sample with topological charge Q. Q_L measured on this ensemble will reach a plateau in this heating procedure, on which Z can be read. If the instanton were stable, the plateau would stay flat forever.

This procedure has been checked and used repeatedly within the field-theoretical method [11,13–15]. The result for Z is shown in Fig. 1 as a function of β for different definitions of $Q_L(x)$. The data for the 0-, 1-, and 2-smeared operators are taken from Ref. [15], and are computed on a one-instanton configuration on a 16^4 lattice. The data for the geometrical definition, are new and are computed with the same procedure. For the geometric definition, Z is compatible with 1 (within two standard deviations). However, the values of $Q_L^{\rm geom}$ have a large spread (as large as $Q \pm 10$), showing that it can assume values different from the original Q on configurations which are presumed to belong to that sector. Only the average satisfies $\langle Q_L \rangle = Q$, but not the value configuration, by configuration. Moreover, on a given configuration, the value of $Q_L^{\rm geom}$ depends on the interpolation used to define it [10].

III. TOPOLOGICAL SUSCEPTIBILITY

The lattice topological susceptibility is written as

$$\chi_L = \sum_x \langle Q_L(x) Q_L(0) \rangle = \frac{Q_L^2}{V}, \tag{20}$$

and analogously for $Q_L^{\rm geom}$. To make a connection to the continuum susceptibility as defined by Eq. (5), in general, there will be an additive renormalization due to the singularity at $x \rightarrow y$ and a multiplicative residual renormalization ($x \neq y$) which will simply be the square of Z computed in Sec. II.

As a matter of fact, $\langle Q_L(x) Q_L(0) \rangle$ is expected to be negative due to reflection positivity at $x \neq 0$, since $Q_L(x)$ changes its sign under time reversal [16]. In fact, this holds at distances larger than the extension of the operator if it is smeared. Figures 2 and 3 show that this is indeed the case

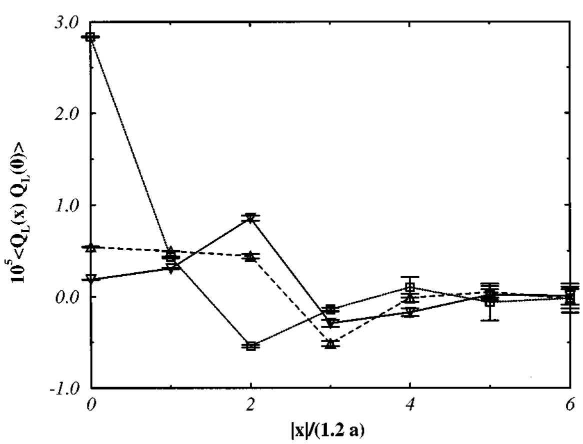

FIG. 2. Correlation function $\langle Q_L(x) Q_L(0) \rangle$ as a function of $|x|/(1.2a)$ for the 0-, 1-, and 2-smeared topological charges (squares, up-triangles, and down-triangles, respectively) at $\beta = 2.57$.

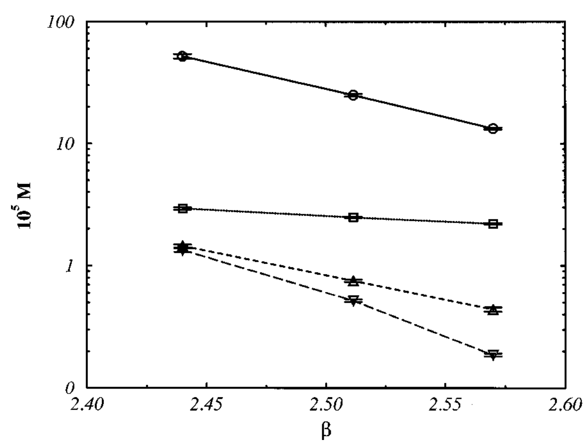

FIG. 4. Values of M as obtained by the heating method for the geometric and 0-, 1-, and 2-smeared field-theoretic topological charges (circles, squares, up-triangles, and down-triangles, respectively).

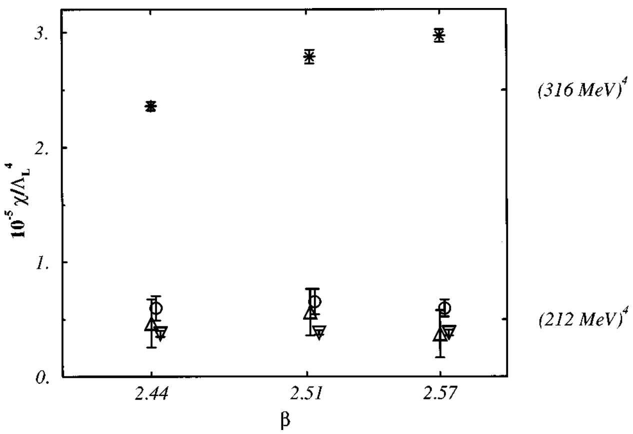

FIG. 5. χ in Λ_L and MeV units for the unsubtracted geometrical charge (stars), subtracted geometrical charge (circles), and 0- and 2-smeared charges (up and down triangles).

both for the geometric operator and the field-theoretical definition. Since Q_L^2 is positive, its value is determined mainly by the point at $x=0$, i.e., by the singularity of the product at $x\to 0$. This peak is there, no matter how $Q_L(x)$ is defined, and its height depends on the definition used. In Figs. 2 and 3 the values for $\langle Q_L(x)Q_L(0)\rangle$ have been summed over all points x inside a shell at distance $|x|$ from the origin $x=0$. The width of this shell was $1.2a$.

Thus, in general [6,7],

$$\chi_L=Z(\beta)^2a^4\chi+M(\beta). \tag{21}$$

$M(\beta)$ will describe a mixing with all scalar operators of dimension $\leqslant 4$ [$\overline{\beta}(g)$ is the beta function]:

$$M(\beta)=A(\beta)\left\langle\frac{\overline{\beta}(g)}{g}F^a_{\mu\nu}F^a_{\mu\nu}\right\rangle a^4+P(\beta)\times 1. \tag{22}$$

M is the value of χ_0 in Eq. (12) in the lattice regularization.

To match the prescription of Eq. (5), χ has to be zero in the sector $Q=0$. Thus, in that sector $\chi_L=M(\beta)$, and $M(\beta)$ can be determined by measuring χ_L in it. This is again done

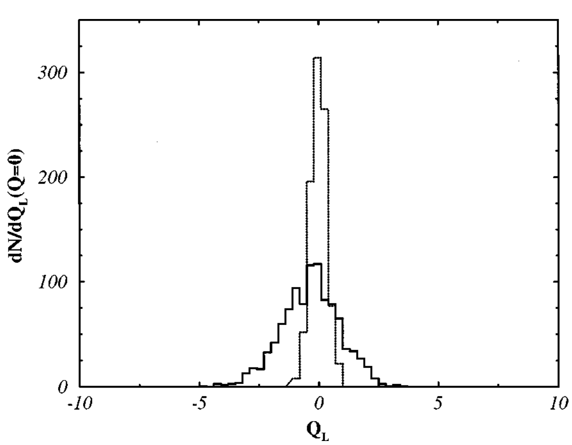

FIG. 6. Distribution of Q_L in the zero-topological charge sector $Q=0$ for the 0-smeared (solid line) and 2-smeared (dotted line) topological charge densities at $\beta=2.57$.

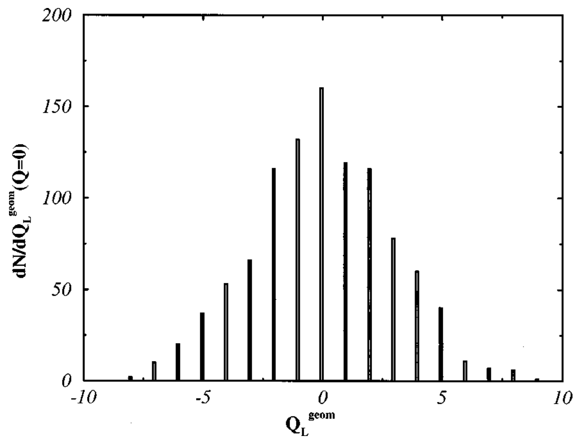

FIG. 7. The same as in Fig. 6 for the geometrical topological charge.

by a heating procedure [8]. The flat, zero-field configuration [$U_\mu(x)=1$] can be dressed with local quantum fluctuations, which do not change its topological content, by the usual updating procedure at the desired value of β. χ_L will soon reach a plateau: if the sector were stable the plateau would persist forever. Instead, a nonvanishing topological charge can be created on the lattice, and care must be taken to eliminate configurations where this happens. Again this must be done by cooling and checks can be done to test the consistency of the procedure. Figure 4 shows the determination of $M(\beta)$ for the geometric definition and for three different field-theoretical definitions. Analogously to Eq. (15), from Eq. (21) we obtain

$$a^4\chi=\frac{\chi_L-M(\beta)}{Z(\beta)^2}. \tag{23}$$

χ_L, M, and Z depend on the choice of the regulator as well as on the choice of the action; a depends on the choice of the action, but χ must be independent of all of it. Figure 5 shows that this is the case. In this figure we have used the data of Ref. [15] for the 0- and 2-smeared field-theoretical charges. The data for the geometric definition has been obtained on a 16^4 lattice with the same updating procedure (heat bath) and compatible statistics (5000 configurations). The result of the simulations is in fact χ/Λ_L^4. Usually, people determine Λ_L by computing the string tension σ/Λ_L^2, and by assuming the physical value for σ. This allows one to express $\chi^{1/4}$ in physical units. We do the same in order to compare our

TABLE I. χ_L, Z, and M for the 0-smeared, 1-smeared, 2-smeared, and geometric topological charge density operators at $\beta=2.57$.

Operator	$10^5\times\chi_L$	Z	$10^5\times M$
geometric	16.6(3)	0.937(26)	13.26(23)
0-smeared	2.320(52)	0.240(26)	2.200(32)
1-smeared	1.010(49)	0.507(9)	0.440(18)
2-smeared	1.165(64)	0.675(8)	0.187(5)

result with other people's determinations. The scale is determined from the data of Refs. [17,18]. The data at 2 smearings yield $(\chi)^{1/4} = 198 \pm 2 \pm 6$ MeV for the $SU(2)$ gauge group, the first error being statistical and the second one coming from the error in Λ_L. The ''naïve'' unsubtracted geometric definition does not scale, and is almost one order of magnitude larger than the subtracted value. In the jargon of the geometrical method, this is called an effect of dislocations. It is the mixing with the identity operator which indeed describes these dislocations, which have dimensions lower than 4. There is, however, an additional mixing in Eq. (22) which has the same dimension as χ and still must be subtracted: checking only by dimension is not sufficient to ensure that χ_L is indeed equal to the physical χ, as defined by Eq. (5).

Figures 6 and 7 show the distribution of values for Q_L in the sector with trivial topology. Its variance is, apart from a normalization factor, a measure of $M(\beta)$. A good operator $Q_L(x)$ is one for which the subtraction $M(\beta)$ is small compared to χ_L. On the other hand, also having $Z \approx 1$ is more reassuring than having a small Z.

Table I shows χ_L, Z, and M for the 0-, 1-, and 2-smeared field-theoretical charges and the geometric charge at $\beta = 2.57$. The 2-smeared definition of $Q_L(x)$ is the best among these choices. The geometric definition is good with respect to Z, but is definitively bad with respect to the additive renormalization M.

IV. DISCUSSION

The main conclusion of the above analysis is that with any definition of topological charge density on the lattice, an additive renormalization for the topological susceptibility and a multiplicative one are necessary. If properly renormalized, all definitions bring about the same physical value for χ.

Confusion on this subject in the past was generated by a mistreatment of renormalization. On the one hand, the geometric definition was believed to be free from renormalizations because it always gave integer values for the total topological charge. This seems to be true for the multiplicative renormalization. Having integer values, however, does not exempt one from having singularities at a short distance in the product which defines χ_L. Figure 5 clearly proves that.

The field-theoretical definition started as a naïve definition. Z was not noticed and set equal to 1; $P(\beta)$ was subtracted by use of perturbation theory. As a result, $Z^2\chi$ was determined instead of χ itself, and found to be much smaller than the expectation [Eq. (16)] [19].

The idea was then put forward that the naïve definition might not be correct and the geometric method [9,20], the cooling method [21,22] and the Atiyah-Singer-based methods [23] were developed. The naïve method was promoted to the field-theoretic method only after introducing Z and a correct subtraction M [6,7]. The non-perturbative determinations of these constants [8], as explained above, finally brought about a reliable determination of χ, which is indeed regulator independent.

The cooling method automatically performs the additive subtraction because it gives $\chi_L = 0$ on the trivial sector; and also brings Z to 1 by freezing the quantum fluctuations. The problem with this was that instantons could be lost in the procedure, leading to an underestimation of χ. Cooling with improved forms of the action [24,25] seems to have eliminated this problem, and indeed gives results which confirm the field-theoretic determination. The same seems to be true for the modern versions of the Atiyah-Singer procedure [26].

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