A critical comparison of different definitions of topological charge on the lattice

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Abstract

A detailed comparison is made between the field–theoretic and geometric definitions of topological charge density on the lattice. Their renormalizations with respect to continuum are analysed. The definition of the topological susceptibility $\chi$, 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.

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1 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 rigour as for any other operator of the theory.

In QCD

$$Q(x) = \frac{g^2}{64\pi^2} \epsilon_{\mu\nu\rho\sigma} F_{\mu\nu}^a(x) F_{\rho\sigma}^a(x).$$

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

$$\partial_\mu J^5_\mu(x) = -2N_f Q(x),$$

$$J^5_\mu(x) = \sum_{i=1}^{N_f} \bar{\psi}_i(x) \gamma_\mu \gamma_5 \psi_i(x).$$

$N_f$ is the number of light flavours. Eq.(2) provides a solution to the $U_A(1)$ problem of Gell–mann’s quark model in which $J^5_\mu$ 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 the inequality $m_{\eta'} \leq \sqrt{3}m_\pi$ is satisfied, which would correspond to a spontaneous breaking à la Goldstone.

Eq.(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 is absent being $O(1/N_c)$, 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 $\eta'$. The prediction is [1, 5]

$$\chi = \frac{f_\pi^2}{2N_f} \left( m_\eta^2 + m_{\eta'}^2 - 2m_K^2 \right)$$

(3)
where
\[ \chi = \int d^4x (0|T(Q(x)Q(0))|0) \quad (4) \]
is the topological susceptibility of the vacuum in the unperturbed \((N_c = \infty)\) theory. This means, among other facts, quenched approximation, fermion loops being \(O(g^2N_f) \sim O(N_f/N_c)\).

In fact, as we shall discuss in detail below, \(\chi\) 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
\[ \chi = \int d^4(x - y)\partial_\mu \partial_\nu (0|T(K_\mu(x)K_\nu(y))|0) \quad (5) \]
where \(K_\mu(x)\) is the Chern current
\[ K_\mu = \frac{g^2}{16\pi^2} \epsilon_{\mu\nu\rho\sigma} A_\nu^a \left( \partial_\rho A_\sigma^a - \frac{1}{3}gf^{abc} A_\rho^b A_\sigma^c \right) \quad (6) \]
related to \(Q(x)\) by the equation
\[ \partial_\mu K_\mu(x) = Q(x) \quad (7) \]
The prescription Eq.(3) eliminates all the \(\delta\)-like singularities in the product \(K_\mu(x)K_\nu(y)\) as \(x \to y\). In any regularization scheme the prescription Eq.(3) only leaves a multiplicative renormalization \(Z^2\) for \(\chi\), \(Z\) being the possible renormalization of \(Q(x)\). Eq. (7) implies that the total topological charge
\[ Q \equiv \int d^4x Q(x) \quad (8) \]
has integer values.

The regularized version of \(Q(x), Q_L(x)\), does not obey in general (7). According to the general rules of renormalization theory (in pure gauge theory)
\[ Q_L(x) = ZQ(x). \quad (9) \]
In general \(Z \neq 1\) unless Eq. (7) is preserved by regularization. To determine \(Z\) it is sufficient to measure \(\langle Q_L \rangle = a^4Z\langle Q \rangle\) on a state belonging to a definite eigenvalue of \(Q\) (see section 2).

The product \(Q_L(x)Q_L(y)\) will not satisfy the prescription Eq. (3) 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)

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

(10)

we will have

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

(11)

where the first term corresponds to the prescription Eq. (5). Taking the v.e.v. of Eq. (11) gives

$$\chi_L = a^4 Z^2 \chi + \chi_0$$

(12)

with

$$\chi_0 = \langle 0 | \delta \chi | 0 \rangle.$$  

(13)

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

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

(14)

It is a generally accepted wisdom that renormalization effects produced by short range quantum fluctuations are practically independent of the semi-classical 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 $\chi_0$ can be determined from Eq. (12) as $\langle q_n = 0 | \chi_L | q_n = 0 \rangle$, i.e. as expectation value of $\chi_L$ on the trivial topological sector.

From Eq. (12)

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

(15)

It is with this prescription that $\chi$ is expected to be

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

(16)

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

In this paper we will show that, if the prescription Eq.(3) is properly implemented, all methods which have been proposed to determine $\chi$ on the lattice give the same result. We shall do this by comparing the geometric method [8, 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).
2 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 (naive) limit $a \to 0$

$$Q_L(x) \sim a^4 Q(x) + O(a^6). \quad (17)$$

A prototype definition is

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

$\tilde{\epsilon}_{\mu\nu\rho\sigma}$ 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 $Q_L^{(i)}$, ($i = 0, 1, 2$) 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 [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 $\leq 4$ being $Q(x)$ itself,

$$Q_L(x) = Z Q(x). \quad (19)$$

The naive expectation for $Z$ would be $Z = 1$ since $Q$, as an integer, should not renormalize. As first realized in [3] 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 [3]. A better way is to measure $\langle Q_L \rangle$, $Q_L$ being 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 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, 14, 15]. The result for $Z$ is shown in Fig. 1 as a function of $\beta$ for different definitions of $Q_L(x)$. The data for the 0–, 1– and 2–smeared operators are taken from ref. [13] and are computed on a 1–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 $Q_{L}^{\text{geom}}$ 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 $Q_{L}^{\text{geom}}$ depends on the interpolation used to define it [10].

3 The topological susceptibility

The lattice topological susceptibility is written as

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

and analogously for $Q_{L}^{\text{geom}}$. To make 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 the previous section.

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. Figs. 2 and 3 show that this is indeed the case both for the geometric operator and the field–theoretical definition. Since \( Q^2 \) 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 1.2 \( a \).

Thus in general \[\chi_L = \chi_0^2 + M(\beta). \tag{21}\]

\( M(\beta) \) will describe a mixing with all scalar operators of dimension \( \leq 4 \) (\( \beta(g) \) is the beta function),

\[
M(\beta) = A(\beta)\left(\frac{\beta(g)}{g} F_{\mu\nu} F^{\mu\nu}\right) a^4 + P(\beta) \cdot 1. \tag{22}
\]

\( M \) is the value of \( \chi_0 \) in Eq.(12) in the lattice regularization.

To match the prescription of Eq.(5), \( \chi \) has to be zero in the sector \( Q = 0 \). In that sector thus \( \chi_L = M(\beta) \) and \( M(\beta) \) can be determined by measuring \( \chi_L \) in it. This is again done by a heating procedure. 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 \( \beta \). \( \chi_L \) will soon reach a plateau: if the sector were stable the plateau would persist forever. Instead non–vanishing 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. Fig. 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

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

\( \chi_L, M \) 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 \( \chi \) must be independent of all of it. Fig. 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 \(\chi/\Lambda_L^4\). Usually people determine \(\Lambda_L\) by computing the string tension \(\sigma/\Lambda_L^2\) and by assuming the physical value for \(\sigma\). This allows to express \(\chi^{1/4}\) in physical units. We do same in order to compare our result with other people’s determinations. The scale is determined from the data of [7, 8]. The data at 2–smearings yield \((\chi)^{1/4} = 198 \pm 2 \pm 6 \text{ MeV}\) for \(SU(2)\) gauge group, the first error being statistical and the second one coming from the error in \(\Lambda_L\). 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 to the identity operator which indeed describes these dislocations, having dimension lower than 4. There is however an additional mixing in Eq. (22) which has the same dimension as \(\chi\) and still must be subtracted: checking only by dimension is not sufficient to ensure that \(\chi_L\) is indeed equal to the physical \(\chi\), as defined by Eq. (5).

Figs. 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 \(\chi_L\). On the other hand, also having \(Z \approx 1\) is more reassuring than having a small \(Z\).

Table I shows \(\chi_L\), \(Z\) and \(M\) for the 0–, 1–, 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 \(M\).

4 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 \(\chi\).

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 gave always integer values for the total topological charge. This seems to be true for the multiplicative renormalization. Having integer values, however, does not exempt from having singularities at short distance in the product which defines $\chi_L$. Fig. 5 is clearly proving that.

The field-theoretical definition started as a naïve definition. $Z$ was not noticed and put equal to 1; $P(\beta)$ was subtracted by use of perturbation theory. As a result $Z^2\chi$ was determined instead of $\chi$ 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 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 $\chi$, 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 it was that instantons could be lost in the procedure, leading to an underestimation of $\chi$. Cooling with improved forms of the action [24, 25] seems to have eliminated this problem and gives indeed 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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Figure captions

Figure 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).

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

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

Figure 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).

Figure 5. $\chi$ in $\Lambda_L$ and MeV units for the unsubtracted geometrical charge (stars), subtracted geometrical charge (circles) and 0– and 2–smeared charge (up and down triangles).

Figure 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 $\beta = 2.57$.

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

Table caption

Table I. $\chi_L$, $Z$ and $M$ for the 0–, 1–, 2–smeared and geometric topological charge density operators at $\beta = 2.57$. 

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| 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)       |
Fig. 2
Fig. 3

\[ \langle Q_L \rangle \]

\[ \langle Q_{L_{\text{geom}}} (x) \rangle \]

\[ |x|/(1.2 a) \]
Fig. 4
Fig. 5

\[ 10^{-5} \chi/\Lambda_L^4 \]

\( \beta \)
Fig. 6

$dN/dQ_L (Q=0)$ vs. $Q_L$.
Fig. 7

The graph shows a distribution of $dN/dQ_{L_{\text{geom}}}$ for $Q = 0$. The x-axis represents $Q_{L_{\text{geom}}}$ ranging from -10 to 10, while the y-axis represents the number of occurrences, ranging from 0 to 200. The distribution is skewed, with a peak around $Q = 0$.