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Topological charge on the lattice: a field theoretical view of the geometrical approach

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Abstract

We construct sequences of "field theoretical" lattice topological charge density operators which formally approach geometrical definitions in 2D $\mathbb{C}P^{N-1}$ models and 4D $SU(N)$ Yang–Mills theories. The analysis of these sequences of operators suggests a new way of looking at the geometrical method, showing that geometrical charges can be interpreted as limits of sequences of field theoretical (analytical) operators. In perturbation theory, renormalization effects formally tend to vanish along such sequences. But, since the perturbative expansion is asymptotic, this does not necessarily lead to well-behaved geometrical limits. It indeed leaves open the possibility that non-perturbative renormalizations survive. © 1997 Elsevier Science B.V.

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1. Introduction

The investigation of the topological properties of 4D $SU(N)$ gauge theories requires non-perturbative calculations. Lattice techniques represent our best source of non-perturbative calculations. However, investigating the topological properties of QCD on the lattice is a non-trivial task. Topology on the lattice is strictly trivial, and one relies on the fact that the physical topological properties should be recovered in the continuum limit.

In the so-called field theoretical method [1], one constructs a local analytical function $q_L(x)$ of the lattice fields which has the topological charge density $q(x)$ as its classical continuum limit:

$$q_L(x) \longrightarrow a^d q(x) + O(a^{d+1}). \tag{1}$$

$q_L(x)$ is not unique, indeed infinitely many choices differing for higher-order $O(a^{d+1})$ terms can be conceived. In this quite straightforward approach the major drawback is that

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related physical quantities, such as the topological susceptibility, can only be obtained after removing cut-off dependent lattice artifacts. The classical continuum limit must be in general corrected by including a renormalization function [2],

$$q_L(x) \longrightarrow a^d Z(g_0^2) q(x) + O(a^{d+1}), \tag{2}$$

where $Z(g_0^2)$ is a finite function of the bare coupling g_0^2 going to one in the limit $g_0^2 \to 0$. The relation of the zero-momentum correlation of two $q_L(x)$ operators,

$$\chi_L = \sum_x \langle q_L(x) q_L(0) \rangle, \tag{3}$$

with the topological susceptibility χ_t is further complicated by an unphysical background term,

$$\chi_L(g_0^2) = a^d Z(g_0^2)^2 \chi_t + M(g_0^2), \tag{4}$$

which eventually becomes dominant in the continuum limit. So in order to extract χ_t from this relation one needs to evaluate $Z(g_0^2)$ and $M(g_0^2)$, which is a hard task.

In order to overcome the problems caused by the above cut-off effects, other methods have been proposed. The so-called geometrical method [3,4] meets the demands that the topological charge on the lattice have the classical correct continuum limit and be an integer for every lattice configuration in a finite volume with periodic boundary conditions. In 4D $SU(N)$ gauge theories this can be achieved by performing an interpolation of the lattice field, from which the principal fiber bundle is reconstructed. Since on the lattice each configuration can be continuously deformed into any other, integer valued geometrical definitions cannot have an analytical functional dependence on the lattice field. Due to their global topological stability, geometrical definitions should not be affected by (perturbative) renormalizations. On the other hand, as a drawback of their non-local nature (leading to non-analyticity), they may be plagued by topological defects on the scale of the lattice spacing, dislocations [5,6], whose non-physical contribution may either survive in the continuum limit (as in the $SU(2)$ gauge theory with Wilson action [6]), or push the scaling region for the topological susceptibility to large-β values.

Field theoretical and geometrical definitions may appear as two quite different approaches to the problem of studying physical topological properties. An interesting connection between them can be conceived by exploiting the following consideration. Noting that geometrical definitions Q_g can be written as a sum of local non-analytical terms, $Q_g = \sum_x q_g(x)$, one can construct sequences of field theoretical (analytical) definitions $q_L^{(k)}(x)$ formally approaching $q_g(x)$ as $k \to \infty$. An example of such sequences has been already given for 2D $\mathbb{C}\mathrm{P}^{N-1}$ models [7].

The construction and analysis of these sequences lead to a new interpretation of the geometrical charges. They can be considered as limits of appropriate sequences of analytical operators, whose perturbative renormalizations formally tend to vanish along the sequences. The asymptotic nature of the perturbative expansion, which emerges from explicit calculations of the renormalizations, does not necessarily lead to well-behaved geometrical limits. It indeed leaves open the possibility of a residual non-perturbative renormalization, which would manifest itself in the contribution of lattice defects (the so-called dislocations) to the geometrical charge. We cannot prove that the expectation values involving the operators of the sequences constructed in this paper converge to the corresponding geometrical limit. However, a numerical analysis seems to show that such a convergence actually occurs at least for sufficiently large β. Within this interpretation one may clarify the meaning of the geometrical charge from a field theoretical point of view, and account for possible discrepancies with other approaches. Moreover, with increasing k, one may hope that $q_L^{(k)}$ and their correlations enjoy a progressive suppression of the renormalization effects, while for not too large k their sensitivity to lattice topological defects is reduced. The convergence of the sequence of topological susceptibilities to the corresponding geometrically defined quantity would imply that, for k sufficiently large, non-perturbative renormalization effects must eventually arise when the geometrical charge is affected by dislocations. We shall exhibit some numerical evidence of this phenomenon.

Our study is mainly done in the context of 2D $\mathbb{C}\mathrm{P}^{N-1}$ models [8,9], which are very useful theoretical laboratories for testing non-perturbative numerical methods conceived to study topological properties. We present an analysis based on large-N and perturbative calculations, and numerical simulations. We then sketch an extension to QCD, where we shall construct a sequence of analytical topological charge density operators approaching Lüscher's geometrical definition [4].

2. Sequences of topological charge density operators in two-dimensional $\mathbb{C}\mathrm{P}^{N-1}$ models

2.1. Topology in two-dimensional $\mathbb{C}\mathrm{P}^{N-1}$ models

Two-dimensional $\mathbb{C}\mathrm{P}^{N-1}$ models are defined by the action

$$S = \frac{N}{2f} \int d^2x\, \overline{D_\mu z} D_\mu z \,, \tag{5}$$

where z is an N-component complex scalar field subject to the constraint $\bar{z}z = 1$, and the covariant derivative $D_\mu = \partial_\mu + iA_\mu$ is defined in terms of the composite field $A_\mu = i\bar{z}\partial_\mu z$. Like QCD, they are asymptotically free and present non-trivial topological structures (instantons, anomalies, θ vacua). A topological charge density operator $q(x)$ can be defined,

$$q(x) = \frac{1}{2\pi}\varepsilon_{\mu\nu}\partial_\mu A_\nu, \tag{6}$$

with the related topological susceptibility

$$\chi_t = \int d^2x \langle q(x) q(0) \rangle. \tag{7}$$

A pleasant feature of these models is the possibility of performing a $1/N$ expansion. A large-N analysis of the topological susceptibility shows that $\chi_t = O(1/N)$. One indeed finds [10]

$$\chi_t \xi_G^2 = \frac{1}{2\pi N}\left(1 - \frac{0.3801}{N}\right) + O\left(\frac{1}{N^3}\right), \tag{8}$$

where ξ_G is the second-moment correlation length.

Most lattice studies of 2D $\mathbb{C}\mathrm{P}^{N-1}$ models have been performed using the following actions:

$$S_L = -N\beta \sum_{n,\mu} |\bar{z}_{n+\mu} z_n|^2, \tag{9}$$

where $\beta = 1/(2f)$, z_n is an N-component complex vector, constrained by the condition $\bar{z}_n z_n = 1$, and

$$S_L^{(g)} = -N\beta \sum_{n,\mu} \left(\bar{z}_{n+\mu} z_n \lambda_{n,\mu} + \bar{z}_n z_{n+\mu} \bar{\lambda}_{n,\mu} - 2\right), \tag{10}$$

where, beside the field z, a $U(1)$ gauge field $\lambda_{n,\mu}$ has been introduced, satisfying $\bar{\lambda}_{n,\mu}\lambda_{n,\mu} = 1$. The latter lattice formulation, $S_L^{(g)}$, turns out to be particularly convenient for a large-N expansion (see Ref. [11] for a review).

The original geometrical construction for the topological charge proposed by Berg and Lüscher [4] is

$$Q_g = \sum_n q_n,$$
$$q_n = \frac{1}{2\pi}\mathrm{Im}\left[\ln \mathrm{Tr}(P_{n+\mu+\nu} P_{n+\mu} P_n) + \ln \mathrm{Tr}(P_{n+\nu} P_{n+\mu+\nu} P_n)\right], \quad \mu \neq \nu, \tag{11}$$

where $P_n = \bar{z}_n \otimes z_n$ and the imaginary part of the logarithm is to be taken in $(-\pi, \pi)$. For the lattice formulation (10) an alternative geometrical definition can be given in terms of the "gauge" field $\lambda_{n,\mu}$. Introducing the plaquette operator

$$u_{\lambda,n} = \lambda_{n,\hat{1}}\, \lambda_{n+\hat{1},\hat{2}} \bar{\lambda}_{n+\hat{2},\hat{1}} \bar{\lambda}_{n,\hat{2}}, \tag{12}$$

one defines $Q_{g,\lambda}$ by

$$Q_{g,\lambda} = \sum_n q_{\lambda,n}, \qquad u_{\lambda,n} = \exp(i2\pi q_{\lambda,n}), \tag{13}$$

where $q_{\lambda,n} \in (-\frac{1}{2}, \frac{1}{2})$. In view of large-$N$ and perturbative calculations, we write the infinite volume limit of $q_{\lambda,n}$ in the form

$$q_{\lambda,n} = \frac{1}{4\pi}\varepsilon_{\mu\nu}(\theta_{n,\mu} + \theta_{n+\mu,\nu} - \theta_{n+\nu,\mu} - \theta_{n,\nu}), \tag{14}$$

where $\theta_{n,\mu}$ is the phase of the field $\lambda_{n,\mu}$, i.e. $\lambda_{n,\mu} \equiv e^{i\theta_{n,\mu}}$.

On a finite volume and for periodic boundary conditions q_n and $q_{\lambda,n}$ generate integer values of the total topological charge for each configuration. They are not analytical functions of the lattice fields z and λ, and fail to be defined on a zero-measure set of "exceptional" configurations. The main feature that makes these functions different from the ones which we term "analytical" is the absence of single valuedness.

Many Monte Carlo studies of the topological properties of 2D $\mathbb{CP}^{N-1}$ models have been presented in the literature. A wide range of values of N has been considered, both small and large in order to test large-N calculations. The present state of art is briefly summarized in the following.

For $N = 2$, that is for the $O(3)$ non-linear σ model, recent simulations using the so-called classical perfect action [12,13] and for a relatively large range of values of β seem to favor what is suggested by semiclassical arguments, that is that χ_t would not be a physical quantity for this model, in that a non-removable ultraviolet divergence affects the instanton size distribution. On the lattice this would manifest itself in the fact that lattice estimators of χ_t do not properly scale approaching the continuum limit. Earlier claims of scaling [14] were probably originated by the relatively small range of values of β considered, and therefore scaling violations could easily be hidden behind the statistical errors.

For $N > 2$ χ_t should be a physical quantity. At $N = 4$ the apparent failure of the geometrical method is probably caused by a late approach to scaling of the geometrical definition (11) when using standard lattice actions such as (9) and (10) [15-17,7]. Evidences of scaling and consistent results have instead been obtained by employing the field theoretical and cooling methods using action (10) and its Symanzik improvement [7], and a geometrical method in the context of the classical perfect action approach [18].

At larger N, $N \gtrsim 10$, the geometrical estimator (11) shows scaling already at reasonable values of the correlation length using both action (10) and its Symanzik improvement [7,19]. The available Monte Carlo data at $N \gtrsim 10$ show that the dimensionless quantity $\chi_t \xi_G^2$ approaches, although slowly, the large-N asymptotic behavior (8), and quantitative agreement (within a few per cent of statistical errors) is found at $N = 21$.

In the following we shall construct sequences of operators approaching the geometrical definitions (11) and (13), and study their main features.

2.2. Sequences of operators approaching geometrical definitions

To begin with, we consider, within the lattice formulation (10), a sequence of analytical operators $q^{(k)}_{\lambda,n}$ approaching the geometrical definition $q_{\lambda,n}$ expressed in terms of $\lambda_{n,\mu}$ fields. By taking appropriate combinations of the plaquette operator $u_{\lambda,n}$ (cf. Eq. (12)), one can define a sequence of local operators $q^{(k)}_{\lambda,n}$ which differ from $q_{\lambda,n}$ by higher and higher-order terms [7]

$$q^{(k)}_{\lambda,n} = \frac{1}{2\pi} \sum_{l=1}^{k} \frac{(-1)^{l+1}}{l} \binom{2k}{k-l} \frac{2}{\binom{2k}{k}} \mathrm{Im}(u_{\lambda,n})^l$$

$$= q_{\lambda,n} - \frac{k!^2}{(2k+1)!}(2\pi)^{2k} q_{\lambda,n}^{2k+1} + O(q_{\lambda,n}^{2k+3}). \tag{15}$$

Similarly, one may define

$$u_{1,n} = \frac{\mathrm{Tr}(P_{n+\hat{1}+\hat{2}}P_{n+\hat{1}}P_n)}{|\mathrm{Tr}(P_{n+\hat{1}+\hat{2}}P_{n+\hat{1}}P_n)|}, \qquad u_{2,n} = \frac{\mathrm{Tr}(P_{n+\hat{2}}P_{n+\hat{1}+\hat{2}}P_n)}{|\mathrm{Tr}(P_{n+\hat{2}}P_{n+\hat{1}+\hat{2}}P_n)|}, \tag{16}$$

and the quantities $q_{j,n}$ $(j = 1,2)$ by

$$u_{j,n} = \exp(i2\pi q_{j,n}) \tag{17}$$

$(q_{j,n} \in (-\frac{1}{2}, \frac{1}{2}))$, so that one can write

$$q_n = q_{1,n} + q_{2,n}. \tag{18}$$

A sequence of operators approaching the geometrical definition (11) can then easily be constructed by

$$q_n^{(k)} = q_{1,n}^{(k)} + q_{2,n}^{(k)},$$

$$q_{j,n}^{(k)} = \frac{1}{2\pi}\sum_{l=1}^{k} \frac{(-1)^{l+1}}{l} \binom{2k}{k-l} \frac{2}{\binom{2k}{k}} \mathrm{Im}(u_{j,n})^l$$

$$= q_{j,n} - \frac{k!^2}{(2k+1)!}(2\pi)^{2k} q_{j,n}^{2k+1} + O(q_{j,n}^{2k+3}). \tag{19}$$

Strictly speaking these functions are not analytical everywhere (they are not polynomials in the fields), but preserve the property of single valuedness.

Once the above definitions are given, one can consider sequences of lattice topological susceptibilities, either in terms of λ or z fields:

$$\chi^{(k)} \equiv \sum_n \langle q_n^{(k)} q_0^{(k)} \rangle = \lim_{p^2 \to 0} \langle \tilde{q}^{(k)}(p) \tilde{q}^{(k)}(-p) \rangle. \tag{20}$$

Under some general assumptions, which essentially amount to assuming the applicability of an OPE to the correlation $q_L(x)q_L(y)$ when $x \to y$, the relation between $\chi^{(k)}$ and the continuum topological susceptibility χ_t is

$$\chi^{(k)}(\beta) = a^2 Z^{(k)}(\beta)^2 \chi_t + M^{(k)}(\beta), \tag{21}$$

where $M^{(k)}$ can be written in terms of the identity I and the trace of the energy-momentum tensor operator $T \equiv \frac{\beta(f)}{2f^2}\overline{D_\mu z} D_\mu z$, plus higher-order terms in a [20],

$$M^{(k)}(\beta) = P^{(k)}(\beta)\,\langle I \rangle + a^2 A^{(k)}(\beta)\,\langle T \rangle\; + O(a^4). \tag{22}$$

The expression of the background term M in terms of the identity and of the trace of the energy-momentum tensor (which are the only RG invariant operators of lower or equal dimensions sharing the same quantum numbers of χ_t) may be obtained by comparing the OPE's of $q_L(x)q_L(y)$ and $q(x)q(y)$, and by taking their difference.

2.3. Large-N and perturbative analysis

The sequence $q^{(k)}_{\lambda,n}$ is particularly suitable for analytical calculations, which will show the main features of such constructions. The reasons that make things easier are the following. In the lattice formulation (10) and in both $1/N$ and perturbative expansion the variable $\theta_{n,\mu}$ (defined by $\lambda_{n,\mu} \equiv e^{i\theta_{n,\mu}}$) is used as a fundamental field, whose propagator can be easily derived [11]. In the infinite volume limit the expression of the geometrical charge density $q_{\lambda,n}$ is linear in terms of $\theta_{n,\mu}$ (cf. Eq. (14)), therefore one can easily obtain the propagator of $q_{\lambda,n}$. The use of the $q_{\lambda,n}$ propagator simplifies considerably the study of the large-N behavior of the renormalization effects in the sequence $q^{(k)}_{\lambda,n}$, in that $q^{(k)}_{\lambda,n}$ can be written as polynomials in $q_{\lambda,n}$ (cf. Eq. (15)). The leading non-trivial orders of the corresponding $Z^{(k)}_\lambda(\beta)$, $P^{(k)}_\lambda(\beta)$, and $A^{(k)}_\lambda(\beta)$ can be obtained by evaluating tadpole-like diagrams, whose lines are the $q_{\lambda,n}$ propagators, and whose vertices are the coefficients of the powers of $q_{\lambda,n}$ in Eq. (15). This occurs also in the evaluation of the leading non-trivial order in standard perturbation theory.

In the large-N limit one can unambiguously identify the terms associated to $Z^{(k)}(\beta)$, $P^{(k)}(\beta)$, and $A^{(k)}(\beta)$. It has been explicitly demonstrated that $Q_{g,\lambda}$ and the corresponding susceptibility χ_λ in the infinite volume limit are not subject to renormalizations in the large-N limit [21], that is

$$\chi_\lambda = \sum_n q_{\lambda,n} q_{\lambda,0} \to a^2 \chi_t \tag{23}$$

in the continuum limit (the same has been shown for the definition (11) too). Using Eqs. (13) and (23), one can deduce the following relationship valid in the lowest non-trivial order of $1/N$ expansion:

$$\chi^{(k)}_\lambda \equiv \sum_n \langle q^{(k)}_{\lambda,n} q^{(k)}_{\lambda,0}\rangle \approx a^2\chi_t \left[1 + 2(2k+1)\alpha_k \langle q^{2k}_{\lambda,0}\rangle\right] + \alpha_k^2 \sum_n \langle q^{2k+1}_{\lambda,n} q^{2k+1}_{\lambda,0}\rangle\,, \tag{24}$$

where $\alpha_k = -(2\pi)^{2k} k!^2/(2k+1)!$.

An asymptotic expansion in powers of the large-N mass [11], m_0, allows one to separate the mixing with the identity from the term of dimension two (i.e. proportional to a^2) in Eq. (21), which contains the physical signal. This is achieved by expanding the $q_{\lambda,n}$ propagator in powers of m_0,

$$\langle \widetilde{q}_\lambda(p)\widetilde{q}_\lambda(-p)\rangle = D_0 + m_0^2 D_1 + O(m_0^4). \tag{25}$$

Using results of Ref. [11], the calculation of the functions D_0 and D_1 is quite straightforward. Then by comparing Eq. (24) with Eqs. (21) and (22), one can write down explicit analytical expressions for $P^{(k)}_\lambda(\beta)$, $Z^{(k)}_\lambda(\beta)$, and $A^{(k)}_\lambda(\beta)$ in the lowest non-trivial order of $1/N$ [22]. In the following we shall discuss some of their properties. We shall not report their complete expressions because they would not be very illuminating.

The zero-dimensional mixing with the identity, which dominates the Monte Carlo signal in the continuum limit, turns out to be

$$P_\lambda^{(k)}(\beta) = O\left(\frac{1}{N^{2k+1}}\right). \tag{26}$$

The renormalization functions corresponding to the terms of dimension two turn out to be

$$Z_\lambda^{(k)}(\beta) = 1 + O\left(\frac{1}{N^k}\right), \tag{27}$$

$$A_\lambda^{(k)}(\beta) = O\left(\frac{1}{N^{2k+1}}\right). \tag{28}$$

In order to derive the lowest non-trivial order contribution to $A_\lambda^{(k)}(\beta)$, we have used the fact that in the $1/N$ expansion $\langle T\rangle = O(1)$, indeed one finds [11]

$$\langle T\rangle\, \xi_G^2 = \frac{1}{3\pi} + O\left(\frac{1}{N}\right). \tag{29}$$

In the $\beta \to \infty$ limit the large-N expressions of $P_\lambda^{(k)}(\beta)$, $Z_\lambda^{(k)}(\beta)$, and $A_\lambda^{(k)}(\beta)$ reduce to formulas that could have been obtained by standard weak-coupling perturbation theory. The correspondence between large-N expansion and standard perturbation theory is obvious for $Z^{(k)}(\beta)$ and $P^{(k)}(\beta)$: it suffices to recognize that for $m_0 = 0$ and $\beta \to \infty$ the large-N θ-propagator reduces to the corresponding perturbative propagator. This correspondence has been explicitly verified also for $A^{(k)}(\beta)$. One obtains

$$Z^{(k)}(\beta) = 1 - k!\left(\frac{1}{\beta N}\right)^k + O\left[\left(\frac{1}{\beta N}\right)^{k+1}\right], \tag{30}$$

and for large k

$$P^{(k)}(\beta) \simeq \frac{k!^4(4k+2)!}{(2k+1)!^3}\left(\frac{1}{\beta N}\right)^{2k+1} + O\left[\left(\frac{1}{\beta N}\right)^{2k+3}\right] \sim (2k)!\left(\frac{1}{\beta N}\right)^{2k+1}, \tag{31}$$

$$A^{(k)}(\beta) \sim (2k)!\left(\frac{1}{\beta N}\right)^{2k+1}. \tag{32}$$

Eqs. (30)-(32) show the mechanism of systematic improvement of the local operators $q_\lambda^{(k)}$. As $k \to \infty$, $q_\lambda^{(k)} \to q_\lambda$ and the lowest-order renormalizations are proportional to higher and higher powers of $1/\beta$. However, the coefficients of the leading non-trivial term grow so fast with k that the convergence to zero of $Z^{(k)}(\beta) - 1$, $P^{(k)}(\beta)$ and $A^{(k)}(\beta)$ cannot be uniform for $\beta \to \infty$. This fact leaves open the possibility that for fixed β some non-perturbative renormalization effects may eventually survive as $k \to \infty$, i.e. as the sequence approaches the geometrical definition.

Inspired by this phenomenon, we suggest the following general picture. The geometrical charge can be interpreted as the limit of a sequence of field theoretical (analytical) operators. As far as (at a given β) the renormalization effects tend to vanish along the sequence, the geometrical object provides a well-behaved lattice estimator of the topological charge. If on the contrary the renormalization effects do not disappear for

$k \to \infty$, some pathology should arise in the geometrical method, such as the contribution of short-distance topological defects. The asymptotic nature of the perturbative expansion, which manifests itself in the growing of the corresponding coefficients, leaves open the possibility of a background term behaving, for example, as $\sim \exp(-c\beta)$, which does not get suppressed in the limit $k \to \infty$. According to the value of c, either this term is suppressed in the continuum limit, or it survives and spoils the expected asymptotic behavior of χ_t, which should behave as a quantity of dimension d. The absence of non-perturbative effects at finite β would be guaranteed by a convergent perturbative expansion of the renormalizations. A good continuum limit of the geometrical definition would be assured by a perturbative expansion in which the limit $k \to \infty$ commutes with the continuum limit $\beta \to \infty$.

The calculation of the renormalizations is more involved for the sequence expressed in terms of the z fields, but the conclusions are qualitatively the same. In particular, since the expansion of q_n in terms of perturbative fields (for example in Valent's parametrization [23]) starts with a bilinear term, it is easy to see from Eq. (15) that $Z^{(k)}(\beta) - 1$ and $P^{(k)}(\beta)$ will get the leading contribution from diagrams with $2k$ and $2k+2$ loops, respectively. Therefore,

$$Z^{(k)}(\beta) = 1 + O\left[\left(\frac{1}{N\beta}\right)^{2k}\right], \tag{33}$$

$$P^{(k)}(\beta) = O\left[\left(\frac{1}{N\beta}\right)^{2k+2}\right]. \tag{34}$$

These results hold for both lattice actions (9) and (10).

2.4. Numerical analysis by heating method

Since estimators involving the field $\lambda_{n,\mu}$ are subject to large fluctuations in Monte Carlo simulations, in our numerical analysis we shall consider the sequence approaching the geometrical definition in terms of z fields only, i.e. $q_n^{(k)}$ defined in Eq. (19). We present a numerical investigation of the corresponding renormalization effects by using the so-called heating method [24,25] (see Ref. [7] for an implementation of this method to 2D $\mathbb{C}\mathrm{P}^{N-1}$ models). The study of the renormalization effects by heating method relies on the possibility of somehow separating the various contributions in Eq. (21) in off-equilibrium simulations. This is made possible when they are originated by lattice modes which behave differently under local thermalization (large vs. small scale modes, Gaussian vs. topological modes). Assuming such a distinction of lattice modes, estimates of the multiplicative renormalization $Z^{(k)}$ are obtained by measuring $Q^{(k)} = \sum_n q_n^{(k)}$ on ensembles of configurations constructed by heating an instanton-like configuration (carrying a definite topological charge $Q^{(k)}$) for the same number n_u of local updating steps. The plateaus showed after a few heating steps by data plotted as a function of n_u give the desired estimates of $Z^{(k)}$. Similarly, the background signal $M^{(k)}$ can be estimated by measuring $\chi^{(k)}$ on ensembles of configurations constructed by heating the flat configuration. Again, the plateaus of data as function of n_u, if observed, should provide estimates of $M^{(k)}$ [25,26].

We performed our simulations on a 100^2 lattice. This lattice size should be sufficiently large in order to estimate Z and M even at large β, in that they are expected to be short ranged (scaling with a), and therefore have very small finite size effects. On the other hand, in order to determine χ_t, one must take lattices with $L \gg \xi$. In the following we describe the main results we have obtained for $N = 4$ and $N = 10$ using the lattice action $S_L^{(g)}$ (cf. Eq. (10)).

For $\beta \simeq 1$ (where the correlation length is sufficiently large to expect scaling to hold [7]), the multiplicative renormalization $Z^{(k)}$ turns out to be very close to one for small values of k already. For example for $N = 4$ and at $\beta = 1.25$ (which corresponds to $\xi_G \simeq 28$) we found $Z^{(1)} \simeq 0.96$, $Z^{(2)} \simeq 0.98$, $Z^{(3)} \simeq 0.99, \ldots$, suggesting a smooth limit to one for $k \to \infty$. For comparison we mention that the polynomial topological charge density definition considered in Ref. [7],

$$q_n^{(p)} = -\frac{i}{2\pi} \sum_{\mu\nu} \epsilon_{\mu\nu} \mathrm{Tr}\left[P_n \Delta_\mu P_n \Delta_\nu P_n\right] \tag{35}$$

(where $\Delta_\mu P(x) = \frac{1}{2}[P_{n+\mu} - P_{n-\mu}]$), has $Z^{(p)} \simeq 0.42$ at this value of β. At larger N, $Z^{(k)}$ get closer to one, as expected from their dependence on N. For example, at $N = 10$ and $\beta = 1.0$ (corresponding to $\xi_G \simeq 17$) we found $Z^{(1)} \simeq 0.985$, $Z^{(2)} \simeq 1.000$, $Z^{(3)} \simeq 1.0000, \ldots$, and $Z^{(p)} \simeq 0.35$.

When using the action (10), at $N = 4$ and $\beta \simeq 1.25$ the geometrical definition (11) is affected by spurious contributions from short-ranged lattice structures, which turn out not to be negligible in order to determine χ_t from $\chi_g = \frac{1}{V}\langle Q_g^2\rangle$ [7]. This fact emerges clearly also by observing the behavior of χ_g in the heating of the flat configuration, in that the initial global geometrical charge (which is zero) appears to be soon modified by the local thermalization process even if the correlation length is rather large, as it occurs at $\beta \simeq 1.25$. In the same heating process, data of $\chi^{(k)}$ appear strongly correlated to those of χ_g, indicating that the above-mentioned short-ranged configurations contribute somehow to $\chi^{(k)}$ too (even for small k). In the analysis of $\chi^{(k)}$ such spurious contributions may be interpreted as renormalization effects, but at these values of N and β we were not able to estimate them by using the heating method. It is possible that in this case the required sharp distinction of the lattice modes contributing to the different terms in Eq. (21) does not occur, or it is not sufficient to make the heating method work.

In a sense, the so-called lattice defect contributions to the geometrical definition χ_g may be seen as the limit $k \to \infty$ of the mixings in $\chi^{(k)}$, which does not seem to vanish at $N = 4$ and values of β corresponding to $\xi_G \lesssim 10^2$. Their effect probably disappears in the large-β limit. Indeed at $\beta = 1.6$, where the correlation length should be about one order of magnitude larger than at $\beta = 1.25$, we found no trace of short-ranged topological defects in the heating procedure. We got the following estimates of the mixing contribution $M^{(k)}$ to $\chi^{(k)}$: $M^{(1)} \simeq 3 \times 10^{-7}$, $M^{(2)} \lesssim 5 \times 10^{-8}$, $M^{(3)} \lesssim$

$10^{-8}, \ldots$, while for the lattice susceptibility associated with the operator (35) we found $M^{(p)} \simeq 7 \times 10^{-6}$. $\beta \gtrsim 1.6$, and therefore $\xi \gtrsim 10^2$, may then be sufficiently large for the geometrical definition (11) to be effective in the determination of χ_t. We also quote some data at $\beta = 2$ where the correlation length should be about two orders of magnitude larger than at $\beta \simeq 1.25$, we found $M^{(1)} \simeq 2.5 \times 10^{-8}$, $M^{(2)} \lesssim 2 \times 10^{-10}$, $M^{(3)} \lesssim 10^{-11}, \ldots$, and $M^{(p)} \simeq 2.9 \times 10^{-6}$. Notice that in order to determine χ_t at $\beta = 1.6$ one would need to perform simulations on a very large lattice with $L \gg \xi$, and therefore $L > 10^3$ in order to avoid sizeable finite size effects. These numerical results are consistent with the picture outlined in the previous subsection.

Of course the onset of scaling for χ_g depends on the lattice action. In this respect actions better than (10) may exist. A substantial improvement with respect to action (10) has been observed when using its Symanzik tree improvement [7].

As suggested by Eq. (34), things get improved with increasing N. For $N \gtrsim 10$ (using the action (10)) the geometrical definition (11) seems to provide a good estimator of χ_t already at reasonable values of the correlation length [7]. For example at $N = 10$, $\chi_g \xi_G^2$ shows good scaling for $\xi_G \gtrsim 10$ [7], and for shorter and shorter ξ_G at larger values of N. At $N = 10$ and $\beta = 1.0$, the heating procedure provided the following estimates of the background signal $M^{(k)}$ in $\chi^{(k)}$: $M^{(1)} \simeq 0.5 \times 10^{-6}$, $M^{(2)} \lesssim 0.5 \times 10^{-7}$, $M^{(3)} \lesssim 0.5 \times 10^{-8}$, $M^{(4)} \lesssim 10^{-9} \ldots$, and $M^{(p)} \simeq 0.7 \times 10^{-5}$ for the operator (35). The mixings in Eq. (21) rapidly disappear with increasing k. The sequence of $\chi^{(k)}$ approaches χ_g which in this case appears to be free of lattice artifact contributions. Taking into account that for $N = 10$ we have $\chi_t \xi_G^2 \simeq 0.017$ [7], at $\beta = 1.0$ renormalization effects turn out to be very small and negligible for $k = 1$ already (in the evaluation of $a^2 \chi_t$ renormalizations for $k = 1$ lead to corrections of about one per cent).

From the above discussion it seems that, at least when using the action (10), little practical improvement is achieved by the use of the operators defined by the sequences $q_n^{(k)}$. Indeed at low N (and at least for $\beta \simeq 1$) they appear to be sensitive to short-ranged lattice defects, whose contributions to renormalization effects seem as difficult to evaluate as for the corresponding geometrical definition (the heating method apparently fails in these cases). The use of standard polynomial or smeared field theoretical operators (smeared operators similar to those defined in Ref. [27] and with the same features can be easily constructed for $\mathbb{C}\mathrm{P}^{N-1}$ models) and the cooling method [28] appears more convincing when this phenomenon occurs. When the geometrical definition provides a good estimator of topological activity, as at large N, the behavior of $q^{(k)}$ is that formally predicted by perturbation theory. But in this case it would be more convenient to use the corresponding geometrical definition, whose use is further justified by our analysis. However, when the renormalization effects do not tend to vanish (at fixed β) along the sequence, we cannot take for granted that the physical predictions based on the use of the corresponding geometrical definition will be correct.

In order to construct improved field theoretical operators one may put together both the idea of smearing the operators [27] and that of defining sequences approaching geometrical definitions. This may be achieved by constructing sequences of operators in terms of smeared fields, instead of lagrangian fields. This should provide optimal field theoretical operators with a more effective suppression of the renormalization effects, and corresponding geometrical limits probably less sensitive to unphysical short-distance lattice topological defects. We mention that for 4D $SU(2)$ gauge theory a geometrical charge defined on appropriate blocked variables has been tested [29]. Unlike the original geometrical charges, which turned out to be affected by dislocations, the blocked definition produced a topological susceptibility consistent with that obtained by alternative cooling and field theoretical methods.

3. Construction of the sequence for $SU(N)$ Yang–Mills theories

We sketch an extension of the above study to $SU(N)$ Yang-Mills theories in four dimensions. Among the different geometrical definitions of lattice topological charge available in the literature, we consider that one proposed by Lüscher in Ref. [4]. In the following we will heavily refer to this work. Lüscher's geometrical definition can be written as a sum of local terms $Q_g = \sum_n q_n$, where q_n is a gauge invariant function of the link variables. We show that it is possible to define a sequence of operators $q_n^{(k)}$ sharing the following properties.

(i) For each k, $q_n^{(k)}$ is a gauge invariant, polynomial function of the link variables of the single elementary hypercube $c(n)$, possessing the appropriate (classical) continuum limit;

(ii) The operators $q_n^{(k)}$ tend, at least formally, to q_n for $k \to \infty$.

q_n is obtained by the lattice fields of the hypercube $c(n)$ through a complicated interpolation procedure. An essential ingredient is the raising of link variables to fractional powers (this is the non-analytical step in the definition), according to the following prescription. For $u \in SU(N)$, setting

$$u = \exp(ig\omega_a\lambda_a), \tag{36}$$

one may define the fractional power u^y, $0 \leqslant y \leqslant 1$, as

$$u^y = \exp(iyg\omega_a\lambda_a) \tag{37}$$

(for convenience, we explicitly introduced the bare coupling constant g, in terms of which the perturbative weak-coupling expansion is defined).

We construct a sequence of gauge invariant analytical operators $q_n^{(k)}$, which differ from the geometrical definition q_n by $O(g^{k+1})$, i.e.

$$q_n^{(k)} = q_n + O\left(g^{k+1}\right). \tag{38}$$

To this purpose, we consider a polynomial approximation $u_{[j]}(y)$ of u^y, of degree j in u and $u^\dagger$, so that

$$u^y = u_{[j]}(y) + O(g^{2j+1}). \tag{39}$$

The polynomial functions $u_{[j]}(y)$ can be easily constructed. We then make the appropriate substitutions $u^y \to u_{[j]}(y)$ in the expression of Lüscher's topological charge density

q_n, so as to obtain $q_n^{(k)}$ as an approximation $O(g^{k+1})$ of q_n that contains polynomials of minimum degree in the link variables.

The lattice susceptibilities $\chi^{(k)} = \sum_n \langle q_n^{(k)} q_0^{(k)} \rangle$ should be related to the continuum topological susceptibility χ_t by

$$\chi^{(k)}(\beta) = a^4 Z^{(k)}(\beta)^2 \chi_t + M^{(k)}(\beta), \tag{40}$$

where

$$M^{(k)}(\beta) = P^{(k)}(\beta)\, \langle I \rangle + a^4 A^{(k)}(\beta)\, \langle T \rangle \; + O(a^6). \tag{41}$$

Assuming (perturbative) non-renormalization for the geometrical definition q_n, and using Eq. (38) one can infer that ($\beta = 2N/g^2$)

$$Z^{(k)}(\beta) = 1 + O\left(\frac{1}{\beta^l}\right), \tag{42}$$

$$P^{(k)}(\beta) = O\left(\frac{1}{\beta^{l+2}}\right), \tag{43}$$

where

$$\begin{aligned} l &= \frac{k}{2} \qquad \text{for even } k, \\ l &= \frac{k+1}{2} \qquad \text{for odd } k. \end{aligned} \tag{44}$$

An analysis of the behavior of the coefficients $z^{(k)}$ and $p^{(k)}$ of the leading non-trivial order in $Z^{(k)}$ and $P^{(k)}$ can be more easily carried out for even k, for which all the corresponding diagrams are substantially tadpoles. A rough estimate of the behavior of $p^{(k)}$ and $z^{(k)}$ may be obtained by counting all the contractions to form $k/2$ tadpoles,

$$p^{(k)} \sim z^{(k)} \sim \frac{k!}{(k/2)!}. \tag{45}$$

Here the dependence on N has been overlooked, in that all contractions have been considered as giving the same contribution. This is true only in the case of commuting generators, as in the case of $U(1)$ gauge theory. Nevertheless, Eq. (45) should give an idea of the behavior at large k, at least for not too large N. On the other hand, at large N, contractions of non-sequential generators in the traces are suppressed by powers of $1/N$, so that the contractions contributing at $N = \infty$ are considerably reduced, leading probably to $p^{(k)} \sim z^{(k)} \sim O(1)$.

Then, as already observed for the sequences constructed within the $\mathbb{C}P^{N-1}$ models, the lowest-order renormalizations are proportional to higher and higher powers of $1/\beta$. However, at finite N the corresponding coefficients of the leading non-trivial order grow so fast with k that the convergence to zero of the renormalization functions cannot be uniform for $\beta \to \infty$. Again, with increasing N, renormalization effects should be further suppressed in the sequence, suggesting that at least at large N the geometrical charge should be free from dislocations.

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