QCD topology using scale controlled cooling:
Densities and cooling invariant observables

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ABSTRACT: We aim at reducing the uncertainties inherent in the analysis of the topological structure by using scale controlled smoothing and observables independent on the “microscopic” description of the instanton ensemble.

Investigating the role of instantons in the QCD vacuum by lattice simulations is a challenging problem. Instantons are involved in the $U_A(1)$ symmetry breaking (cf the Witten - Veneziano formula which relates quenched topological susceptibility and $\eta'$ mass) and in chiral symmetry breaking (via zero modes of the Dirac operator), and they lead to dynamical effects at intermediate distances. Global properties like susceptibility and charge distributions afford direct tests, while the features of the local structure (ensemble, size and distance distributions) are ingredients for dynamical models [1]. To recall, an $\mathbb{R}^4$ (anti-)instanton $(A)I$ of size $\rho$ located at $x = 0$ has charge $(q)$ and action $(s)$ densities:

$$q(x) = \frac{1}{8\pi^2} F^* F = \frac{6Q}{\pi^2\rho^4} \left[1 + \sum_{\mu=1}^{4} \left(\frac{x\mu}{\rho}\right)^2\right]^{-4}$$

$$Q = \int d^4x \, q(x), \quad S = \int d^4x \, s(x) = |Q| S_0$$

$$s(x) = S_0 |q(x)|, \quad S_0 = 8\pi^2, \quad Q = \pm \text{integer}.$$  \hfill (1)

“Superpositions” of $N$ I’s or A’s lead to higher minima of the action: $S = NS_0$. However pairs I-A are not minima and, e.g., under unrestricted cooling they decay, the sooner the smaller their action $S^{IA} = 2S_0 - S^{IA}_{int} < S_0$ is, where $S^{IA}_{int}$ depends in particular on the “overlap” $\omega = (\rho + \rho_A)/d_{IA}$, $d_{IA}$ being the I - A distance.

In analyzing the topology by lattice methods we need to deal with the roughness of the Monte Carlo configurations at short scales and to identify the physically relevant topological structure. UV lattice artifacts (dislocations) and close I-A pairs, indistinguishable from short range density fluctuations, have small action and can be easily produced. To smooth out in a controlled way high frequency fluctuations in Monte Carlo configurations the method of Restricted Improved Cooling (RIC) has been developed in [2] as a gauge invariant low pass filter. RIC introduces a parameter directly related to a physical scale above which fluctuations will be preserved. Since it uses an “improved” action RIC has as fixed point non-trivial classical configurations. But since it preserves all structures above the chosen scale it also retains, e.g., I-A pairs with overlap smaller than a threshold depending on the smoothing scale.

The identification of the uncovered topological structure poses special problems. Usually a “microscopic” description in terms of I’s and A’s is attempted. This, however, becomes increasingly ill defined at small scales, particularly if close pairs abound. Therefore it is interesting to avoid the necessity of such a description and ob-
tain the phenomenological parameters appearing in the instanton models from observables which can be directly measured on the lattice.

We here suggest to study properties of instantons in lattice simulations using observables objectively defined in continuum QCD. Rather than investigating instantons microscopically by inspecting lattice field configurations, we shall consider "macroscopic" observables which in a pure instanton vacuum can directly be related to properties of the instanton ensemble. One such class of quantities are ratios of VEV's of chirally odd operators, which are purely non-perturbative quantities, and (at least in a dilute instanton vacuum) are independent on the instanton density and can directly be related to moments of the instanton size distribution. Assuming the latter to be a well defined property of the topological structure, we expect these ratios to remain approximately constant under cooling, at least after achieving a certain, minimal degree of smoothing. Using RIC we can rephrase this question in terms of the physical scale of the relevant topological fluctuations.

Scale Controlled Smoothing. Cooling [3] is an iterative, local minimization of the action, which proceeds sweep-wise and can be defined to converge onto (non-trivial) classical configurations. It acts as a diffusion process with the length scale of smoothing growing like the square root of the number of iterations [4].

Restricted Improved Cooling (RIC) [2] is a scale controlled smoothing procedure involving two ingredients:

a) - Improved minimization action with practically scale invariant instanton solutions, and

b) - Restriction of cooling to allow a certain amount of (Euclidean) "energy" above the minimum, homogeneously distributed over the lattice.

Our improved action [2], [5] is correct to order $O(a^6)$ and is completely flat for instanton sizes larger than $\rho_0 \sim 2.3a$, below which it drops - see Fig. 1. It then follows from a) that:

- Below the "dislocation threshold" $\rho_0$ short range topological structure is eliminated. Note that $\rho_0 \to 0$ in continuum.
- Above $\rho_0$, instantons are stable to cooling.
- The correspondingly improved charge density leads to a charge approaching an integer already after a few cooling sweeps and stable thereafter.

Figure 1. Improved (5Li) and Wilson action vs instanton size given in lattice units - these are SU(2) results, but they are representative also for SU(3).

The restriction b) is introduced as the following modification of the local updating rule for a link:

$$U \to V \quad \text{iff} \quad \Delta \equiv \text{Tr}(WW^\dagger - (UW^\dagger)^2) \geq \delta^2$$

where $W$ is the staple connected to $U$ and $V$ the group projection of $W$ (for SU(2) $V = W/||W||$). It naturally leads to gradual saturation and eventual stop of cooling after a number of sweeps depending on $\delta$. RIC thus acts as a frequency filter for the field fluctuations. Since $\Delta$ is the square of the lattice equations of motion it has a continuum limit and therefore the cooling parameter $\delta$ can be related to a physical scale.
Table 1
RIC results for SU(3).

| \(\delta\) (fm\(^{-3}\)) | \(r_c\) (fm) | \(\chi^{1/4}\) (MeV) | Sat. sw. | Plaq. | \(|P|\) |
|---------------------------|-----------|----------------|--------|------|-------|
| no cooling                | 144(2)    | 0              | .5754  | .01  |
| 411.3                     | .27(5)    | 176(3)         | 8      | .9846| .04   |
| 290.8                     | .34(6)    | 178(3)         | 16     | .9888| .04   |
| 145.4                     | .41(7)    | 181(3)         | 30     | .9939| .05   |
| 51.41                     | .67(9)    | 183(3)         | 67     | .9976| .07   |

Figure 2. Mass gap \(M(t) = \sigma L\) vs lattice distance \(t\) (\(L\): spatial lattice size). The horizontal band indicates standard results for this lattice.

For this we calculate the string tension \(\sigma\) from correlations of spatial Polyakov loops at separation \(t\) in time, measured on configurations RIC-cooled with \(\delta\). We determine \(r_c(\delta)\) as the the minimal distance \(t\) at which the string tension is recovered, taking the first cooling curve as reference. See Fig. 2; for details and for SU(2) results see [2]. The data presented here concern SU(3) and have been obtained on a \(12^4\), pbc lattice at \(\beta = 5.85\) (\(a = 0.135\) fm), using 900 configurations separated by 600 sweeps (after 50000 thermalization sweeps). The line in Fig. 3 corresponds to \(r_c(\delta) \approx 2.3 \delta^{-1/3}\).

The restriction b) does not affect significantly the behavior of single instantons under RIC but does affect the behavior of I-A pairs. There is a well defined relation between \(\Delta\) and the I-A “interaction” \(S_{\text{int}}^{IA} = 16\pi^2 - S^{IA}\) [2]. As a result RIC with given \(\delta\) preserves pairs depending on their interaction, hence on their overlap. Generally, physics on scales larger than \(r_c\) is expected to remain unaffected by RIC. How RIC affects small and large scales is also illustrated by the values of the Plaquette and Polyakov loop (\(|P|\)) in Table 1. The distribution of the latter after cooling stays compatible with confinement (see Fig. 4).

An extended topology analysis for SU(2) using RIC has been provided in [2], here we add some further results for SU(3).

The topological charge distribution is Gaussian and is stable under cooling - see Fig. 5.
Table 1 we give the topological susceptibility of SU(3) for various $\delta$ (the phenomenological expectation is $\chi^{1/4} \sim 180$ MeV). On Fig. 6 we plot the SU(3) density correlations $\langle q(x) q(0) \rangle$ at various values of $\delta$. Due to the improved charge density even non-cooled data can be obtained, they show however strong UV renormalization effects. Notice that $\langle q(x) q(0) \rangle < 0$ for disjoint supports [7]. With progressing smoothing this effect disappears indicating gradual loss of support properties.

From the RIC analysis of SU(2) [2] it appeared that one can speak of a typical size, but that a “microscopic” description of the instanton ensemble is problematic since topological excitations cannot be separated at small scales from short range fluctuations. We observed at small $r_c$ a strongly growing $I(A)$ density, with more and more peaks of alternating charge and increasingly large overlap showing up at distances in the $r_c$ range. This may also affect the size determination and explain the differences in the detail of the size distribution found in the literature [6]. To avoid the uncertainties introduced by this situation in the determination of the instanton size we look for an independent determination of the typical size using “macroscopic” observables.

“Macroscopic” observables for topology. The relevance of instantons to chiral symmetry breaking is due to the fact that a single $I(A)$ induces a localized (i.e., normalizable) zero mode of the Dirac operator of definite chirality:

$$i \nabla (A_{I(A)}) \Phi_{\pm}(x) = 0, \quad \gamma_5 \Phi_{\pm}(x) = \pm \Phi_{\pm}(x).$$

(3)

Instanton models usually proceed from a simple picture of the Yang–Mills vacuum as a dilute “medium” of $I$‘s and $A$‘s:

$$\bar{\rho}^4 \Omega \ll 1, \quad \text{or} \quad \bar{\rho}/\bar{R} \ll 1$$

(4)

where $\bar{\rho}$ is the average size, $\bar{R}$ the average distance and $\Omega = N/V$ the density of the instantons. The ratio $\bar{\rho}/\bar{R}$ can be used as a small parameter to classify non-perturbative effects generated by the medium of instantons [9], [10]. In this picture chiral symmetry breaking can be understood as a collective effect involving all instantons in the ensemble [11], [12] (this can be seen as a consequence of the cumulative effect of the chirally
odd ‘t Hooft vertices of individual instantons, result-
ing in the appearance of a dynamical quark mass). The chiral order parameter is then [12]:
\[
\langle \bar{\psi} \psi \rangle \sim \bar{\rho}^{-3} (\bar{\rho}^4 \Omega)^{1/2} \sim \bar{\rho}^{-3} (\bar{\rho}/\bar{R})^2
\] (5)

Generally, the VEV’s of any chirally odd operator can serve as order parameter for chiral symmetry breaking. Since they are purely non-perturbative quantities which acquire a non-zero value only because of the spontaneous breaking of chiral symmetry they provide good probes of the instanton effects. So, for instance, in an instanton medium we have:
\[
\langle \bar{\psi} \mathcal{F}[F] \Gamma \psi \rangle \sim \bar{\rho}^{-d} (\bar{\rho}^4 \Omega)^{1/2} \sim \bar{\rho}^{-d} (\bar{\rho}/\bar{R})^2
\] (6)

where \( \mathcal{F}[F] \) is a function of the gauge fields, \( \Gamma = 1, \gamma_5, \sigma_{\mu\nu} \) a chirally odd Dirac matrix and \( d \) is the mass dimension of the operator. Note that while these VEV’s depend differently on the instanton size, they all show the same dependence on the instanton density as the usual quark condensate. Therefore in ratios of such VEV’s the dependence on the instanton density cancels:
\[
X \equiv \frac{\langle \bar{\psi} \mathcal{F}[F] \Gamma \psi \rangle}{\langle \bar{\psi} \psi \rangle} \sim \bar{\rho}^{-d+3}
\] (7)

For example one finds in the large-\( N_c \) limit, where all instantons are of size \( \rho = \bar{\rho} \), [13]:
\[
\langle \bar{\psi} F_{\mu\nu} \sigma_{\mu\nu} \psi \rangle / \langle \bar{\psi} \psi \rangle = 4 \bar{\rho}^{-2}
\] (8)

In the instanton vacuum such ratios can thus directly be related to properties of the instanton size distribution, with no reference to the density. (A non-zero density is needed only for numerator and denominator to be non-zero individually.) Therefore we expect quantities of the type (7) to be approximately “invariant” under cooling.

We plan to measure the cooling behavior of ratios of the type (7) using RIC. Since we can control the smoothing scale we can test the dependence of our derivation on the assumption of diluteness by observing the saturation of the ratios, and then obtain an estimation of the typical instanton size independently on a microscopic description of the ensemble. (A lattice simulation for (8) has been performed with limited statistics in [14].)

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REFERENCES