Spatial Correlation of the Topological Charge in Pure SU(3) Gauge Theory and in QCD

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Abstract

We study the spatial correlator of the topological charge density operator in pure SU(3) gauge theory and in two flavor QCD. We show that the data for distances up to about 1 fm is consistent with a vacuum consisting of individual instantons and closely bound pairs. The percentage of paired objects is twice as large on the dynamical configurations than on the pure gauge ones, implying increased molecule formations due to fermionic interactions.
Our understanding of the QCD vacuum has increased considerably in the last few years. Lattice calculations using different algorithms have consistent predictions for the topological susceptibility in pure gauge QCD \([1]\), and the first results in dynamical systems have been published recently \([2]\,[3]\). Results concerning the density and size distribution of instantons are less consistent, but there is increasing evidence that the pure gauge QCD vacuum is filled with instantons of average radius \(\sim 0.3 \text{ fm}\), with a density of about \(1 \text{ fm}^{-4}\) \([4]\,[5]\,[6]\).

Instanton Liquid Models (ILM) describe the phenomenological properties of instantons in the QCD vacuum closely \([6]\). Even the Random ILM provides an accurate description of the pure gauge instanton vacuum indicating that the gauge interaction and consequently the spatial correlation between instantons is small. The situation is quite different for systems with dynamical light quarks. In the zero quark mass limit the topological susceptibility is zero and there are no unpaired topological objects in the vacuum. Yet one expects instantons to be present. Chiral symmetry is spontaneously broken, \(\langle \bar{\psi}\psi \rangle \neq 0\) in the zero quark mass limit. According to the Casher-Banks formula, the chiral condensate (summed over quark flavors) is \([7]\)

\[
\langle \bar{\psi}\psi \rangle = \pi \rho(0),
\]

implying that \(\rho(0)\), the density of the eigenmodes of the Dirac operator at eigenvalue zero, is finite. Since instantons are the leading candidates to create near-zero eigenmodes of the Dirac operator, the vacuum is likely to be filled with instantons. Fermions create an attractive force between oppositely charged instantons. It is therefore natural to expect that the instantons of the zero quark mass vacuum form instanton-antiinstanton pairs, molecules. In the case of finite quark mass the topological susceptibility does not vanish but it is proportional to the quark mass \([8]\)

\[
\chi = \langle \bar{\psi}\psi \rangle > m_q n_f = \frac{f_\pi^2 m_q^2}{4n_f} + O(m_q^4),
\]

where \(f_\pi = 132\text{MeV}\) is the pion decay constant. The vacuum in this case has unpaired objects in addition to the molecules.

Even though the above picture describing spatial correlation between instantons sounds very natural, no evidence from lattice calculations has supported it so far. The culprit is most likely the lattice approach. In order to reveal individual topological objects, vacuum fluctuations have to be removed, the vacuum has to be smoothed. Almost all smoothing procedures distort the vacuum, they destroy molecules especially easily. In addition the smoothed configurations are frequently analyzed by a pattern-recognition algorithm to identify individual instantons. Most algorithms have a built-in cut-off which limits the nearest objects it can resolve, further limiting the possibility of finding closely bound pairs.
In this paper we study the topological density correlator

\[ C(r) = \frac{1}{V} \int d^4x q(x)q(x+z), \quad r = |z|, \]  

(3)

where \( q(x) \) is the topological charge density measured using the improved charge operator of Ref. [5],[9]. We measured \( C(r) \) on two sets of configurations with similar lattice spacings. The first set is a pure gauge ensemble of \( 16^3 \times 32 \) configurations at \( \beta = 6.0 \), the is a dynamical ensemble of the same size, generated with two flavors of staggered fermions at \( \beta = 5.7 \) with \( ma = 0.01 \). The lattice spacing of the pure gauge ensemble is \( a \approx 0.095 \) fm, of the dynamical ensemble is \( a \approx 0.11 \) fm. Both ensembles are from the NERSC QCD archive[10]. For this study 170 of the pure gauge configurations [11] and 83 of the dynamical configurations [12] (the entire available data set) were used.

The gauge configurations have to be smoothed to reveal the topological content. Here we used APE smearing [13] with parameter \( c = 0.45 \) as the properties of this smoothing has been extensively tested in Refs. [5],[9]. \( N \) steps of APE smearing smooths a configuration to distance \( d_s \sim a\sqrt{Nc/3} \) [14] but preserves the properties of the vacuum at longer distances. First we will compare the topological density correlators on the pure gauge and dynamical configurations after the same number, \( N = 30 \), APE steps. Since the lattice spacings of the two ensembles are approximately the same, that corresponds to about the same physical smoothing and even observables that change with smoothing can be compared. Afterwards we will vary \( N \) between 10 and 60 to justify the above assumption.

First we consider the topological susceptibility. The susceptibility is largely independent of the number of smoothing steps on both configuration sets. Several previous studies found that the topological charge has very large autocorrelation time on dynamical configurations, sometimes hundreds of molecular dynamics time units. We did not find this problem here. The average charge on the dynamical configurations is \( \langle Q \rangle = 0.16 \pm 0.25 \) and the charge distribution also appears standard. We found \( \chi^{1/4} = 193(4) \) MeV on the pure gauge ensemble and \( \chi^{1/4} = 130(5) \) MeV on the dynamical ensemble. This decrease of the susceptibility is expected according to Eq. 2. Using the published pion mass value \( m_\pi a = 0.25 \) of the dynamical ensemble [12] in Eq. 3 we obtain \( f_\pi = (105 \pm 20) \) MeV, fairly close to the experimental value \( f_\pi = 132 \) MeV. (Note that Eq. 3 differs from the equivalent equation of Ref.[2].)

Figures 1 and 2 show \( C(r) \) versus \( r \) for both configuration sets after \( N = 30 \) APE smoothing steps. The inserts of the figures enlarge the large \( r \) tail. At this smoothing level the vacuum fluctuations are largely removed. A few properties of the instanton vacuum can be immediately deduced from the figures. At small distances \( C(r) \) is dominated by the auto-correlator of individual instantons and

\footnote{The author is indebted to Peter Hasenfratz for checking Eq. 3.}
Figure 1: Spatial correlation of the topological charge density on pure gauge configurations. The insert enlarges the large $r$ region. The solid line corresponds to the four parameter fit described in the text.

Figure 2: Same as Figure 1 but for the dynamical ensemble.
Table 1: The results of the four parameter fit for the pure gauge and the dynamical configurations.

| Parameter | Pure gauge | Dynamical |
|-----------|------------|-----------|
| $N_0/V$ [fm$^{-4}$] | 1.0±0.05 | 0.35±0.02 |
| $\bar{\rho}$ [fm] | 0.25±0.01 | 0.30±0.01 |
| $d$ [fm] | 0.53±0.03 | 0.61±0.02 |
| $2n_p/N_0$ | 0.16±0.02 | 0.29±0.03 |

$C(r)$ can be approximated by a dilute gas. In the dilute gas approximation the height of the correlator is proportional to the number of topological objects of the configuration, $N_0$, and the width is related to the average radius of the instantons, $\bar{\rho}$. At distances $r \approx 2\bar{\rho}$, the correlator probes the close neighbors of the instantons. If there is no spatial correlation between topological objects, $C(r)$ should be about zero for $r \geq 2\bar{\rho}$\footnote{In the continuum reflection positivity requires $C(r) < 0$ for all $r \neq 0$. On the lattice that is not the case for small $r$. Since smoothing removes most of the vacuum fluctuations one expects $C(r)$ to be dominated by non-perturbative vacuum structures.}. If pairing of oppositely charged objects occur, $C(r)$ is expected to be negative, reaching its minimum around $r \sim 2\bar{\rho}$. Comparing now the pure gauge and dynamical correlators of figures 1 and 2 we observe that the widths of the correlators are almost identical but the height at $r = 0$ is very different. This implies that $\bar{\rho}$ is approximately the same for the two ensembles but the dynamical configurations have about three times fewer topological objects. The tails of the two distributions reveal further differences. While $C(r)$ on the pure gauge ensemble is consistent with zero for $r \geq 0.7fm$, $C(r)$ on the dynamical ensemble shows an unmistakable negative dip signaling opposite-charge correlation.

To quantify these differences, we model the vacuum with a simple picture. Assume that there are $N_0$ topological objects in the vacuum with uniform radius $\bar{\rho}$. If the topological density of a single instanton of radius $\bar{\rho}$ centered at the origin is $q_0(x)$ and the instantons are non-overlapping, the topological density of the configuration in this model is

$$\tilde{q}(x) = \sum_{i=1}^{N_0} s_i q_0(x - x_i), \quad (4)$$

where $x_i$ is the center of the $i$th topological object and $s_i = \pm 1$ depending on whether it is an instanton or antiinstanton. The topological correlator is

$$\tilde{C}(z) = \sum_{i,j} s_i s_j C_{\rho}(z - x_i + x_j) \quad (5)$$

where $C_{\rho}(z)$ is the topological correlator of a single instanton. If the instantons are randomly distributed, averaging over configurations will give

$$<\tilde{C}(z)> = N_0 C_{\rho}(z). \quad (6)$$
If only $N_0 - n_p$ objects are randomly distributed and the other $n_p$ objects form molecules (i.e. $2n_p$ oppositely charged instantons are paired), the average of the topological correlator is
\[
\langle \hat{C}(z) \rangle = N_0 C_\rho(z) - n_p C_d(z),
\]

where $C_d(z)$ is the correlator of an instanton-instanton pair separated by distance $d$, averaged over the direction of $d$. $C_\rho$ and $C_d$ can be calculated using the analytical form of the single instanton charge distribution. If the instanton size is $\bar{\rho} \sim 0.3$ fm and the pairs are closely bound, i.e. $d \sim 0.6$ fm, this model can be valid in the $0 \leq r \leq 0.6 - 0.9$ fm range. The measured $C(r)$ then can be fitted with the four parameters $N_0$, $n_p$, $\bar{\rho}$ and $d$. In the fit we keep data with $0 \leq r/a \leq 5 - 8$ as for $r/a \geq L/2 = 8$ finite size effects become important. Varying the upper range of the fit between $r/a = 5$ and 8 hardly effects the fit parameters, it changes the $\chi^2$ of the fit only. The solid lines in figures 1 and 2 correspond to the best fit. The fit parameters listed in table 1 confirm our earlier observations. The average instanton size on both ensembles is about 0.3 fm. The instanton density on the pure gauge ensemble is about 1 fm$^{-4}$, in agreement with expectations, while the density on the dynamical configurations is about a third of that. On both ensembles we observe pairs at a distance of about $2\bar{\rho}$. On the pure gauge configurations 15 percent of the instantons are in pairs, while on the dynamical configurations close to 30 percent are paired up. It is not surprising to find pairs even on the pure gauge configurations, as there is an attractive gauge interaction between oppositely charged instantons, but pairing is clearly enhanced on the dynamical ensemble.

Until now we have compared the dynamical and pure gauge ensembles at the same level of APE smoothing. In the remainder of this paper we study the dependence on the level of smoothing. The smoothing has two different effects on a configuration: it removes vacuum fluctuations and it also distorts and annihilates instantons. These two effects cannot be separated. The first effect is the important one for small amounts of smoothing, but as the configuration is smoothed many times, the second one becomes more relevant. We have measured the correlator $C(r)$ at $N = 10, 20, 30, 40, 50$ and $60$ levels of APE blocking on both ensembles and also at $N = 15$ on the dynamical configurations only. The same level of APE smoothing can have very different effect at different lattice spacing. The smearing distance $d_s = a\sqrt{Nc/3}$ characterizes the removal of vacuum fluctuations but it is not clear what is the variable (if one exists at all) that describes how instantons are annihilated or otherwise distorted by APE smoothing at different lattice spacings. In the following we report the results as the function of the smearing distance. The qualitative form of the correlator is the same at all levels of smearing and we fit the data with four parameters as described above. The fit is excellent in every case except at the $N = 60$ level smoothing where the smearing distance is comparable to the lattice size and finite size effects become important.

Figure 3 shows the ratio of paired objects and $N_0$ as the function of $d_s$. 
The ratio decreases rapidly up to $d_s \sim 0.2$ fm but changes slower after that, indicating that most of the vacuum fluctuations have been removed and further change is due to the annihilation of topological objects. Comparing data at the same smoothing distance even increases the previously observed difference between the pure gauge and dynamical ensembles; the dynamical configurations show more than twice the pairing rate of the pure gauge ones.

It is interesting to ask, which instantons contribute to the topological susceptibility, all of them or only the unpaired ones? Figure 4 shows the density of the unpaired objects, $(N_0 - 2n_p)/V$ as a function of the smearing distance $d_s$. The horizontal lines indicate the value of the corresponding topological susceptibilities in $\text{fm}^{-4}$. The agreement implies that the unpaired instantons follow a Poisson distribution and only they contribute to the topological susceptibility.

We have studied only one set of dynamical ensemble with two quark flavors. It would be important to extend this work to include different, preferably smaller quark masses and four quark flavors. In both cases one expects the fermionic effects to be stronger. We mention here that the NERSC archive contains two smaller (less than 50 configurations) dynamical configuration sets, both at heavier quark masses. We have analyzed the available configurations, but within errors they show no significant difference compared to the dynamical
Figure 4: \((N_0 - 2n_p)/V\) as the function of the smearing distance for the dynamical (diamonds) and pure gauge (crosses) ensembles. The horizontal lines indicate the value of the corresponding topological susceptibilities.

In summary, we have demonstrated important differences between pure gauge and dynamical QCD configurations. On the dynamical configurations the topological susceptibility is considerably smaller than on the pure gauge configurations. This is due both to the decreased density of instantons and to the stronger pairing of oppositely charged objects. In the case we studied here we found that the density of instantons decreased by about a factor of three while pairing occurred twice as frequently on the dynamical configurations.

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