Are Topological Charge Fluctuations in QCD Instanton Dominated?

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Abstract

We consider a recent proposal by Horváth et al. to address the question whether topological charge fluctuations in QCD are instanton dominated via the response of fermions using lattice fermions with exact chiral symmetry, the overlap fermions. Considering several volumes and lattice spacings we find strong evidence for chirality of a finite density of low-lying eigenvectors of the overlap-Dirac operator in the regions where these modes are peaked. This result suggests instanton dominance of topological charge fluctuations in quenched QCD.
I. INTRODUCTION

Understanding the mechanisms of confinement and chiral symmetry breaking in QCD has been a major goal of non-perturbative field theory for many years. A good candidate for the source of chiral symmetry breaking are topological fluctuations of the gauge fields associated with instantons and anti-instantons. Through mixing, the “would be zero modes” from the instantons and anti-instantons become the small modes that lead, when present with a finite density, to chiral symmetry breaking. Many of the low energy properties of QCD can be explained phenomenologically by the interactions of the fermions with instantons and anti-instantons [1,2]. To our knowledge, confinement, though, is not one of those properties.

However, as pointed out by Witten [3], there is an inconsistency between instanton based phenomenology and large-$N_c$ QCD. Instantons would produce an $\eta'$ mass that vanishes exponentially for large $N_c$, while considerations based on large-$N_c$ chiral dynamics suggest that the $\eta'$ mass should be of order $1/N_c$. The topological charge fluctuations then should be associated not to instantons but rather some other, confinement-related vacuum fluctuations. And the strong attraction produced by these confinement-related fluctuations would also induce the breaking of chiral symmetry.

In an attempt to settle the issue, whether topological charge fluctuations are instanton dominated or not, Horváth, Isgur, McCune and Thacker [4] investigated the response of fermions by considering low lying eigenmodes of a lattice discretized Dirac operator and quantifying the extent to which, in the peak regions of these eigenmodes they are chiral, as would be expected if the almost zero modes around instantons dominate these low lying eigenmodes. They introduced a local “chiral orientation” parameter, or “chirality” parameter, $X(x)$, via the definition

$$\tan\left(\frac{\pi}{4}(1 + X(x))\right) = \left(\frac{\psi_L^\dagger(x)\psi_L(x)}{\psi_R^\dagger(x)\psi_R(x)}\right)^{1/2},$$

where $\psi_L(x)$ and $\psi_R(x)$ are the left- and right-handed components of the eigenmode. Chirality near ±1 would be obtained from almost zero modes due to instantons and anti-instantons, lifted from being exact zero modes by their mixing.

Horváth et al. [4] chose the Wilson discretization for their lattice Dirac operator and claim to have found evidence against instanton dominance of topological charge fluctuations from the behavior of the chirality parameter. However, the Wilson-Dirac operator explicitly breaks chiral symmetry at any finite lattice spacing $a$. As a consequence, the Wilson-Dirac operator does not have exact (chiral) zero modes in gauge fields with a non-trivial topological charge. And the discretization effects responsible might well also strongly affect the chirality parameter. To our knowledge, the magnitude of such distortion effects at the presently accessible lattice spacings are not known. However, the scaling violations for hadron masses due to the $O(a)$ lattice artifacts at the lattice spacing used by Horváth et al. ($a \simeq 0.17$ fm at $\beta = 5.7$) are known to be as large as 30–40% [5].

In a response to [4] DeGrand and Hasenfratz presented evidence that is suggestive of instanton dominance of topological charge fluctuations [6]. They used a variant of the overlap-Dirac operator, proposed and investigated in [7], for the lattice Dirac operator. The overlap-Dirac operator [8], and any variant that substitutes the Wilson-Dirac operator used
in its construction by another suitable Wilson-like discretization of the Dirac operator, has
the chiral and topological properties of the continuum Dirac operator even at finite lattice
spacing, e.g. exact chiral zero modes in gauge fields with a non-trivial topological charge.
However, DeGrand and Hasenfratz coupled their overlap fermions not directly to the “rough”
lattice gauge fields, but rather to “APE smeared” gauge fields, essentially Gaussian smeared
fields with fixed width in lattice units. While such a fermion action is local and therefore
does not change universality class, the distortions the smearing procedure might induce at
finite lattice spacings are not known. Indeed, the level of smearing used by DeGrand and
Hasenfratz removes ultraviolet fluctuations in the gauge field to an extend where pure gauge
observables start to “feel” and be able to identify instanton-like topological excitations that
on the “rough” lattice gauge fields are completely obscured by the dominant ultraviolet
fluctuations. For example, the naive topological charge measurements gives results that are
clearly peaked around integer values.

In an earlier paper, using the same variant of the overlap-Dirac operator, DeGrand and
Hasenfratz produced evidence that the chiral density \( \omega(x) = \psi^\dagger \gamma_5 \psi(x) \) comes in lumps on
the lattice [9], and furthermore that the correlation function of the chiral density with itself
is similar in shape to the correlation function of the chiral density \( \omega(x) \) with the topological
charge density \( Q(x) \) obtained from an APE-smeared operator. But, since APE-smearing
is involved, these results are not beyond doubt. Indeed, the authors of Ref. [4] argue that
the “lumpiness” observed in the correlation function of the chiral density \( \omega(x) \) could occur
without these lumps being purely right-handed or left-handed.

Here we address these questions using the standard overlap-Dirac operator [8] with the
fermions coupled to the original lattice gauge fields. We thereby avoid potential distortions
due to smearing while we retain all chiral properties including existence of exact zero modes
and thus avoid the lattice artifacts, unknown in magnitude and significance, of Wilson
fermions.

II. SETUP

We consider the standard massless overlap-Dirac operator [8]

\[
D(0) = \frac{1}{2} \left[ 1 + \gamma_5 \epsilon(H_w(M)) \right] 
\]

with \( H_w(M) = \gamma D_w(-M) \) and \( D_w(M) \) the usual Wilson-Dirac operator. Then, \( H^2(0) = D(0)D(0) \) commutes with \( \gamma_5 \) and can be simultaneously diagonalized [11,111]. \( H^2(0) \) can have zero eigenvalues with chiral eigenmodes, which are also eigenmodes of \( D(0) \), due to
global topology. The non-zero eigenmodes of \( H^2(0) \) are doubly degenerate and have opposite
chirality,

\[
H^2(0) \psi_{1,\lambda} = \lambda^2 \psi_{1,\lambda} , \quad \gamma_5 \psi_{1} = \psi_{1} , \quad \gamma_5 \psi_{\lambda} = -\psi_{\lambda} ,
\]

with \( 0 < \lambda \leq 1 \). The non-zero (right) eigenmodes of \( D(0) \) are then easily obtained as

\[
\psi_{\pm} = \frac{1}{\sqrt{2}} \left( \psi_{1} \pm i \psi_{\lambda} \right) 
\]
The “chirality” parameter of eq. (1) is then given by

\[ \tan \left( \frac{\pi}{4} (1 + X(x)) \right) = \left( \frac{\psi_1^\dagger(x) \psi_1(x)}{\psi_1^\dagger(x) \psi_1(x)} \right)^{1/2}, \]

and is equal for the two related modes \( \psi_\pm \). In the following they will be therefore counted as one mode. The exact zero modes, of course, have \( X(x) \equiv 1 \).

We computed low-lying eigenmodes \( \psi_{1,1} \) of \( H^2(0) \) with the Ritz functional algorithm of Ref. [12]. For the sign function \( \epsilon(H_W) \) in eq. (2) we used the optimal rational approximation of [10,11] with “projection of low-lying eigenvectors of \( H_w \)” to ensure sufficient accuracy.

### III. RESULTS

We computed the 20 eigenmodes \( \psi_{1,1} \) of \( H^2(0) \) with smallest \( \lambda \) on ensembles of \( 8^3 \times 16 \) pure gauge Wilson action configurations with \( \beta = 5.7 \) and 5.85, and Wilson-Dirac mass of \( M = 1.65 \). The gauge configurations have lattice spacing of about 0.17 and 0.125 fm, respectively, and hence volumes of about 7 and 2 fm\(^4\). We also computed the 20 lowest eigenmodes on an ensemble of \( 6^3 \times 12 \) lattices with \( \beta = 5.7 \), with a volume of about 2.2 fm\(^4\), fairly close to the volume of the \( \beta = 5.85 \) ensemble.

In Fig. 1 we show the chirality histograms for the lowest two non-zero modes at the 2.5% of the lattice sites with the largest \( \psi^\dagger \psi(x) \). In this, and in all similar figures, the histograms are normalized such that the area under the histogram is equal to the fraction of sites considered. In their peaks, the lowest two eigenmodes are fairly chiral. Comparing the two ensembles with the same gauge coupling (and hence lattice spacing) we see a dramatic dependence on the physical volume. In an instanton liquid picture of the vacuum, the number of instantons and anti-instantons, and hence the number of almost zero modes grows linearly with the volume. Then it is not surprising that the lowest modes become increasingly chiral in their peaks with increasing volume. Comparing the two ensembles with almost equal volume in physical units, we notice a tendency of the peaks to become more chiral as the lattice spacing is decreased.

Comparing with Fig. 1 of Ref. [12] we see that in their peaks the lowest two non-zero eigenmodes of the overlap-Dirac operator appear to be more chiral than the real modes of the Wilson-Dirac operator. Considering that Ref. [12] used a lattice with larger volume of about 35 fm\(^4\) and the dramatic volume dependence of the chirality histogram observed here leads one to suspect that the chiral symmetry breaking lattice artifacts of the Wilson-Dirac operator are truly significant at the lattice spacing used.

Comparing with Fig. 1 of Ref. [6], on the other hand, where a physical volume of about 3.5 fm\(^4\) was used, indicates that the APE smeared fields used by DeGrand and Hasenfratz enhance the chirality in the peaks of the lowest-lying non-zero modes somewhat. DeGrand and Hasenfratz already noted a slight dependence on the smearing of gauge fields (see Fig. 4...
FIG. 1. Chirality histograms for the lowest two non-zero modes of the overlap-Dirac operator at the 2.5% sites with the largest $\psi^\dagger\psi(x)$ on the three ensembles with Wilson gauge action.
of \( \psi \), though the effect appears much smaller than the effects of the lattice artifacts from using Wilson fermions.

Considering also the next two higher modes while further restricting the peak region gives the chirality histograms for the two smaller lattices shown in Fig. 2. These modes appear still rather chiral in their peaks. On the larger volume, as expected, a larger number of modes are chiral in their peak, as seen in Fig. 3.

To confirm the trends with volume and lattice spacing, we would like to consider a still larger volume, as well as a lattice at smaller lattice spacing. Unfortunately, the numerical implementation of overlap fermions becomes increasingly difficult and costly, due to the finite density of modes with almost zero eigenvalues of the underlying Wilson-Dirac operator \([13]\). It is believed that these modes are caused by lattice artifact dislocations in the gauge fields generated with Wilson like gauge actions. It is known \([13, 14, 15]\) that these same small modes are responsible for the residual chiral symmetry breaking observed for domain wall fermions with finite 5-th dimension \( L_s \). It was found that improving the gauge action via the Symanzik improved action suppresses the dislocations and decreases the density of small modes \([13]\). It has also been observed that the residual chiral symmetry breaking for domain wall fermions on gauge fields generated with an improved gauge action is much reduced \([15, 16, 17]\). And in Ref. \([18]\) it was noted that the cost of implementing the overlap-Dirac operator on gauge fields with a tree-level Symanzik improved gauge action is lowered.

We made a study of various gauge actions to find which one lowered the density of small modes and would consequently lower the cost of implementing the overlap-Dirac operator. The density of zero eigenvalues of the hermitian Wilson-Dirac operator \( \rho(0) \) at the mass \( M = 1.65 \) was determined for quenched backgrounds from the Iwasaki \([21]\), tree-level tadpole-improved and 1-loop tadpole-improved Lüscher-Weisz gauge action \([22, 23]\). Comparisons were made with the Wilson gauge action at two scales determined by the string tension. The results shown in Table \([2]\) show the quenched Iwasaki gauge action to have the lowest \( \rho(0) \).
For example, at the lattice spacing equivalent to Wilson gauge action $\beta = 5.7$ the $\rho(0)$ is reduced by a factor of about 23.

We therefore generated gauge field ensembles with Iwasaki’s action with $\beta = 2.2782$ and 2.45, chosen to give the same lattice spacing, in units of the string tension, as the ensembles already considered with Wilson action at $\beta = 5.7$ and 5.85. As expected, since the density of small modes of the Wilson-Dirac operator used in the overlap fermion construction were considerably reduced, the overlap fermion computation became much faster. For example, at the lattice spacing equivalent to Wilson $\beta = 5.7$ and lattice size $8^3 \times 16$ the cost of the inner conjugate-gradient step in applying the overlap-Dirac operator was reduced from between 200 to 400 iterations to between 120 to 170 iterations. The average time per configuration to compute the 20 lowest eigenvectors was reduced by roughly a factor of 3. This made it feasible to consider lattices of size $12^3 \times 16$, giving a volume of about 23.6 fm$^4$ at $\beta = 2.2782$ and 6.7 fm$^4$ at $\beta = 2.45$, i.e. about the same volume as the $8^3 \times 16$ lattice at $\beta = 2.2782$. We also generated a $12^3 \times 16$ at $\beta = 2.65$, chosen such that the volume is about 2.1 fm$^4$, the same volume as the smallest lattice at the other two gauge couplings. The lattice size and volume, both in lattice and physical units, as well as the average number of zero modes and the fluctuation of the topological charge, obtained from the number of zero modes, of all ensembles considered are listed in Table II.

The chirality histograms of the two lowest non-zero modes at the 2.5% of sites with largest $\psi^\dagger \psi(x)$ for all six ensemble with Iwasaki glue are shown in Fig. 4. The physical volume of the systems shown in the left column are approximately the same. Comparing the three
TABLE I. Comparison of the density of zero eigenvalues $\rho(0)$ of the hermitian Wilson-Dirac operator for various gauge actions. The comparisons were made at the same lattice spacings as the Wilson gauge action $\beta = 5.85$ and 5.7. The scale was set using the string tension. Shown are the results for the Wilson, Iwasaki, tree-level and 1-loop tadpole-improved Lüscher-Weisz gauge actions. The string tensions for the Wilson gauge action were taken from Ref. [24]. The string tension for the 1-loop tadpole-improved Lüscher-Weisz gauge action comes from an interpolation of previous results, while the others were computed in this work. All tests used a Wilson-Dirac mass of $M = 1.65$. The Iwasaki gauge action has the lowest $\rho(0)$ at fixed $a\sqrt{\sigma}$.

<table>
<thead>
<tr>
<th>action</th>
<th>$\beta$</th>
<th>$V a^4$</th>
<th>$a\sqrt{\sigma}$</th>
<th>$\rho(0) \times 10^5$</th>
</tr>
</thead>
<tbody>
<tr>
<td>Wilson</td>
<td>5.70</td>
<td>$8^3 \times 16$</td>
<td>0.3917</td>
<td>162(9)</td>
</tr>
<tr>
<td></td>
<td>5.85</td>
<td>$8^3 \times 16$</td>
<td>0.2864</td>
<td>21(3)</td>
</tr>
<tr>
<td></td>
<td>6.00</td>
<td>$24^3 \times 32$</td>
<td>0.2197</td>
<td>2.3(2)</td>
</tr>
<tr>
<td>Iwasaki</td>
<td>2.2872</td>
<td>$8^3 \times 16$</td>
<td>0.3885(95)</td>
<td>7(1)</td>
</tr>
<tr>
<td></td>
<td>2.45</td>
<td>$12^3 \times 16$</td>
<td>0.2840(53)</td>
<td>2.4(9)</td>
</tr>
<tr>
<td>0-loop TI LW</td>
<td>7.26</td>
<td>$8^3 \times 16$</td>
<td>0.3900(76)</td>
<td>58(6)</td>
</tr>
<tr>
<td></td>
<td>7.60</td>
<td>$12^3 \times 16$</td>
<td>0.2872(39)</td>
<td>4.3(8)</td>
</tr>
<tr>
<td>1-loop TI LW</td>
<td>7.79</td>
<td>$8^3 \times 16$</td>
<td>0.3917</td>
<td>44(5)</td>
</tr>
<tr>
<td></td>
<td>8.13</td>
<td>$12^3 \times 16$</td>
<td>0.2864</td>
<td>3.9(7)</td>
</tr>
</tbody>
</table>

TABLE II. The gauge ensembles with Wilson glue in the first three lines and with Iwasaki glue in the rest. Listed are the volume in lattice units and in units of fm$^4$, the average number of zero modes and the average of the square of the global topological charge as obtained from the number of zero modes.

| $\beta$ | $V [a^4]$ | $V [fm^4]$ | $\langle |Q| \rangle$ | $\langle Q^2 \rangle$ |
|---------|-----------|------------|-----------------|-------------------|
| 5.70    | $6^3 \times 12$ | 2.2        | 1.2(2)          | 2.8(5)            |
| 5.70    | $8^3 \times 16$ | 7.0        | 2.0(2)          | 7.1               |
| 5.85    | $8^3 \times 16$ | 2.0        | 1.3(1)          | 2.6(4)            |
| 2.2872  | $6^3 \times 12$ | 2.2        | 1.0(1)          | 1.7(2)            |
| 2.2872  | $8^3 \times 16$ | 7.0        | 2.0(2)          | 5.1               |
| 2.2872  | $12^3 \times 16$ | 23.6       | 4.2(9)          | 25(8)             |
| 2.45    | $8^3 \times 16$ | 2.0        | 1.0(1)          | 1.8(2)            |
| 2.45    | $12^3 \times 16$ | 6.7        | 2.3(4)          | 8(1)              |
| 2.65    | $12^3 \times 16$ | 2.1        | 1.3(2)          | 2.4(6)            |
FIG. 4. Chirality histograms for the lowest two non-zero modes of the overlap-Dirac operator at the 2.5\% sites with the largest $\psi^\dagger\psi(x)$ on the six ensembles with Iwasaki gauge action. The systems in the left column all have approximately the same volume in physical units. The systems in the top two panels in the right column also have the same, about a factor of 3 larger, volume, while the system in the lower right hand corner panel has the largest volume.
FIG. 5. Chirality histogram similar for the lowest six non-zero modes at the 2.5% sites with the largest $\psi^\dagger\psi(x)$ on the two lattices with volume of about 7 fm$^4$.

histograms confirms the trend, already observed with Wilson glue, that the lowest non-zero modes tend to become more chiral in their peaks as the lattice spacing is decreased. This strongly suggests that the behavior observed here will survive the continuum limit. Comparing the three histograms for $\beta = 2.2872$, on the other hand, confirms the strong volume dependence already observed with Wilson glue.

In Fig. 5 we show the chirality histogram of the lowest six non-zero modes on the two systems with physical volume of about 7 fm$^4$ and in Fig. 6 the chirality histogram from all non-zero modes out of the 20 lowest modes that we computed (there are between 11 and 20 non-zero modes per configuration). Comparing with the histograms in the left column of Fig. 4 indicates that the number of non-zero modes with similar chirality histograms grows roughly like the physical volume so that there is a finite density of modes which are chiral in their peaks. This is good evidence that we are not observing a finite volume effect that would disappear in the infinite volume limit.

IV. ABELIAN GAUGE THEORIES

To contrast the results for quenched QCD of the previous section we considered the chirality parameter also for quenched U(1) theories in two and four dimensions. In 2d, also considered in Ref. [4], topology plays a crucial role and one expects local chirality in the peaks of low-lying modes. This is clearly seen in Fig. 7, where the 10 lowest non-zero modes have been kept. Comparing with Figs. 6 and 7 of Ref. [4] demonstrates again the superiority of the overlap-Dirac operator over the Wilson-Dirac operator for the purpose of investigating chirality properties. The histogram in Fig. 7 for the 10 lowest non-zero modes shows better chirality peaks than Fig. 6 of [4] for the real modes of the Wilson-Dirac operator, the “should be zero modes”, were it not for the explicit chiral symmetry breaking from the Wilson term.

In 4d U(1), in the confined phase, chiral symmetry is spontaneously broken, and a finite
FIG. 6. Chirality histogram for all the non-zero modes out of the 20 lowest modes at the 2.5% sites with the largest $\psi^\dagger \psi(x)$ on the lattice at $\beta = 2.2872$ with the largest volume.

FIG. 7. Chirality histogram for the lowest ten non-zero modes of the overlap-Dirac operator at the 6% sites with the largest $\psi^\dagger \psi(x)$ on $24^2$ U(1) configurations at $\beta = 1.9894$. 
density of near zero modes exists. But there are no instantons, and so one would not expect the near zero modes to be dramatically chiral even in their peak regions. There do exist exact zero modes of the overlap-Dirac operator, which again, of course, are chiral, although their origin is not completely understood \cite{23}. We analyzed, stored eigenmodes from Ref. \cite{23}. The chirality histogram for the lowest two non-zero modes is shown in Fig. 8. We note that while there is some mild indication of chirality peaking, the proportion of sites showing this behavior is much reduced compared to the SU(3) case and appears to be of a qualitatively different nature than seen before. In the U(1) case the small peaking could conceivably come about from the scenario outlined by Horvath, et. al. - namely from the confinement inducing vacuum fluctuations.

V. CONCLUSIONS

Horváth \textit{et al.} \cite{4} proposed an observable, the “chirality” parameter, designed to answer the question whether topological charge fluctuations in (quenched) SU(3) gauge theory are instanton dominated or not by the response of fermions. Chirality of the low lying modes near $\pm 1$ in the regions where they have the largest magnitude would signal instanton dominance. Using Wilson fermions, afflicted by potentially strong lattice artifacts, they claimed evidence that the topological charge fluctuations are \textit{not} instanton dominated. We took up this question using overlap fermions, a lattice fermion formulation known to have the same chiral properties as continuum fermions, and therefore much less afflicted by lattice artifacts and better suited to the study of properties closely related to chiral symmetry.

Considering several volumes and lattice spacings, we found convincing evidence for chirality of the low lying modes in their peak region, confirming results of Ref. \cite{6} obtained using overlap fermions coupled to smoothened gauge fields. We note that improving the
gauge action did not significantly change the degree of chirality at fixed lattice spacing and lattice size. Our results give evidence that the number of modes which are chiral in their peaks grows linearly with the volume so that there is a \emph{finite density} of such modes, and that the chirality of the modes becomes more pronounced as the lattice spacing is decreased. Therefore, our observations should remain valid in the continuum limit.

That the results of Ref. \cite{4} are strongly affected by lattice artifacts was confirmed by the very recent paper of Hip \emph{et al.} \cite{24}. These authors consider an improved chirality parameter for Wilson fermions, clover improved Wilson fermions, and lattices at smaller lattice spacing than Ref. \cite{4}. With these reductions of lattice artifacts, they conclude that instanton dominance of topological charge fluctuations is not ruled out by the response of (improved) Wilson fermions. Together with the results from overlap fermions presented in this paper and the lack of significant chirality enhancement in the 4-d U(1) model where instantons should not exist, the case for instanton domination in 4-d SU(3) gauge theory, as measured by the chirality parameter, becomes even more compelling.

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