Role of the Wilson mass parameter in the overlap Dirac topological charge density

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The negative Wilson mass parameter is an input parameter to the overlap Dirac operator. We examine the extent to which the topological charge density, revealed by the overlap definition, depends on the value of the negative Wilson mass. A strong dependence is observed, which can be correlated with the topological charge density obtained from the gluonic definition, with a variable number of stout-link smearing sweeps. The results indicate that the freedom typically associated with fat-link fermion actions, through the number of smearing sweeps, is also present in the overlap formalism, through the freedom in the Wilson mass parameter.
1. Introduction

By simulating the theory of quantum chromodynamics on a four-dimensional space-time lattice, one can directly probe the topological structure of the quantum vacuum. An integral component of the continuum theory is the realization of an exact chiral symmetry in the massless limit. Ideally, Lattice QCD calculations should also observe this symmetry. Unfortunately, simple transcriptions of the fermion action explicitly break this symmetry at the order of the lattice spacing.

The famous Nielsen-Ninomiya “no-go” theorem [1] explains the difficulties with implementing chiral symmetry on the lattice. In the early 80’s, Ginsparg and Wilson [2] proposed that the smoothest way to break chiral symmetry on the lattice was to obey the Ginsparg-Wilson relation,

\[ D\gamma_5 + \gamma_5 D = aDR\gamma_5 D. \]  

(1.1)

A popular solution to Eq. (1.1) is the overlap Dirac operator [3, 4],

\[ D = \frac{m}{a} \left( 1 + \frac{D_W(-m)}{\sqrt{D_W^*(-m)D_W(-m)}} \right), \]  

(1.2)

where the Wilson-Dirac operator \( D_w \), with a negative Wilson mass \(-m\), is the standard choice of input kernel. The overlap operator is known to observe an exact chiral symmetry on the lattice, and satisfies the Atiyah-Singer index theorem, where the total topological charge \( Q \) is equal to the difference of Dirac zeromodes with opposite chirality.

The topological charge density can be extracted from the trace of the overlap operator,

\[ q_{ov}(x) = -\text{Tr} \left[ \gamma_5 \left( 1 - \frac{a}{2m} D \right) \right], \]  

(1.3)

which allows one to investigate QCD vacuum structure through studies of the \( \langle q_{ov}(x)q_{ov}(0) \rangle \) correlator [5, 6] and the topological charge density itself [7, 8]. An ultraviolet cutoff can be introduced through the spectral representation [5, 9],

\[ q_{\lambda, uv}(x) = -\sum_{|\lambda| < \lambda, uv} \left( 1 - \frac{\lambda}{2m} \right) \psi^\dagger_\lambda(x) \gamma_5 \psi_\lambda(x). \]  

(1.4)

We begin these proceedings by highlighting recent research results [10] comparing the UV filtered overlap topological charge density to the long established gluonic definition,

\[ q_{sm}(x) = \frac{g^2}{16\pi^2} \text{Tr} \left( F_{\mu\nu} \tilde{F}_{\mu\nu} \right), \]  

(1.5)

obtained after smearing the gauge field. Following this, we consider the extent to which the negative Wilson mass parameter used in the Wilson-Dirac input kernel of Eq. (1.2) affects the overlap topological charge density.

2. Stout-link smearing and the overlap Dirac operator

The gluonic definition of the topological charge density in Eq. (1.5) is only valid on “smooth” gauge fields. Many prescriptions exist for smoothing a gauge field, however discretization errors
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Figure 1: The overlap $\langle q(x)q(0) \rangle$ correlator from the full topological charge density and the corresponding smeared correlator [10]. The match can be further fine tuned by varying the smearing parameter.

can skew the results. For studies of QCD vacuum structure, it is important to choose a topologically stable smearing algorithm, such as the over-improved stout-link smearing algorithm [11]. This is a modification of the original stout-link algorithm, in which the standard plaquette is replaced by a combination of plaquettes and rectangles, tuned to preserve topological objects in the vacuum whilst smearing. We use the parameters proposed in Ref. [11] and refer the reader to that publication for full details of the algorithm and its efficiency. The topological charge density is then extracted using Eq. (1.5) in combination with an $O(a^4)$-improved field strength tensor.

In comparisons between the gluonic and overlap topological charge densities, the gluonic definition may not always provide an integer topological charge $Q$. For this reason, it is common to apply a multiplicative renormalization factor $Z$, $q_{sm}(x) \rightarrow Z q_{sm}(x)$, where $Z$ is chosen such that $Q_{sm} = \sum_x q_{sm}(x)$ equals $Q_{ov}$, which is always an exact integer. The renormalization factors are typically close to 1. The interested reader is encouraged to consult Ref. [10] for the values.

We begin with a comparison of the $\langle q(x)q(0) \rangle$ correlator, which should be negative for any $x > 0$ [12, 13, 6]. This was first observed for the overlap in Ref. [6], and it was later shown in Ref. [14], that this behavior can be reproduced with the gluonic definition. Figure 1 shows the overlap correlator and the best smeared match using a smearing parameter of $\rho = 0.06$ with 5 sweeps of over-improved stout-link smearing. We note that by varying the magnitude of $\rho$ this match can be further fine tuned. This matching of the $\langle q(x)q(0) \rangle$ enables high statistics studies using the computationally efficient smearing algorithm, and was used in Ref. [15] to explore the effect of dynamical quarks on QCD vacuum structure.

Ilgenfritz et al. [10] further explored the correlation between the gluonic and overlap topological charge density using the spectral representation of the overlap operator, Eq. (1.4). They found a direct connection between the number of stout-link smearing sweeps applied to the gauge field and the strength of the UV cutoff. In Fig. 2 we present a sample of that work, the best match for a cutoff of $\lambda_{cut} = 634$ MeV.

3. Role of the negative Wilson mass parameter

The (negative) Wilson mass parameter enters the definition of the overlap operator through the Wilson-Dirac input kernel. At tree level the allowed range for the Wilson mass is $0 < m < 2$. 
Figure 2: The overlap topological charge density (left) calculated using an UV cutoff of $\lambda_{\text{cut}} = 634$ MeV. On the right is the best smeared match found using 48 sweeps of over-improved stout-link smearing [10, 11].

However, when working at a finite lattice spacing $a$, one must also have $m \gtrsim 1.0$ [18]. Converting this to the more standard $\kappa$ parameter gives an allowed range of $1/6 \lesssim \kappa < 1/4$, since at tree level,

$$\kappa \equiv \frac{1}{2(-m)a + 8r}.$$  \hspace{1cm} (3.1)

By varying $m$ within this range, one has access to a fermionic probe of the gauge background at different scales $\sim 1/m$ [4]. Previous studies have investigated how the total topological charge and topological susceptibility depend on the value of the Wilson mass [3, 16, 17, 18]. We now extend this work to include an analysis of the topological charge density itself. This should provide some useful physical insights since the low-lying modes of the Dirac operator are strongly correlated with the topological charge density [10, 19].

The overlap Dirac operator is an expensive calculation so we consider a single spatial slice from some representative $16^3 \times 32$ configurations. Five $\kappa$ values, 0.17, 0.18, 0.19, 0.21 and 0.23 are used to investigate the effect of the Wilson mass on the topological charge density. As before, we monitor the changes in $q_{ov}(x)$ through direct visualizations.

The topological charge densities, for the five choices of $\kappa$, are presented in Fig. 3. A clear dependence on the Wilson mass is apparent from the figures, with smaller values of $m$ revealing greater topological charge density. This is consistent with expectations, since as $m$ is increased the Dirac operator becomes more sensitive to smaller topological objects.

The changes in $q_{ov}(x)$ as $m$ is varied appear very similar to the way that the gluonic topological charge density depends on the number of smearing sweeps applied, and we now quantify this connection. We use a relatively weak smearing parameter$^1$ of $\rho = 0.01$, and as before, applying a multiplicative renormalization factor. We consider two choices for $Z$, firstly a calculated $Z$,

$$Z = \frac{\sum_x |q_{ov}(x)|}{\sum_x |q_{sm}(x)|}.$$ \hspace{1cm} (3.2)

This will be compared with a fitted $Z$ where $Z$ is found by minimizing,

$$\sum_x |q_{ov}(x) - Z q_{sm}(x)|.$$ \hspace{1cm} (3.3)

$^1$To be compared with the usual $\rho = 0.06$ for over-improved stout-link smearing, or $\rho = 0.1$ for standard stout-link smearing
Figure 3: The overlap topological charge density $q_{ov}(x)$ calculated with five choices for the Wilson mass $m$. From left to right, we have $\kappa = 0.23, 0.21, 0.19$ on the first row, with 0.18, and 0.17 on the second. There is a clear dependence on the value of $m$ used, with larger values revealing a greater amount of topological charge density.

Figure 4: The best smeared matches (right) compared with three of the overlap topological charge densities (left) in order of increasing $m$, where $q_{om}(x)$ is renormalized using the calculated $Z$. 
The best smeared matches for all five \( \kappa \) values considered. Results for two configurations are reported in Table (a) (left) and (b) (right). There is a definite correlation between the choice of the Wilson mass and the number of smearing sweeps required to match the topological charge density.

The overlap topological charge densities along with the corresponding best matches found using the calculated \( Z \) are shown in Fig. 4. Due to a lack of space we show only the largest, smallest and middle \( \kappa \) values. As the Wilson mass is increased, and non-trivial topological charge fluctuations are removed, a greater number of smearing sweeps are needed in order to recreate the topological charge density. A summary of the best matches are provided in Table 1a along with the results obtained using a fitted \( Z \) value. We note the good agreement between the two choices for fixing the renormalization factor. Results for a second configuration are provided in Table 1b. A comparison reveals little difference in the number of smearing sweeps required to match the overlap \( q(x) \).

4. Conclusion

The overlap topological charge density displays a clear dependence on the value of the Wilson mass used in the calculation. Although this was not unexpected, we are also able to show how one can correlate the value of \( \kappa \) used in the overlap to a specific number of stout-link smearing sweeps. This implies an intimate relationship between the number of smearing sweeps and the value of \( \kappa \) in the overlap formalism.

We have shown how the smoothness of the gauge field as seen by the overlap operator depends on the value of the Wilson mass. This is similar to fat-link fermion actions where the gauge links are smeared with a small number of smearing sweeps and the smoothness depends on the number of applied sweeps. The results indicate that the freedom typically associated with fat-link fermion actions, through the number of smearing sweeps, is also present in the overlap formalism, through the freedom in the Wilson mass parameter. However the number of smearing sweeps relevant to the overlap operator is small. This connection will be further explored in a forthcoming publication [20].

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