Study of QCD Vacuum Structure Using Ginsparg-Wilson Fermionic Kernels

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Abstract

We have recently presented evidence that in configurations dominating the regularized pure-glue QCD path integral, topological charge associated with overlap Dirac operator organizes into long-range low-dimensional space-time structure. This opened an exciting possibility of studying the QCD vacuum structure *directly* in typical configurations contributing to the regularized QCD path integral. Here we propose to initiate a systematic study which will help to clarify the quantitative (and some qualitative) details of this structure (such as space-time dimensions of its parts) and will help to clarify the physical role of the associated geometric properties. In particular, we propose to calculate the full overlap-based topological charge density on configurations sufficiently close to the continuum limit (a $\approx$ 0.05 fm). This is an important step toward obtaining a definitive picture of topological charge fluctuations in QCD vacuum. The total amount of requested resources is 280,000 processor hours on the FNAL's 128 node single-processor cluster and the proposal should be considered of type (B).

1 Physics Goals of the Calculation

The underlying goal of the proposed calculation is to determine the role of topological charge fluctuations in the physics of strong interactions. It has long been believed that resolving this issue represents an important component in ultimately solving the mystery of the QCD vacuum. However, it is only recently that the exciting developments in lattice field theory offered convincing reasons to believe that an important progress is within the reach. First, the developments in understanding lattice chiral symmetry provided us with the best-founded topological charge density operators [1, 2]. An operator from this class posesses completely continuum-like field-theoretic properties [3], and represents a full-fledged topological field (with associated charge strictly stable) on the lattice [1]. Secondly, it was found that there is an obvious excess of space-time order in distributions of topological charge when such operators are used [4]. (See also Ref. [5].) This is the first time that an observation of space-time structure directly in thermalized configurations of regularized QCD ensembles has been achieved. The conceptual value of this development is that it demonstrates that the direct lattice approach to studying the QCD vacuum structure is possible (and feasible). The aim of the current proposal and request for SciDAC resources is to pursue this avenue of research.

1.1 Geometry and Physics

Direct approach to the QCD vacuum (i.e. one that does not rely on any proposed idealized picture of the QCD vacuum), while truly promising, is in its infancy. Consequently, the associated goals and the nature of the research must be viewed in the appropriate context. At the current stage of development the emphasis must be put on identifying the prominent patterns of the space-time structure. In other words, the emphasis is naturally on the *geometry*. Once the defining geometric features are identified and quantified, their role in determining the physics of the QCD vacuum should be studied. In Ref. [4] the first steps toward describing the geometry of space-time arrangement in topological field have been achieved. It was found that the charge is organized into the sign-coherent locally low-dimensional "sheets". The sheets are geometrically global (see also [6]), spreading over maximal available distances, and fill the macroscopic fraction of the space-time. This sheet structure is built around the supporting substructure – the "skeleton", with analogous geometric properties. Needless to say, there are many geometrical details to be discovered and specified in this overall picture.

When it comes to *physics*, then one can argue that the first attempts to identify the connections to geometry should concentrate on the charge-charge correlator $C(x) \equiv \langle q(0)q(x)\rangle$. Indeed, this correlator encodes the topological susceptibility (related to the $U_A(1)$ problem via Witten-Veneziano relation) and the mass spectrum of pseudoscalar glueballs. One can thus ask in detail how the space-time structure in topological charge distributions results in the particular properties of this correlator. Note that $C(x)$ has not been itself calculated for overlap-based topological charge density, and so this is actually part of the proposed calculation.

1.2 Examples of Specific Goals

While the proposed calculations have to be treated as exploratory we give below the questions that we hope to answer with the computer resources made available for this project.

(1) **Calculate both local and global dimensions involved in the structure.** While it has been demonstrated that the local dimension of the structure is less than four [4] (both in case of sheets and of the skeleton), the calculation of exact dimensions using scaling analysis has not been performed yet. This will be done both for the sheets and the skeleton. Also, it is possible that more than one definite dimension is involved for different parts of the structure. We hope to shed light on this question as well.

(2) **The physical relevance of sheet versus skeleton.** With the data obtained in this calculation it will be possible to determine whether it is the skeleton structure or the sheet structure that is relevant for determining the shape of the charge-charge correlator, and hence responsible for important physical properties of QCD vacuum.

(3) **The calculation and properties of $C(x)$.** As mentioned above, this correlator is crucial for this project and is intimately associated with the structure to be studied. As first pointed out in Ref. [7], $C(x)$ is negative at arbitrary non-zero distances and this served as an important guide for identifying the relevance of low-dimensional structure. We wish to learn in detail how the interplay of positive core and the negative part at non-zero physical distances (both diverging) result in a finite topological susceptibility. It will be possible to determine precisely the nature of the divergence at short distances which is highly interesting theoretically.

(4) **Geometric relation between positive/negative sheets (parts of skeleton).** There is a rich geometric information encoded in the space-time relation between positive and negative part of the structure. While it is known that these have to follow closely one another [4] the exact nature of the relation has not been explored yet in detail. Uncovering the precise form of this relation will add important new information on topological charge fluctuations in the QCD vacuum and hopefully will lead to an understanding of how the global charge in the configuration comes about.

(5) **Relation between the structure at low energy and the fundamental structure.** Using the topological density based on GW fermions, one can naturally define an *effective topological field* describing topological fluctuations at low energy [8]. One can thus ask about the relation between the fundamental structure (involving all fluctuations up to the scale of the cutoff) and the structure at low energy. The scale-dependent picture of QCD vacuum is the new conceptual ingredient that our recent direct studies invoked. The proposed calculation will make it possible to develop this picture in much finer detail.

ensemble	a [fm]	V	#configs	#eigenmodes	#full densities
$\mathcal{E}_1$	0.165	8^4	50	100	30
$\mathcal{E}_2$	0.110	12^4	50	100	15
$\mathcal{E}_3$	0.082	16^4	50	100	5
$\mathcal{E}_4$	0.055	24^4	50	100	0

Table 1: Ensembles of Iwasaki gauge configurations with the associated number of overlap eigenmodes per configuration that will be available for the construction of effective topological densities. The number of configurations with full densities currently available is given in the right column.

2 The computational strategy

2.1 Context of the proposed calculation – existing data

As discussion above indicates, our inquiry into the nature of topological fluctuations in QCD involves two computationally separate but physically intertwined lines which need to be developed simultaneously. The first is the computation of effective densities for several ensembles with sufficiently large physical volume. This involves the calculation of large number of eigenmodes for the overlap Dirac operator [9]. This part of the project has been almost completed, and the most extensive part of the calculation is currently proceeding using SciDAC resources at FNAL. We work with quenched Iwasaki ensembles at fixed physical volume $V_p = 3$ fm^4 and four different lattice spacings. Upon completion, we will have the pool of eigenmodes summarized in Table 1. These will allow the study of effective topological densities up to the cutoff $\Lambda = 1$ GeV across the range of lattice spacings considered.

The second line of computation within this project involves calculation of full (fundamental) densities on the identical (sub)ensembles. This part of the project has also already begun using other resources of the Kentucky group and the current status of this calculation is summarized in the right column of Table 1. Note that in this second part it is not feasible (nor necessary) to calculate the overlap densities for full ensembles. (We will come back to the question of sufficiency later in this proposal.) Indeed, our plan is to eventually generate full densities for 50, 50, 12, 7 configurations from ensembles $\mathcal{E}_1, \ldots, \mathcal{E}_4$ respectively by the end of next year. The current proposal involves the calculation of full densities for 7 configurations of the ensemble $\mathcal{E}_4$, which is computationally the most intensive part of this project.

2.2 Other details

To calculate the topological density on configurations from the above ensembles we will use the overlap Dirac operator [9] with negative mass $\rho = 1.368$ ($\kappa = 0.19$) in the Zolotarev implementation. The density is given by $q_x = \frac{1}{2\rho}\mathtt{Tr}\gamma_5 D_{x,x}$. Since the overlap operator is implicitly defined, the required matrix elements have to be computed via acting with D on point sources, i.e.

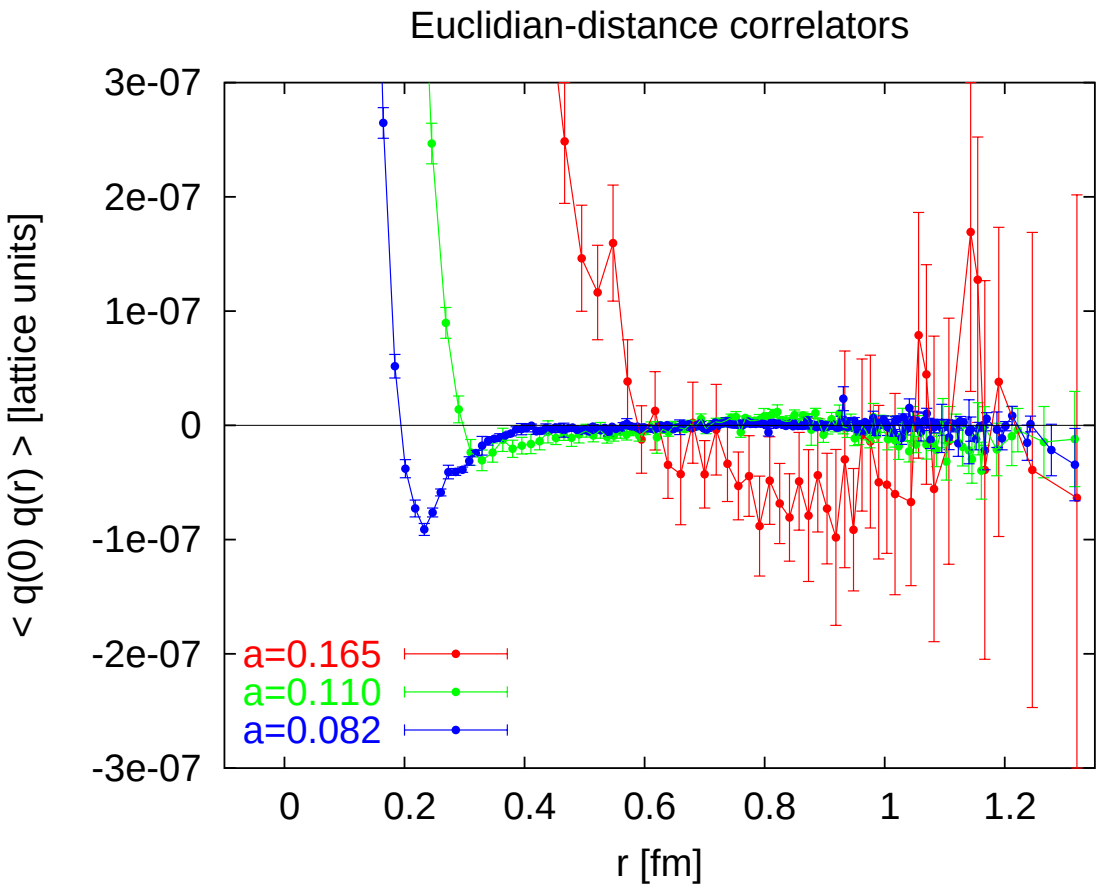

Figure 1: $C(x)$ correlators at three different lattice spacings.

$$D^{\mu a,\nu b}_{x,y} \;=\; (\eta^{\mu a}_x)^+ \, D \, \eta^{\nu b}_y \tag{1}$$

where $\eta^{\mu a}_x$ is unity at space-spin-color index (x, μ, a) and zero elsewhere. As it stands this is an $O(V^2)$ calculation. This complexity is offset to some degree by the fact that good locality properties of the overlap-Dirac operator allow for several space-distributed sources to be computed simultaneously. Our tests show that on 24^4 lattice it is possible to use the superposition of 16 sources separated by Euclidean distance at least 12. Using our implementation of the overlap operator (with violation of chiral symmetry around 10^{-10} as measured by the residual mass), the use of multiple sources will introduce the local relative error in q_x better than 10^{-5}.

2.3 The need and sufficiency

The calculation we are proposing is non-standard and we would like to clarify certain points in this regard.

The need. While the computation of full densities on 24^4 lattice is computationally quite intensive, it is crucial to carry it out since all of the physics goals listed in Sec. 1.2 depend on it to some degree. This is most apparent for goals (1) and (3). Indeed, in case of dimensions we need in most general case to carry out 3-parameter fits to the form $c_1 + c_2 a^d$ in lattice-spacing dependence. We thus need at least four different lattice spacings for such analysis. Moreover, our first experience with the data indicates that the physical input at lattice spacing around $a \approx 0.05$ fm is necessary to carry out the continuum extrapolation reliably. Similarly, in case of goal (3), we are finding that it is necessary to calculate the correlator at such lattice spacing in order to capture the diverging short-distance behavior of the correlator.

The sufficiency. The proposed calculation involves just 7 configurations on 24^4 lattice which might invoke the impression that it cannot possibly serve our physics purposes. In fact, this is not the case. First of all, what we have found so far is that at the fundamental level (i.e. for full densities), the behavior of the structure is very stable from configuration to configuration. This is another signature of the order present. (Seeing one configuration essentially means seeing them all.) At the quantitative level, we have emphasized that at the current stage the physics focus is on the correlator $C(x)$. In Fig. 1 we show the correlators constructed from the available data quoted in Table 1. Even though the calculation for ensemble $\mathcal{E}_3$ only involves 5 configurations, the quality of the correlator is far better than from 30 configurations for $\mathcal{E}_1$. This is both the result of the fact that an all-to-all correlator from a single configuration closer to the continuum limit samples the behavior with more "statistics" and the fact that the space-time structure simply becomes more robust and universal closer to the continuum limit.

3 Software

The software used for the proposed calculation has already been developed by the χQCD collaboration (mainly Andrei Alexandru) and used in the calculations carried out so far (see Table 1). The package is written in C and is based on publicly available MILC code. This code has been tested thoroughly for the current purpose and has comparable efficiency to the existing version of the CHROMA code in the critical part of the calculation i.e. for overlap operator–vector operation. The tests performed in the context of overlap propagator calculation on JLab clusters indicate that our code runs less than 20% slower than the highly optimized CHROMA code in the setting that will be used in the calculation. We believe that this difference does not justify an extensive effort (and manpower needed) to make the transition to QCD API software at the current stage of the project.

4 Time estimate and requested resources

We have made a direct estimate of the time needed on the FNAL's 128 node (single processor) cluster, where we expect the proposed calculation to be carried out. This is also where our current eigenmode calculation for ensemble $\mathcal{E}_4$ is currently being performed. The results of small test runs show that 40,000 processor-hours per configuration are needed to carry out

the full density calculation on 24^4 lattice. Our total requested time is thus 280,000 processor-hours on the FNAL's 128 node, single-processor cluster (1.5 months of the cluster use). The alternative would be the same amount of processor-hours on the JLab's 256 node cluster.

5 Availability of the data

Given its nature, the results of the proposed calculation will be mainly useful to the part of the community interested in studying the QCD vacuum structure. The data produced as the result of this calculation will be made available to the SciDAC LGT collaboration after the period for the requested allocation ends.

6 Exclusive rights

We would prefer to have an exclusive right for calculations and investigations listed in Sec. 1.2 for 9 months after the period for the requested allocation ends.

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