Topological Charge Evolution in the Markov-Chain of QCD

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The topological charge is studied on lattices of large physical volume and fine lattice spacing. We illustrate how a parity transformation on the $SU(3)$ link-variables of lattice gauge configurations reverses the sign of the topological charge and leaves the action invariant. Random applications of the parity transformation are proposed to traverse from one topological charge sign to the other. The transformation provides an improved unbiased estimator of the ensemble average and is essential in improving the ergodicity of the Markov chain process.

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I. INTRODUCTION

The Markov chain process is the corner stone of modern importance-sampling techniques for generating field configurations in the numerical simulation of quantum field theories. Central to the process is ergodicity; the ability to move through configuration space from any particular field configuration to any other field configuration with finite probability. Vacuum expectation values of observable operators are estimated from the average of field configurations selected with a probability given by the exponentiation of the Euclidean action, $\exp(-S_E)$, governing the quantum field theory.

It is essential that these field configurations are selected based on the action alone, unbiased by the field configuration used to initiate the Markov chain. In practice this is done by updating the field configurations for thousands of sweeps through the lattice, monitoring the autocorrelation of various observables, and selecting a new representative field configuration only after significant evolution through configuration space.

The topological charge of a gauge configuration in lattice QCD has already been identified as a particularly difficult quantity to evolve in the Markov chain process, displaying unusually long autocorrelation times [1, 2, 3, 4]. Some gauge actions such as the renormalization-group block-transform based DBW2 action [5, 6] are notorious for locking in the topological charge at fine lattice spacings [3, 4]. Difficulties associated with the Iwasaki gauge action [7, 8] are presented here.

In this study we address an aspect of the topological charge evolution problem that will present itself for any gauge field action. In particular, we address a problem associated with the approach to the infinite-volume continuum limit in numerical supercomputer simulations of $SU(3)$ gauge theory and QCD in general.

As the physical volume, V, of the lattice increases, the average value of the squared topological charge increases, in accord with the topological susceptibility, given by

$$\chi = \frac{\langle Q^2 \rangle}{V}. \tag{1}$$

In quenched QCD, χ is related to physical hadron masses via the large N_c Witten-Veneziano relation [9, 10]

$$\chi = \frac{f_\pi^2}{2\,N_f} \left(m_\eta^2 + m_{\eta'}^2 - 2\,m_K^2 \right). \tag{2}$$

In full QCD, the quark mass dependence of the topological susceptibility may be related to pseudoscalar meson properties via the Gell-Mann–Oakes–Renner relation as [11, 12, 13, 14]

$$\chi = \frac{f_\pi^2\, m_\pi^2}{2\,N_f} + \mathcal{O}(m_\pi^4). \tag{3}$$

On a sufficiently large volume lattice, the distribution of the topological charge is expected to be Gaussian. Regions of non-trivial topological charge density are uncorrelated for sufficiently large separations and a normal distribution will result. The distribution of Q for the Wilson gauge action has been found to be Gaussian to a very good approximation for both quenched QCD [15, 16] and full QCD where the Wilson gauge action is complemented by the Wilson fermion action [1] or the Wilson-clover action [17].

Alternate distributions of the topological charge can occur in a finite volume if the correlation length of the topological charge density for a particular lattice gauge action approaches the length of the lattice dimensions.

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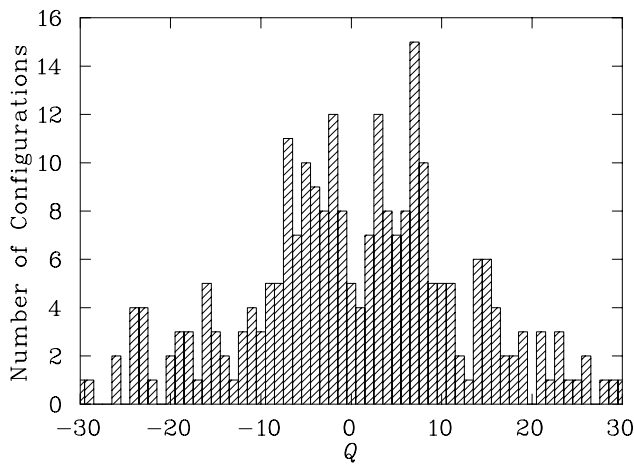§Electronic address: fxlee@gwu.edu

FIG. 1: Histogram illustrating the number of configurations in our ensemble of 250 configurations having a particular topological charge, Q. A suppression of $Q \sim 0$ configurations is observed.
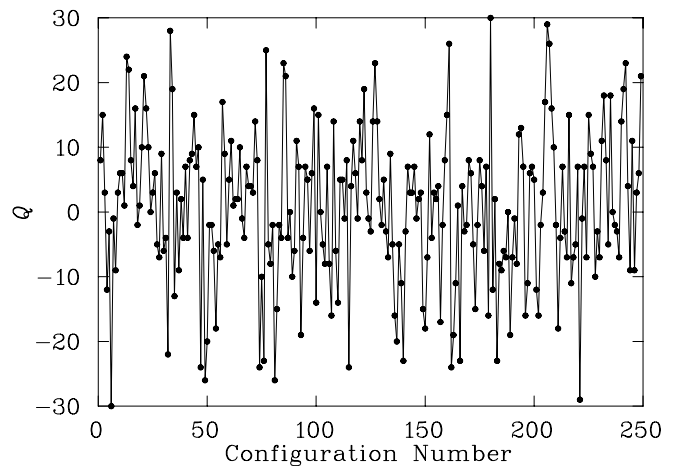

FIG. 2: The time evolution of the topological charge plotted as a function of simulation time as represented by the configuration number. 1000 pseudo-heatbath sweeps are performed between each gauge field sample.

Figure 1 displays a histogram of the topological charge from an ensemble of 250 quenched Iwasaki [7, 8] gauge configurations at $\beta = 9.1674$ on a $28^3 \times 44$ lattice, where the lattice spacing a is 0.113 fm. The topological charge is calculated using the highly-improved, three-loop $\mathcal{O}(a^4)$-improved lattice field-strength tensor [18] on 10-sweep cooled configurations obtained with a three-loop $\mathcal{O}(a^4)$-improved action. The gauge configurations represented in Fig. 1 are separated by 1000 pseudo-heatbath sweeps in an attempt to obtain uncorrelated configurations. Fig. 2 illustrates the time evolution of the topological charge plotted as a function of simulation time, represented by the configuration number. Acceptable movement of the topological charge is indicated by the rapidity and amplitude of the oscillations. To the best of our knowledge, this is the first time a double-peaked structure in the probability distribution of the topological charge has been revealed for a renormalization-group improved gauge action. It would be interesting to examine this distribution for the DBW2 action.

For any lattice action, the distribution of the topological charge will broaden as the volume of the lattice increases, such that

$$\langle Q^2 \rangle = \chi V . \tag{4}$$

As the infinite-volume continuum limit is approached and correlation lengths diverge, it will become increasingly difficult to evolve the topological charge over the broad range demanded by Eq. (4). In particular, a symmetric distribution about $Q = 0$ is required to preserve the symmetries of QCD.

Recognizing the need for improvement in the evolution of the topological charge in the Markov chain process, we present a simple transformation in the following section, that may be applied to a gauge-field configuration of quenched QCD or dynamical-fermion QCD that changes the sign of Q while leaving the action invariant. The transformation provides an improved unbiased estimator of the ensemble average and is essential in improving the ergodicity of the Markov chain process.

II. GAUGE-LINK TRANSFORMATION

The index theorem [19] relates the topological charge Q to the chirality index of the Dirac operator D on a continuum 4-torus as

$$Q = \mathrm{index}(D) \equiv n_- - n_+ . \tag{5}$$

Here n_+ and n_- are the number of exact zero eigenmodes, $D\psi = 0$, with positive, $\gamma_5 \psi = +\psi$, (right-handed) and negative, $\gamma_5 \psi = -\psi$, (left-handed) chiralities respectively.

This link between the topological charge and the chirality (or helicity) of zero eigenmodes of the Dirac operator identifies parity as the transformation for changing the sign of the topological charge while leaving the action invariant. Helicity transforms as a pseudoscalar under rotations, whereas the action of QCD, designed to conserve parity, transforms as a scalar under rotations. For the improper rotation of the parity transformation, the right-handed modes will become the left-handed, and vice versa, changing the sign of Q.

In deriving the transformation of the links under parity, we begin with the transformation of the gauge potential. Under the parity transformation

$$A_i(\vec{x}, t) \rightarrow -A_i(-\vec{x}, t), \quad \text{and} \quad \partial_i \rightarrow -\partial_i , \tag{6}$$

for the spatial indices $i = 1, 2, 3$ and

$$A_4(\vec{x}, t) \rightarrow A_4(-\vec{x}, t), \quad \text{and} \quad \partial_4 \rightarrow \partial_4 . \tag{7}$$

Here the 3×3 colour matrix degrees of freedom of $A_\mu(x)$ are implicit. The non-abelian field strength tensor $F_{\mu\nu}$ is

$$F_{\mu\nu} = \partial_\mu A_\nu - \partial_\nu A_\mu + i\,g\,[A_\mu, A_\nu]\,. \qquad (8)$$

Under parity transformations

$$F_{ij} \to F_{ij}, \quad F_{4j} \to -F_{4j}, \quad \text{and} \quad F_{i4} \to -F_{i4}\,. \qquad (9)$$

Hence the action

$$S = \frac{1}{2} \int d^4x\,\mathrm{Tr}\,(F_{\mu\nu}(x)\,F_{\mu\nu}(x))\,, \qquad (10)$$

is invariant under parity while the topological charge

$$Q = \frac{g^2}{32\pi^2} \int d^4x\,\epsilon_{\mu\nu\rho\sigma}\,\mathrm{Tr}\,(F_{\mu\nu}(x)\,F_{\rho\sigma}(x))\,, \qquad (11)$$

changes sign due to the presence of $\epsilon_{\mu\nu\rho\sigma}$ ensuring the presence of one and only one time component in the field strength tensor product.

The gauge-field links are related to the gauge potential via

$$U_\mu(x) = \exp\left(i\,g \int_0^a A_\mu(x + \lambda\,\hat\mu)\,d\lambda\right)\,, \qquad (12)$$

where $x \equiv (\vec{x}, t)$. Under the parity transformation, the spatial components, $i = 1, 2, 3$, of the links transform as

$$\mathcal{P}\,U_i(x)\,\mathcal{P}^\dagger = \exp\left(-i\,g \int_0^a A_i(-\widetilde{x} - \lambda\hat\imath)\,d\lambda\right)\,, (13)$$

$$= U_i^\dagger(-\widetilde{x} - a\hat\imath)\,, \qquad (14)$$

where

$$-\widetilde{x} \equiv (-\vec{x}, t)\,. \qquad (15)$$

Similarly, the time components transform as

$$\mathcal{P}\,U_t(x)\,\mathcal{P}^\dagger = \exp\left(i\,g \int_0^a A_t(-\widetilde{x} + \lambda\hat{t})\,d\lambda\right)\,, (16)$$

$$= U_t(-\widetilde{x})\,. \qquad (17)$$

The exact nature of the parity transformation on the links follows from the fact that parity is an exact symmetry on the hypercubic lattice.

It is interesting to examine the manner in which the lattice action density and lattice field-strength tensor transform under parity. Consider the product of links about an elementary plaquette located at space-time point x, in the μ - ν plane

$$U_{\mu\nu}(x) \equiv U_\mu(x)\,U_\nu(x + \hat\mu)\,U_\mu^\dagger(x + \hat\nu)\,U_\nu^\dagger(x)\,, \qquad (18)$$

and its transformation under parity. For spatially oriented plaquettes, the untransformed plaquette $U_{ij}(x)$ originates from x, and loops counter-clockwise in the positive $\hat\imath$, $\hat\jmath$ direction

$$U_i(x)\,U_j(x + \hat\imath)\,U_i^\dagger(x + \hat\jmath)\,U_j^\dagger(x)\,. \qquad (19)$$

Under the parity transformation $U_{ij}(x)$ transforms to

$$U_i^\dagger(-\widetilde{x} - \hat\imath)\,U_j^\dagger(-\widetilde{x} - \hat\imath - \hat\jmath)\,U_i(-\widetilde{x} - \hat\jmath - \hat\imath)\,U_j(-\widetilde{x} - \hat\jmath)\,, \quad (20)$$

which is the spatial plaquette originating from $-\widetilde{x}$, looping in a counter-clockwise orientation again, this time in the negative $\hat\imath$, $\hat\jmath$ direction. The space-time oriented plaquettes originating from x and looping counter-clockwise in the positive $\hat\imath$, $\hat{t}$ direction

$$U_i(x)\,U_t(x + \hat\imath)\,U_i^\dagger(x + \hat{t})\,U_t^\dagger(x)\,, \qquad (21)$$

transform to

$$U_i^\dagger(-\widetilde{x} - \hat\imath)\,U_t(-\widetilde{x} - \hat\imath)\,U_i(-\widetilde{x} - \hat\imath + \hat{t})\,U_t^\dagger(-\widetilde{x})\,, \quad (22)$$

which is the space-time oriented plaquette originating from $-\widetilde{x}$ but this time looping clockwise in the negative $\hat\imath$, positive $\hat{t}$ direction.

The connection between these link products and the lattice field strength tensor is provided by

$$g\,F_{\mu\nu}(x) = \frac{1}{8\,i}\left[(\mathcal{O}_{\mu\nu}(x) - \mathcal{O}_{\mu\nu}^\dagger(x))\right.$$
$$\left. -\frac{1}{3}\mathrm{Tr}\,(\mathcal{O}_{\mu\nu}(x) - \mathcal{O}_{\mu\nu}^\dagger(x))\right]\,, \quad (23)$$

where $\mathcal{O}_{\mu\nu}(x)$ is the sum of 1×1 link paths oriented about x in the μ - ν plane

$$\mathcal{O}_{\mu\nu}(x) = U_\mu(x)\,U_\nu(x + \hat\mu)\,U_\mu^\dagger(x + \hat\nu)\,U_\nu^\dagger(x)$$
$$+ \; U_\nu(x)\,U_\mu^\dagger(x + \hat\nu - \hat\mu)\,U_\nu^\dagger(x - \hat\mu)\,U_\mu(x - \hat\mu)$$
$$+ \; U_\mu^\dagger(x - \hat\mu)\,U_\nu^\dagger(x - \hat\mu - \hat\nu)\,U_\mu(x - \hat\mu - \hat\nu)\,U_\nu(x - \hat\nu)$$
$$+ \; U_\nu^\dagger(x - \hat\nu)\,U_\mu(x - \hat\nu)\,U_\nu(x + \hat\mu - \hat\nu)\,U_\mu^\dagger(x)\,. \qquad (24)$$

Taking the Hermitian conjugate of $\mathcal{O}_{\mu\nu}(x)$ changes the orientation of the link products from counter-clockwise to clockwise. Noting further that $F_{\mu\nu}(x)$ is odd under such transformations, we see that the orientations of the link-product parity transformations of Eqs. (20) and (22) are precisely those required to recover the continuum transformations of $F_{\mu\nu}(x)$ in Eq. (9). While the topological charge density undergoes a parity transformation, the magnitude of the topological charge remains invariant, as all lattice sites are summed over. Similarly, the lattice action

$$S = \beta \sum_{\substack{x \\ \mu<\nu}} \frac{1}{6}\,\mathrm{Tr}\,(2 - U_{\mu\nu}(x) - U_{\mu\nu}^\dagger(x))\,, \qquad (25)$$

is even under the orientation transformation $U_{\mu\nu}(x) \to U_{\mu\nu}^\dagger(x)$, and since all sites are summed over, the lattice gauge action is invariant under the lattice parity transformation.

III. NUMERICAL RESULTS

The parity transformations of the gauge links in Eqs. (14) and (17) have been coded in Fortran 90 [20]

and tested on a $12^3 \times 24$ lattice with the tadpole-improved Lüscher-Weisz gauge action [21]. We use three methods to examine the properties of the parity transformed configurations.

The 3-loop improved field strength tensor [18] accompanied by the associated 3-loop improved cooling action are used to provide a determination of the topological charge Q and action S for a cooled gauge configuration and its parity transformed partner. The transformed action and topological charge magnitude agree to machine precision.

The low-lying spectral flow of the hermitian Wilson-Dirac operator $H_W = \gamma_5 D_W$ is examined. Under the parity transformation, the low-lying eigenvalues of H_W change sign such that the slope of the spectral flow (proportional to the topological charge giving rise to the zeromode) changes sign. Since H_W is of even dimension (lattice volume × number of colors × number of Dirac indices), $\det(H_W) = \det(\gamma_5) \times \det(D_W)$ is unaffected by the parity transformation, as required to preserve parity in dynamical fermion QCD simulations.

Finally, the topological charge is determined by counting the exact zeromodes of the massless overlap Dirac operator. Under a parity transformation, the number of exact zeromodes with positive (right-handed) and negative (left-handed) chiralities exchange as expected.

IV. DISCUSSION AND CONCLUSIONS

The manner in which the parity transformation is used in practice will depend on the application at hand for the gauge fields. Often, exact parity can be enforced during the construction of correlation functions by averaging opposite-sign nontrivial momenta of the lattice Green's functions [22]. In other applications, exact parity can be enforced by doubling the number of gauge field configurations, averaging each field configuration with its parity transformed partner. Finally, the transform can be applied in the Markov chain process itself, applying the transform randomly with a 50% probability prior to writing the gauge configuration to disk, or equivalently, following the reading of the configuration to be evolved, from disk.

Motivated by the lattice index theorem, we have illustrated how a parity transformation on the $SU(3)$ link-variables of lattice gauge configurations reverses the sign of topological charge while leaving the action invariant. The transformation provides an improved unbiased estimator of the ensemble average and is essential in improving the ergodicity of the Markov chain process.

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