Numerical study of the lattice index theorem using improved cooling and overlap fermions

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We investigate the topological charge and the index theorem on finite lattices numerically. Using mean field improved gauge-field configurations we calculate the topological charge Q using the gluon field definition with $\mathcal{O}(a^4)$-improved cooling and an $\mathcal{O}(a^4)$-improved field strength tensor $F_{\mu\nu}$. We also calculate the index of the massless overlap fermion operator by directly measuring the differences between the numbers of zero modes with left- and right–handed chiralities. For sufficiently smooth field configurations we find that the gluon field definition of the topological charge is an integer to better than 1%, and furthermore that this agrees with the index of the overlap Dirac operator, i.e., the Atiyah-Singer index theorem is satisfied. This establishes a benchmark for reliability when calculating lattice quantities that are very sensitive to topology.

I. INTRODUCTION

The connection between the topology of a background gauge field and fermion zero modes is related to the axial anomaly and the large η-η' mass splitting in QCD. Lattice gauge theory is the tool best suited to the study of these nonperturbative issues. We study this connection in QCD formulated on a periodic lattice, i.e., on a four-dimensional toroidal mesh. For a fine enough lattice and/or a sufficiently smooth gauge-field configuration we should recover the results for continuum QCD on a four-torus. In particular, we should recover the Atiyah-Singer index theorem [1].

In the continuum the Dirac operator $D = \gamma_\mu (\partial_\mu + i g A_\mu)$ of massless fermions in a smooth background gauge field with a nontrivial topology has eigenmodes with zero eigenvalue (i.e., "zero modes") which are also chiral eigenstates of positive or negative chirality. The Atiyah-Singer index theorem [1] gives the result

$$Q = \text{index}(D), \tag{1.1}$$

where

$$Q = \frac{g^2}{32\pi^2} \int d^4x \, \epsilon_{\mu\nu\rho\sigma} \, \text{tr}(F_{\mu\nu} F_{\rho\sigma}) \tag{1.2}$$

is the topological charge of the background gauge field and where

$$\text{index}(D) \equiv n_- - n_+ \tag{1.3}$$

is the chirality index of the Dirac operator. Here n_+ and n_- are the number of zero eigenmodes with positive (right-

handed) and negative (left-handed) chiralities respectively, i.e., $D\psi = 0$ with $+/-$ chiralities such that $\gamma_5 \psi = \pm \psi$. These results apply to QCD defined on a continuum four-torus, where ultimately we wish to take the size of the four-torus to infinity, i.e., the infinite-volume limit.

However, in the lattice formulation one has ambiguities associated with the discretization and in general one can expect the index theorem of Eq. (1.1) to be satisfied only on a sufficiently fine lattice and/or after sufficient smoothing of the gauge fields. The use of improved operators and actions will lead to the index theorem being satisfied for less stringent conditions on lattice spacing and/or smoothness. There are different ways to calculate Q for a given gauge field configuration, e.g., using the gauge-field tensor definition [2] of Eq. (1.2) or using the geometrical definition [3]. In this study we focus on the definition in Eq. (1.2). On a continuum four-torus the two definitions of topological charge for the gauge field are necessarily identical. However, in the calculation of hadronic observables using typical lattices, the configurations in the ensembles are too coarse for the lattice definitions of Eq. (1.2) to lead to integer topological charge and so the index theorem is not satisfied.

In an arbitrary gauge field, the Wilson fermion operator does not have exact zero modes due to the Wilson term, which removes fermion doublers and breaks chiral symmetry. Attempts to study the index theorem with such an action require one to estimate the number of "zero modes" by looking at low lying real eigenvalues [4]. Because of the difficulties in estimating the index of the Wilson fermion operator in a precise manner, it is difficult to reach a definite conclusion concerning the validity of the index theorem on a finite lattice with Wilson fermions. In the case of Ginsparg-Wilson (GW) Dirac fermions [5–7] there is an exact lattice realization of chiral symmetry [8] and the GW Dirac operator possesses exact zero modes. Hence the ambiguity associated with the need to subjectively estimate the number of "zero modes" of the Wilson fermions is absent. A good review and introduction to many of these issues can be found in Ref. [9].

There are several numerical studies [10–15] of the index theorem on a finite lattice. In Ref. [10] the overlap fermion formalism is used to estimate the probability distribution of

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topological charge $p(Q)$ in pure SU(2) gauge theory by examining the spectral flow of $H(\mu)$, where $H(\mu)$ is the Hermitian Wilson-Dirac operator. The study in Ref. [11] explores the real eigenvalues of the Wilson-Dirac operator, which are identified as the lattice counterparts of the continuum zero modes. These authors studied topology by examining the complete spectrum of the fermion matrix in SU(2) gauge theory on small lattices. Reference [12] uses the spectral flow method to perform a comprehensive study of both quenched SU(3) and dynamical fermion configurations. There the role of the Sheikholeslami-Wohlert term is also examined.

We focus here on Neuberger's overlap Dirac operator, which is an explicit solution of the Ginsparg-Wilson relation, and investigate the Atiyah-Singer index theorem on a finite lattice by numerical methods. In a recent paper [16], Adams performed an analytical study which showed that the index theorem was satisfied by the overlap operator in the continuum limit. We calculate the index of the overlap fermion operator directly by measuring the number of left minus right zero modes of the overlap Dirac operator D.

In measuring the gauge-field definition of the topological charge, Q, we use an $\mathcal{O}(a^4)$-improved definition of the field strength tensor leading to an improved topological charge operator. We also use a mean-field-improved Symanzik gluon action in the quenched approximation to generate our ensemble of configurations. Where we have employed cooling to smooth our configurations, we have used an $\mathcal{O}(a^4)$-improved gluon action in the cooling algorithm. The resulting Q approaches integer values after a few cooling sweeps and has been verified to be stable for hundreds to thousands of cooling sweeps.

The paper is organized as follows. In Sec. II we introduce the details of our calculation of the improved gauge-field topological charge Q. In Sec. III we review the overlap quark propagator and describe our calculation of index(D). Our results are described in Sec. IV and finally our summary and discussion are presented in Sec. V.

II. IMPROVED COOLING AND TOPOLOGY

To investigate the topology of gauge fields on the lattice we first construct an ensemble of gauge-field configurations. In lattice QCD, the gluon fields are represented by SU(3) matrices on each link connecting adjacent lattice sites. These links are parallel transport operators between the lattice sites. We use a parallel Cabibbo-Marinari [17] pseudo-heat-bath algorithm with three diagonal SU(2) subgroups looped over twice and appropriate link partitioning [18].

For typical lattice spacings used in simulations of QCD the link configurations in the ensemble have fluctuations on many scales. In particular, such typical link configurations are not smooth at the scale of the lattice spacing. However, the Boltzmann factor $e^{-S_{\text{gauge}}}$ with $S_{\text{gauge}} \propto 1/g^2$ will ensure that link configurations become increasingly smooth as the continuum limit is approached ($g \to 0$, $a \to 0$). But the cost is that the volumes that one can afford to simulate also become correspondingly smaller.

One common approach to probing the medium to long

range topological structure of typical link configurations is to *cool* them sufficiently that they become approximately smooth at the scale of the lattice spacing [19]. Cooling involves recursively modifying the link values to locally minimize the action. As we sweep repeatedly over the whole lattice we reduce the total action, smoothing out fluctuations on successively larger scales [20]. This quickly eliminates the high-frequency, rough components of the fields, leaving relatively smooth topological structures. Once the link configuration has been cooled sufficiently, we can expect the cooling process to preserve the global topological charge Q. If we cool indefinitely a link configuration on a sufficiently fine lattice such that we preserve the global topological charge Q, then we should converge toward the minimum action solutions with charge Q, i.e., we should converge to self-dual configurations ($F_{\mu\nu} = \tilde{F}_{\mu\nu}$). The resulting self-dual configurations on the four-torus should contain only $|Q|$ instantons (if $Q > 0$) or anti-instantons (if $Q < 0$). The action of an instanton or anti-instanton in infinite space-time is known analytically and is given by $S_0 = 8\pi^2/g^2$. Instantons and anti-instantons have the property that they are scale invariant, i.e., they can have any scale in the infinite four-volume continuum and their action S_0 is unaffected. In infinite space-time in the continuum, a *self-dual* gluon configuration with action S will necessarily have topological charge $|Q| = S/S_0$ and contain only instantons (or anti-instantons). To the extent that the finite volume of a four-torus is sufficiently large compared with the size of the instantons on it, one can expect the above results to hold.

However, it is well established that cooling with the standard Wilson action eventually destroys (anti-)instanton configurations, due to the discretization errors inherent in the Wilson action [21]. The Wilson gluon (i.e., Yang-Mills) action at each lattice site is calculated from the plaquette, a closed product of four link operators

$$S_{\text{Wil}} = \beta \sum_x \sum_{\mu < \nu} \frac{1}{N} \text{Re tr}(1 - U_{\mu\nu}) \qquad (2.1)$$

where the plaquette operator $U_{\mu\nu}$ is

$$U_{\mu\nu} = U_\mu(x) U_\nu(x+\mu) U_\mu^\dagger(x+\nu) U_\nu^\dagger(x). \qquad (2.2)$$

This Wilson plaquette action contains deviations from the continuum Yang-Mills action of $\mathcal{O}(a^2)$ where a is the lattice spacing. This problem may be remedied by improving the action. Tree-level improvement of the classical lattice action combined with mean-field (i.e., tadpole) nonperturbative improvement [22] provides a simple and very effective means of eliminating lowest-order discretization errors. The simplest improvement of the classical gauge action on the lattice is achieved by taking a linear combination of the Wilson plaquette and an $a \times 2a$ rectangle, i.e., Symanzik improvement. Since the plaquette and rectangle have different $\mathcal{O}(a^2)$ errors they can be added in a linear combination in such a way that these $\mathcal{O}(a^2)$ errors cancel, leaving only errors of $\mathcal{O}(a^4)$ in the classical (i.e., tree-level) gauge action. One can preserve this improvement at the nonperturbative level by combining this with mean-field improvement of the links [23]. More recently, DeForcrand *et al.* [24] have used tree-

level improvement to construct a lattice action which eliminates $\mathcal{O}(a^4)$ errors and leaves only $\mathcal{O}(a^6)$ errors, by using combinations of up to five different closed-loop products of link operators (Wilson loops). From these five loops, particular linear combinations were studied in detail and were referred to as three-loop, four-loop, and five-loop improved actions. The difference is the number of nonzero contributions in the linear combination of the five planar loops. They represent the improved action as

$$S_{\text{imp}} = \sum_{i=1}^{5} c_i S_i,\tag{2.3}$$

where the S_i are the actions calculated as per Eq. (2.1), but using five different Wilson loops, and the c_i are the weighting constants tuned to eliminate the $\mathcal{O}(a^2)$ and $\mathcal{O}(a^4)$ errors. Additional details may be found in Ref. [24].

In our work we construct improved actions utilizing the results of DeForcrand *et al*. However, we have chosen to improve the topological charge via an improved field strength tensor. In particular, we employ an $\mathcal{O}(a^4)$-improved definition of $F_{\mu\nu}$ in which the standard clover sum of four 1×1 Wilson loops lying in the μ,ν plane is combined with 2×2 and 3×3 Wilson loop clovers. Bilson-Thompson *et al*. [25] find

$$gF_{\mu\nu} = \frac{-i}{8}\left[\left(\frac{3}{2}W^{1\times1} - \frac{3}{20u_0^4}W^{2\times2} + \frac{1}{90u_0^8}W^{3\times3}\right) - \text{H.c.}\right]_{\text{traceless}},\tag{2.4}$$

where $W^{n\times n}$ is the clover sum of four $n\times n$ Wilson loops and where $F_{\mu\nu}$ is made traceless by subtracting $1/3$ of the trace from each diagonal element of the 3×3 color matrix. This definition reproduces the continuum limit with $\mathcal{O}(a^6)$ errors. We employ the plaquette measure of the mean link

$$u_0 = \langle \tfrac{1}{3}\text{Re tr}\, U_{\mu\nu}\rangle_{x,\mu\neq\nu}^{1/4},\tag{2.5}$$

which is updated after each sweep through the lattice. The mean link u_0 rapidly tends to 1 under cooling, thus reproducing the classical limit. However, early in the cooling procedure, the fields are not classical and u_0 serves to tadpole improve the definition of $F_{\mu\nu}$.

This improved field-strength tensor can be used directly in Eq. (1.2), resulting in a topological charge that is automatically free of discretization errors to the same order as the field-strength tensor. On self-dual configurations, this operator produces integer topological charge to better than 4 parts in 10^4. Furthermore, since the gluon (i.e., Yang-Mills) action is also based upon the field-strength tensor, it is possible to create what we refer to as a *reconstructed action* based upon the improved field-strength tensor. The value of the action calculated with the reconstructed action operator can be compared with the value calculated with the standard improved action operator Eq. (2.3) at each cooling sweep as a double-
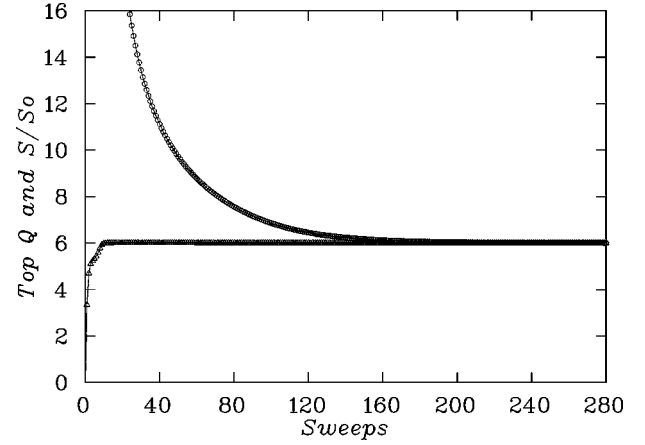

FIG. 1. An example plot of how improved cooling stabilizes the action (circles) and topological charge (triangles) at consistent values. The action has been rescaled by dividing it by S_0, the action of a single instanton.

checking mechanism to ensure that the two different approaches to tree-level improvement removing $\mathcal{O}(a^4)$ errors yield consistent results.

The principal criteria by which we may judge the value of an improvement scheme are how quickly and how closely the results for the topological charge Q approach integer values, and the stability with which they remain at that integer. On a lattice, the discretization errors prevent us from obtaining exactly integer results. However, the more successful the improvement program, the more rapidly we can expect cooling to lead us to a stable Q, and the closer this will be to an integer. Figure 1 shows how both the action and topological charge approach the same integer value as a function of the number of cooling sweeps. This is exactly as we would expect for Q. As we approach self-duality on the four-torus we appear to recover $S/S_0 = |Q|$ just as in the continuum infinite-volume limit. Recall that the positivity of $(F^a_{\mu\nu} \pm \tilde{F}^a_{\mu\nu})^2$ ensures that $0 \leqslant \int d^4x (F^a_{\mu\nu} \pm \tilde{F}^a_{\mu\nu})^2 = 2\int d^4x[(F^a_{\mu\nu})^2 \pm F^a_{\mu\nu}\tilde{F}^a_{\mu\nu}]$ and hence

$$S = \frac{1}{4}\int d^4x (F^a_{\mu\nu})^2 \geqslant \frac{1}{4}\left|\int d^4x F^a_{\mu\nu}\tilde{F}^a_{\mu\nu}\right| = \frac{8\pi^2}{g^2}|Q| = S_0|Q|,\tag{2.6}$$

where we have defined $S_0 \equiv 8\pi^2/g^2$. Self-dual configurations $F^a_{\mu\nu} = \pm\tilde{F}^a_{\mu\nu}$ saturate this identity, i.e., $|Q| = S/S_0$. This result applies independent of the shape of the space-time manifold and so applies on the continuum four-torus as well as for infinite space-time. However, note that Nahm's theorem [26] implies that there is no self-dual $|Q|=1$ configuration possible on the four-torus. In infinite space-time S_0 is the single instanton or anti-instanton action.

While an in-depth comparison of the various cooling schemes is beyond the scope of this report, we summarize by noting that it has been determined [25] that three-loop improved cooling with a three-loop topological charge operator gives excellent results in terms of how close the calculated values of S/S_0 and Q come to integer values, the stability

TABLE I. Parameters of generated lattices.

Action	Volume	N_{therm}	N_{sep}	β	a (fm)	u_0	Physical volume (fm)
Improved	$8^3 \times 16$	5000	500	4.80	0.093	0.89625	$0.75^3 \times 1.50$
Improved	$8^3 \times 16$	5000	500	4.38	0.165	0.87821	$1.32^3 \times 2.64$
Improved	$12^3 \times 24$	5000	500	4.60	0.125	0.88888	$1.50^3 \times 3.0$

with which they remain at that integer, and the speed with which cooling can be performed.

III. OVERLAP FERMIONS AND ZERO MODES

The overlap fermion formalism [27] provides a way of realizing exact chiral symmetry on the lattice. The massless overlap-Dirac operator can be written as

$$D_o(0) = [1 + \gamma_5 \epsilon(H_w)], \qquad (3.1)$$

where $\epsilon(H_w)$ is the matrix sign function

$$\epsilon(H_w) = \frac{H_w}{|H_w|}, \qquad H_w = \gamma_5 D_w, \qquad (3.2)$$

D_w is the usual Wilson-Dirac operator

$$D_w = M_{a\alpha m, b\beta n}$$

$$= \delta_{a,b} \delta_{\alpha,\beta} \delta_{m,n} - \kappa \sum_{\mu=1}^{4} [(1-\gamma_\mu)_{\alpha\beta}$$

$$\times U_\mu(m)_{ab} \delta_{m,n-\hat{\mu}} + (1+\gamma_\mu)_{\alpha\beta}$$

$$\times U_\mu^\dagger(m-\hat{\mu})_{ab} \delta_{m,n+\hat{\mu}}], \qquad (3.3)$$

and κ is the hopping parameter,

$$\kappa = \frac{1}{-2m+8}. \qquad (3.4)$$

The bare mass parameter for the Wilson kernel in the overlap formalism m has to be in the range $(0,2)$ for $D_o(0)$ to describe a single massless Dirac fermion. Note that the m used in this context is the negative of the bare mass used in simulations with the Wilson quark action itself. In principle, any value of m in the above range should give the same continuum theory. But on a finite lattice, where volume and lattice spacing are finite, the results for the overlap action can depend on the value chosen for m. For the purposes of using overlap fermions to be most sensitive to the topology of the background gauge fields [12], m has to be chosen $m > m_1(g^2)$ for some $m_1(g^2)$ going to zero in the continuum limit. For typical gauge configurations $m_1(g^2)$ is slightly less than m_c, where m_c is the critical value of m at which the pion mass extrapolates to zero in a simulation with ordinary Wilson fermions. In the hopping parameter formalism, the κ should be in the range $(\kappa_c, 0.25)$ at tree level. The massless overlap operator $D_o(0)$ has been shown [7] to satisfy the Ginsparg-Wilson relation

$$\{\gamma_5, D_o(0)\} = D_o(0) \gamma_5 D_o(0). \qquad (3.5)$$

Its spectral properties are as follows.

The modulus of the eigenvalue of $D_o(0)$ lies in the range $[0,2]$. It has exact zero eigenvalues which are associated with topology. The corresponding eigenvectors are also eigenvectors of γ_5. They need not occur in pairs. There can be n_+ zero modes with eigenvalues of γ_5 equal to 1 and n_- zero modes with eigenvalues of γ_5 equal to -1. It also has eigenvalues equal to ± 2 which also have definite chirality. Their difference $(n'_+ - n'_-)$ is equal to $(n_- - n_+)$.

Nonzero eigenvalues of $D_o(0)$ are complex, their moduli are less than 2, they come as pairs, and they are conjugate to each other. The associated eigenvectors are not eigenvectors of γ_5.

In practice, we calculate a small number of low-lying eigenvalues and eigenvectors of $D_o^\dagger(0)D_o(0)$. Note that $D_o^\dagger(0)D_o(0)$ commutes with $D_o(0)$ and it is Hermitian and positive definite. It also commutes with γ_5 and can be simultaneously diagonalized. Hence, $D_o^\dagger(0)D_o(0)$ has zero eigenmodes of definite chirality which are also the zero eigenmodes of $D_o(0)$.

We compute low-lying eigenmodes of $D_o^\dagger(0)D_o(0)$ using the Ritz functional algorithm [28]. In the computation of the overlap operator, the time consuming part is the calculation of the matrix sign function $\epsilon(H_w)$. There are several numerical approaches by which to approximate the sign function $\epsilon(z)$ [29–31]. We adopt the optimal rational approximation [30] with a ratio of polynomials of degree 12 in the Remez algorithm. We find the error to the approximation of $\epsilon(z)$ to be within 10^{-6} in the range $[0.04,1.5]$ of the argument z. To improve the accuracy as well as efficiency of computation of the matrix sign function $\epsilon(H_w)$, a number of low-lying eigenvalues of H_w whose absolute values are less than 0.04 are projected out. Since

$$D_o^\dagger(0)D_o(0) = D_o^\dagger(0) + D_o(0), \qquad D_o^\dagger(0) = \gamma_5 D_o(0)\gamma_5, \qquad (3.6)$$

we use chiral states in the Ritz functional algorithm, and hence can save one matrix multiplication [32] per iteration.

IV. RESULTS AND COMPARISON

Configurations have been generated on an $8^3 \times 16$ lattice at both $\beta = 4.80$ and $\beta = 4.38$ as well as on a $12^3 \times 24$ lattice at $\beta = 4.60$. Configurations are selected after $N_{\text{therm}} = 5000$ thermalization sweeps from a cold start and every $N_{\text{sep}} = 500$ sweeps thereafter with the average link u_0 fixed at the time of the first sample configuration being taken. Lattice parameters are summarized in Table I.

We first use the gluon field definition to calculate the topological charge Q by using the three-loop improved field

strength $F_{\mu\nu}$ as described in Sec. II. For each configuration we measure the topological charge by cooling with the three-loop improved action for just enough cooling sweeps that Q is integer to within 1%. This typically requires from one to 30 cooling sweeps depending on the lattice spacing and the particular configuration. We retain both the original uncooled configurations as well as these ''just cooled'' configurations. We denote the topological charge obtained from the ''just cooled'' gluon field configurations as Q_g.

Secondly, we use the overlap formalism to calculate the index of the gauge configurations at two κ values, i.e., $\kappa = 0.19$ corresponding to $m = 1.36$ and $\kappa = 0.2499$ corresponding to $m = 1.999$. The second value approaches the largest allowed value of m to describe a single massless Dirac fermion. We extract the overlap index for both the original uncooled and the ''just cooled'' cooled configurations and denote the results by Q_d and $Q_{d\,cooled}$, respectively.

The results for the small-volume $8^3 \times 16$, $\beta = 4.80$ lattice are collected in Table II. We see that since the physical volume of our lattice is rather small, only a few configurations have nontrivial topology. The index Q_d of the overlap operator calculated at the two different κ values is the same for all 30 configurations. The range of cooling sweeps needed to get Q to within 1% of integer was between 1 and 7 with an average of approximately 3. The index for these ''just cooled'' configurations differs from these for only one of the 30 configurations, i.e., configuration 26. For all of the configurations the gluon topological charge Q_g is identical to the index of the overlap operator extracted from ''just cooled'' configurations $Q_{d\,cooled}$. These results indicate that on such a fine lattice ($a = 0.093$ fm) topology is relatively well represented and the index theorem is ''almost'' valid for uncooled configurations. We see also that for ''just cooled'' configurations the index theorem appears to be perfectly satisfied. Future investigations should explore the possible volume dependence of these results.

We next turn to the coarser ($a = 0.165$ fm), larger-volume $8^3 \times 16$, $\beta = 4.38$ lattice. The results for this lattice are shown in Table III. Since the physical volume of the lattice is larger there is more nontrivial topology than before, which is reflected in the large Q values. We find that Q_d now differs in 30% of cases depending on which value of κ is used in the overlap kernel. In some cases, e.g., for configuration 14, the disagreement is very significant indeed. The range of cooling sweeps needed for this coarse lattice was between 4 and 28 with an average of approximately 12.5. In addition to measuring the gluon topological charge on these ''just cooled'' configurations Q_g, on this lattice we have also attempted to identify the gluon topological charge after just three cooling sweeps, i.e., Q_{g3}. This was done by identifying the nearest integer to the gluon topological charge after just three cooling sweeps and was motivated by the observation that the action density and the reconstructed action density matched within 10% after three sweeps. We see that Q_{g3} is reasonably consistent with the robust Q_g, but there are significant differences. Q_{g3} also has significant differences from the Q_d values. The disagreement between Q_d and Q_g is more significant on this coarse lattice.

TABLE II. Results for $\beta = 4.80$ improved gauge configurations on an $8^3 \times 16$ lattice with spacing $a = 0.093$ fm: Q_d is calculated from the zero modes of the overlap operator on the original uncooled configurations; Q_g is obtained using the improved topological charge operator for the ''just cooled'' configurations (i.e., configurations after just enough improved cooling sweeps to bring Q within 1% of integer); $Q_{d\,cool}$ is also calculated from the zero modes of the overlap operator, but on the ''just cooled'' configurations.

Configuration No.	$Q_d(\kappa = 0.19)$	$Q_d(\kappa = 0.2499)$	Q_g	$Q_{d\,cool}$
1	0	0	0	0
2	0	0	0	0
3	0	0	0	0
4	+1	+1	+1	+1
5	0	0	0	0
6	−1	−1	−1	−1
7	0	0	0	0
8	0	0	0	0
9	0	0	0	0
10	0	0	0	0
11	0	0	0	0
12	0	0	0	0
13	0	0	0	0
14	0	0	0	0
15	0	0	0	0
16	0	0	0	0
17	0	0	0	0
18	0	0	0	0
19	0	0	0	0
20	0	0	0	0
21	0	0	0	0
22	0	0	0	0
23	0	0	0	0
24	−1	−1	−1	−1
25	−2	−2	−2	−2
26	+1	+1	0	0
27	0	0	0	0
28	0	0	0	0
29	0	0	0	0
30	0	0	0	0

These differences may be interpreted by considering the size of the topological objects giving rise to exact zero modes [33]. At $\kappa = 0.19$, the overlap operator will typically miss zero modes associated with small topological objects. Indeed, for the six configurations where $Q_d(\kappa = 0.19) \neq Q_d(\kappa = 0.2499)$, $Q_d(\kappa = 0.2499)$ agrees better with Q_{g3} than with Q_g. This is as one might expect, as further cooling will remove topological objects smaller than the dislocation threshold of the improved cooling algorithm, which is typically two lattice spacings.

These results all suggest that for uncooled configurations on this coarser lattice topology is not well represented and the index theorem is badly violated. However, from the perfect agreement between Q_g and $Q_{d\,cool}$, we see that for ''just cooled'' configurations the index theorem is again perfectly

TABLE III. Results for $\beta=4.38$ improved gauge configurations on an $8^3\times16$ lattice with spacing $a=0.165$ fm: Q_d is calculated from the zero modes of the overlap operator on the original uncooled configurations; Q_g is obtained using the improved topological charge operator for the "just cooled" configurations; Q_{g3} is obtained using the improved topological charge operator for the configurations obtained after just three improved cooling sweeps; $Q_{d\,cool}$ is also calculated from the zero modes of the overlap operator, but on the "just cooled" configurations.

Configuration No.	$Q_d(\kappa=0.19)$	$Q_d(\kappa=0.2499)$	Q_{g3}	Q_g	$Q_{d\,cool}$
1	0	0	+1	0	0
2	+3	+3	+4	+3	+3
3	+1	0	0	0	0
4	0	0	0	0	0
5	0	0	−1	−1	−1
6	−1	−1	−1	−1	−1
7	+5	+4	+4	+6	+6
8	−1	−4	−2	−2	−2
9	+1	+1	+1	+1	+1
10	0	0	−1	0	0
11	−2	−2	−3	−3	−3
12	−1	−1	−1	−1	−1
13	+2	+2	+3	+2	+2
14	+3	−5	−4	−4	−4
15	−3	−3	−3	−3	−3
16	0	0	−1	0	0
17	0	−1	−1	0	0
18	−1	−1	−1	−1	−1
19	+1	+1	+1	+1	+1
20	+1	0	0	−2	−2

TABLE IV. Results for $\beta=4.60$ improved gauge configurations on a $12^3\times24$ lattice with spacing $a=0.125$ fm: Q_d is calculated from the zero modes of the overlap operator on the original uncooled configurations; Q_g is obtained using the improved topological charge operator for the "just cooled" configurations; $Q_{d\,cool}$ is also calculated from the zero modes of the overlap operator, but on the "just cooled" configurations.

Configuration No.	$Q_d(\kappa=0.19)$	Q_g	$Q_{d\,cool}$
1	−1	−1	−1
2	+1	+1	+1
3	−4	−4	−4
4	0	0	0
5	+1	+1	+1
6	−2	−2	−2
7	−2	−2	−2
8	−1	−1	−1
9	0	0	0
10	−2	−2	−2
11	+1	+1	+1
12	0	0	0
13	−3	−3	−3
14	−4	−3	−3
15	−2	−4	−4
16	−1	−2	−2
17	−5	−5	−5
18	−2	−3	−3
19	−5	−5	−5
20	−4	−4	−4

satisfied. In that sense, we conclude that our "just cooled" configurations are indeed smooth enough.

We now present in Table IV the results for the third lattice with an intermediate lattice spacing $a=0.125$ fm corresponding to $\beta=4.60$ and with lattice size $12^3\times24$. This lattice has the largest physical volume. The range of cooling sweeps needed for this medium-spaced lattice was between 2 and 14 with an average of approximately 8. As we might anticipate, the agreement of Q_g with Q_d in this case is worse than for the fine lattice but better than for the coarse lattice. We do not have results for the large $\kappa=0.2499$ case here, since on this larger lattice this marginal choice of κ proved numerically difficult. Calculating $Q_{d\,cool}$ with its "just cooled" configurations gives perfect agreement with Q_g for all configurations.

It is expected that $\langle Q^2\rangle$ should scale approximately as the volume V for large volumes, since the topological susceptibility is given by $\langle Q^2\rangle/V$ and should be volume independent. The ratio of this four-volume to that for the coarse lattice is 1.66. The mean Q^2 per configuration for this lattice is easily seen from Table IV to be $\langle Q^2\rangle=7.3$, whereas for the coarser, smaller-volume lattice in Table III we find $\langle Q^2\rangle=4.85$. We see that $\langle Q^2\rangle_{big}/\langle Q^2\rangle_{small}=1.51$ which is approximately equal to $V_{big}/V_{small}=1.66$. This level of agreement seems reasonable for such modest volume lattices and small numbers of configurations.

We also observe that for this largest lattice there appears to be a significant imbalance in the sign of Q in the ensemble and in particular the sign is consistently negative for the last eight configurations in the ensemble. If the configurations were uncorrelated, this would be very unlikely to occur. This suggests that for larger lattices, when measuring quantities that are very sensitive to topology, one should use an increased number of thermalization and separation sweeps. To balance the topological charge in the ensemble one should perhaps consider doubling the ensemble size by adding parity-transformed link configurations [34] which leave the action invariant but reverse the sign of Q.

V. CONCLUSIONS AND DISCUSSION

We have shown that overlap fermions are suitable for use in the study of topology and the Atiyah-Singer index theorem in lattice simulations. We have shown that with an improved gluon action and an improved definition of the gluon topological charge operator we can obtain near integer topological charge (within 1%) within a relatively small number of cooling sweeps. The finer the lattice the fewer cooling sweeps are needed to obtain these "just cooled" configurations. We found that for lattice spacings of $a=0.093$, 0.125, and 0.165 fm we needed on average 3, 8, and 12.5 improved cooling sweeps, respectively. For all

configurations on all lattices, we found the index theorem satisfied for these ''just cooled'' configurations. Even for the finest lattice and with an improved topological charge operator some small number of cooling sweeps was needed to obtain an integer gluon topological charge. On the finest lattice the index of the overlap operator appeared independent of κ and agreed with the ''just cooled'' overlap index 29 out of 30 times. This lattice appears then to be almost fine enough that the index theorem has meaning without cooling. For all lattices the index theorem appeared to be fully satisfied for the ''just cooled'' configurations. This provides us with a clear benchmark for smoothness and lattice spacing when calculating lattice quantities that are very sensitive to topology.

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