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Topological susceptibility from overlap fermion*

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We numerically calculate the topological charge of the gauge configurations on a finite lattice by the fermionic method with overlap fermions. By using the lattice index theorem, we identify the index of the massless overlap fermion operator to the topological charge of the background gauge configuration. The resulting topological susceptibility χ is in good agreement with the anticipation made by Witten and Veneziano.

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1. Introduction

Topology plays a fundamental role in quantum chromodynamics (QCD). One of the most intriguing features of QCD is its topological vacuum structure which results in phenomenological consequences such as the breaking of the axial $U_A(1)$ and chiral symmetries. The connection between the topology of a background gauge field and fermion zero modes is related to the axial anomaly and the large $\eta-\eta'$ mass splitting in QCD. In the $1/N_c$ expansion, the anomaly acts as a perturbation, displacing the pole of the $U_A(1)$ Goldstone boson to the actual mass of the η'. The mass splitting of $\eta-\eta'$ can be related to the strength of the topological fluctuations:[1,2]

$$\chi_{\rm t} \equiv \frac{\langle Q^2\rangle}{V} = \frac{f_\pi^2}{2N_{\rm f}}\left(m_\eta^2 + m_{\eta'}^2 - 2m_{\rm K}^2\right) \sim (180\,{\rm MeV})^4. \quad (1)$$

This is to leading order in $N_{\rm c}$ and so the value of $\chi_{\rm t}$ is the quenched value.

In the continuum the Dirac operator, $D = \gamma_\mu(\partial_\mu + {\rm i}A_\mu)$, of massless fermions in a smooth background gauge field with 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[3] gives the result

$$Q = {\rm index}(D), \quad (2)$$

where

$$Q = \frac{1}{32\pi^2}\int {\rm d}^4x\, \epsilon_{\mu\nu\rho\sigma}\,{\rm tr}(F_{\mu\nu}F_{\rho\sigma}) \quad (3)$$

is the topological charge of the background gauge field and where

$${\rm index}(D) \equiv n_- - n_+ \quad (4)$$

is the chirality index of the Dirac operator. Here n_+ and n_- are the numbers of zero eigenmodes with positive (right-handed) and negative (left-handed) chiralities respectively, i.e. $D\psi = 0$ with $+/-$ chiralities such that $\gamma_5\psi = \pm\psi$.

There are different ways to calculate Q for a given gauge field configuration on a finite lattice, for example using the gauge-field tensor definition[4] of Eq.(3) or using the geometrical definition.[5] On the typical lattices which are used in the calculation of hadronic observables, the configurations in the ensembles are too coarse for lattice definition of Eq.(3) to lead to the integer topological charge Q, so the cooling method is always employed.[6]

In this study we focus on the fermionic method, i.e. by using the index theorem with Eq.(2) to identify the topological charge Q of the background gauge field to the index of the Dirac operator. This was developed as early as 1987 using the Wilson fermion operator.[7] However, 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 topological fluctuation with such an action

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requires one to estimate the number of "zero modes" by looking at low-lying real eigenvalues.[7] Due to the difficulties in estimating the index of the Wilson fermion operator in a precise manner, it is difficult to reach a definite conclusion. In the case of Ginsparg–Wilson (GW) Dirac fermions[8−10] there is an exact lattice realization of chiral symmetry[11] 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.[12].

We focus here on Neuberger's overlap fermion operator, which is an explicit solution of the GW relation. There are several numerical studies[13−15] of topological charge on a finite lattice using overlap fermion. In Ref.[13] the overlap fermion formalism is used to estimate the probability distribution of the 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. Reference [14] also uses the spectral flow method to perform a comprehensive study of both quenched $SU(3)$ and dynamical fermion configurations. There the role of the clover term is also examined. In our work, we will 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.

2. Overlap fermions and zero modes

The overlap fermion formalism[10] provides a way of realizing exact chiral symmetry on the lattice. The massless overlap Dirac operator can be written as

$$D_{\rm o}(0) = (1 + \gamma_5 \epsilon(H_{\rm w})), \tag{5}$$

where $\epsilon(H_{\rm w})$ is the matrix sign function

$$\epsilon(H_{\rm w}) = \frac{H_{\rm w}}{|H_{\rm w}|}, \qquad H_{\rm w} = \gamma_5 D_{\rm w}, \tag{6}$$

and $D_{\rm w}$ is the usual Wilson–Dirac operator

$$\begin{aligned} D_{\rm w} =& M_{a\alpha m, b\beta n} \qquad (7)\\ =& \delta_{a,b}\delta_{\alpha,\beta}\delta_{m,n} \\ & - \kappa \sum_{\mu=1}^{4} [(\mathbf{1} - \gamma_\mu)_{\alpha\beta} U_\mu(m)_{ab} \delta_{m,n-\hat{\mu}} \\ & + (\mathbf{1} + \gamma_\mu)_{\alpha\beta} U^\dagger_\mu(m - \hat{\mu})_{ab} \delta_{m,n+\hat{\mu}}] \qquad (8) \end{aligned}$$

and where κ is the hopping parameter,

$$\kappa = \frac{1}{-2m + 8}. \tag{9}$$

The bare mass parameter for the Wilson kernel in the overlap formalism m has to be in the range $(0, 2)$ for $D_{\rm o}(0)$ to describe a single massless Dirac fermion. 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,[14] m has to be chosen as $m > m_1(g^2)$ 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 $m_{\rm c}$, where $m_{\rm c}$ 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 ($\kappa_{\rm c}$, 0.25) as tree level. The massless overlap operator $D_{\rm o}(0)$ has been shown[10] to satisfy the GW relation[8]

$$\{\gamma_5, D_{\rm o}(0)\} = D_{\rm o}(0)\gamma_5 D_{\rm o}(0). \tag{10}$$

Its spectral properties are:

• The modulus of the eigenvalue of $D_{\rm o}(0)$ 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. They also have eigenvalues equal to ± 2 which also have definite chirality. Their difference $(n'_+ - n'_-)$ is equal to $(n_- - n_+)$.

• Non-zero eigenvalues of $D_{\rm o}(0)$ are complex, their moduli are less than 2, they come as pairs and 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 $D^\dagger_{\rm o}(0)D_{\rm o}(0)$. Note that $D^\dagger_{\rm o}(0)D_{\rm o}(0)$ commutes with $D_{\rm o}(0)$ and it is hermitian and positive definite. It also commutes with γ_5 and can be simultaneously diagonalized. Hence, $D^\dagger_{\rm o}(0)D_{\rm o}(0)$ has zero eigenmodes of definite chirality, which are also the zero eigenmodes of $D_{\rm o}(0)$.

3. Numerical results

One hundred configurations have been generated on an $8^3 \times 16$ lattice using renormalization-group-improved Iwasaki[16] gauge action. The β is chosen to be 8.558. Configurations are selected after

$N_{\rm therm} = 10\,000$ thermalization sweeps from a cold start and every $N_{\rm sep} = 1000$ sweeps thereafter. Lattice parameters are summarized in Table 1. The lattice spacing a is determined from the static quark potential with a string tension $\sqrt{\sigma}$=440 MeV.

Table 1. Parameters of generated lattices.

Action	Size	$N_{\rm therm}$	$N_{\rm sep}$	β	a/fm	Physical volume/fm
Iwasaki	$8^3 \times 16$	10 000	1000	8.558	0.150	$1.20^3 \times 2.40$

We compute the low-lying eigenmodes of $D_{\rm o}^{\dagger}(0)$ $D_{\rm o}(0)$ using the Ritz functional algorithm.[17] The κ is taken to be 0.19, which corresponds to m=1.36. In the computation of the overlap operator, the time consuming part is the calculation of the matrix sign function $\epsilon(H_{\rm w})$. We use the optimal rational approximation with a 14th order Zolotarev expansion to calculate the matrix sign function,

$$\epsilon(H) = H \cdot \sum_{i=1}^{14} \frac{c_i}{H_w^{\dagger} H_w + b_i}. \qquad (11)$$

The multi-shift conjugate gradient (CG) algorithm is used to implement the matrix inversion. The deflation technique is used to accelerate the CG iteration, i.e. we project out a number of low-lying eigenstates of $H_{\rm w}$ to improve the condition number of $H_{\rm w}$. The step will reduce the CG iteration sweeps. Since

$$D_{\rm o}^{\dagger}(0) D_{\rm o}(0) = D_{\rm o}^{\dagger}(0) + D_{\rm o}(0), D_{\rm o}^{\dagger}(0) = \gamma_5 D_{\rm o}(0) \gamma_5, \qquad (12)$$

we use chiral states in the Ritz functional algorithm, and thus it saves one matrix multiplication[18] per iteration.

The results of the topological charge Q are listed in Table 2. Because Q are identified as the indexes of the overlap fermion operator, they are strictly integers. The resulting topological susceptibility χ are

$$\chi = \frac{\langle Q^2 \rangle}{V} = [(177 \pm 45) {\rm MeV}]^4 . \qquad (13)$$

Here the statistical error is rather big, because the ensemble of gauge configurations is small due to the large computer resources being needed to attack the overlap fermions. However, the central value of the topological susceptibility χ is in good agreement with the expectation.[1,2]

Table 2. Topological charge $|\,Q\,|$ of 50 gauge configurations.

Configuration	$\lvert\, Q \,\rvert$
1, 4, 6, 8 − 10, 20, 48, 49, 51, 56, 59, 61, 67, 78, 92, 98	0
2, 3, 11, 12, 15, 17, 18, 23 − 28, 32, 33, 35, 36, 40, 41, 43, 44, 47, 50, 53 − 55, 64, 66, 68, 70, 73 − 76, 83, 85 − 91, 96, 97, 99	1
5, 7, 13, 14, 16, 21, 29, 30, 34, 37 − 39, 42, 45, 52, 57, 58, 60, 63, 65, 69, 71, 79 − 82, 93, 94, 100	2
19, 46, 72, 77, 95	3
22, 31, 62, 84	4

4. Summary

In this paper, we work on a $8^3 \times 16$ lattice at a = 0.15 fm, with a total of 100 gauge configurations. By using the lattice index theorem, we have calculated the topological charge of the background gauge configurations by directly estimated the index of the overlap fermion operator. Although the lattice size is not big, the gauge configurations are not smooth, and the ensemble of configurations is not large, the resulting topological susceptibility is in good agreement with the expectation. This demonstrates that the overlap fermions are suitable for use in the study of topological fluctuations on the lattice. Because of the chiral symmetry, the overlap fermion operator has zero modes which can be identified unambiguously. The topological charge Q can be calculated on any gauge configuration, and they are strictly integers. The only drawback of the method is that the large computer time is needed to calculate the sign matrix function. This prevents us from working on large lattices with more gauge configurations at the current stage.

The MC simulations were performed at the University of Adelaide, Australia.

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