Topological susceptibility in 2+1 flavors lattice QCD with domain-wall fermions

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Abstract

We measure the topological charge and its fluctuation for the gauge configurations generated by the RBC and UKQCD Collaborations using 2+1 flavors of domain-wall fermions on the $16^3 \times 32$ lattice ($L \simeq 2$ fm) with length 16 in the fifth dimension at the inverse lattice spacing $a^{-1} \simeq 1.62$ GeV. From the spectral flow of the Hermitian operator $H_w(2 + \gamma_5 H_w)^{-1}$, we obtain the topological charge $Q_t$ of each gauge configuration in the three ensembles with light sea quark masses $m_q a = 0.01, 0.02,$ and $0.03,$ and with the strange quark mass fixed at $m_s a = 0.04$. From our result of $Q_t$, we compute the topological susceptibility $\chi_t = \langle Q_t^2 \rangle / \Omega$, where $\Omega$ is the volume of the lattice. In the small $m_q$ regime, our result of $\chi_t$ agrees with the chiral effective theory. Using the formula $\chi_t = \Sigma / (m_u^{-1} + m_d^{-1} + m_s^{-1})$ by Leutwyler-Smilga, we obtain the chiral condensate $\Sigma^{\overline{MS}}(2 \text{ GeV}) = [259(6)(9) \text{ MeV}]^3$.

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I. INTRODUCTION

In Quantum Chromodynamics (QCD), the topological susceptibility ($\chi_t$) is the most crucial quantity to measure the topological charge fluctuation of the QCD vacuum, which plays an important role in breaking the $U_A(1)$ symmetry. Theoretically, $\chi_t$ is defined as

$$\chi_t = \int d^4x \langle \rho(x)\rho(0) \rangle, \quad (1)$$

where

$$\rho(x) = \frac{1}{32\pi^2}\epsilon_{\mu\nu\lambda\sigma} \text{tr}[F_{\mu\nu}(x)F_{\lambda\sigma}(x)], \quad (2)$$

is the topological charge density expressed in term of the matrix-valued field tensor $F_{\mu\nu}$. With mild assumptions, Witten [1] and Veneziano [2] obtained a relationship between the topological susceptibility in the quenched approximation and the mass of $\eta'$ meson (flavor singlet) in unquenched QCD with $N_f$ degenerate flavors, namely,

$$\chi_t(\text{quenched}) = \frac{f_\pi^2m_{\eta'}^2}{4N_f}, \quad (3)$$

where $f_\pi = 131$ MeV, the decay constant of pion. This implies that the mass of $\eta'$ is essentially due to the axial anomaly relating to non-trivial topological charge fluctuations, which can turn out to be nonzero even in the chiral limit, unlike those of the (non-singlet) approximate Goldstone bosons.

Using the Chiral Perturbation Theory (ChPT), Leutwyler and Smilga [3] obtained the following relation in the chiral limit

$$\chi_t = \frac{\Sigma}{\left(\frac{1}{m_u} + \frac{1}{m_d} + \frac{1}{m_s}\right)} + \mathcal{O}(m_u^2), \quad (N_f = 2 + 1), \quad (3)$$

where $m_u, m_d,$ and $m_s$ are the quark masses, and $\Sigma$ is the chiral condensate. This implies that in the chiral limit ($m_u \to 0$) the topological susceptibility is suppressed due to internal quark loops. Most importantly, [3] provides a viable way to extract $\Sigma$ from $\chi_t$ in the chiral limit.

From (11), one obtains

$$\chi_t = \frac{(Q_t^2)}{\Omega}, \quad Q_t \equiv \int d^4x \rho(x), \quad (4)$$
where $\Omega$ is the volume of the system, and $Q_t$ is the topological charge (which is an integer for QCD). Thus, one can determine $\chi_t$ by counting the number of gauge configurations for each topological sector. Furthermore, we can also obtain the second normalized cumulant

$$c_4 = -\frac{1}{\Omega} \left[ \langle Q_t^4 \rangle - 3 \langle Q_t^2 \rangle^2 \right], \quad (5)$$

which is related to the leading anomalous contribution to the $\eta' - \eta'$ scattering amplitude in QCD, as well as the dependence of the vacuum energy on the vacuum angle $\theta$. (For a recent review, see for example, Ref. [4] and references therein.)

However, for lattice QCD, it is difficult to extract $\rho(x)$ and $Q_t$ unambiguously from the gauge link variables, due to their rather strong fluctuations.

To circumvent this difficulty, one may consider the Atiyah-Singer index theorem [5]

$$Q_t = n_+ - n_- = \text{index}(D), \quad (6)$$

where $n_\pm$ is the number of zero modes of the massless Dirac operator $D \equiv \gamma_\mu (\partial_\mu + igA_\mu)$ with $\pm$ chirality.

For lattice QCD with exact chiral symmetry, it is well-known that the overlap Dirac operator [6, 7] in a topologically non-trivial gauge background possesses exact zero modes (with definite chirality) satisfying the Atiyah-Singer index theorem. Thus we can obtain the topological charge from the index of the overlap Dirac operator. Writing the overlap Dirac operator as

$$D = m_0 \left( 1 + \gamma_5 \frac{H_w}{\sqrt{H_w^2}} \right), \quad (7)$$

where $H_w$ is the standard Hermitian Wilson operator with negative mass $-m_0$ ($0 < m_0 < 2$), then its index is

$$\text{index}(D) = \text{Tr} \left[ \gamma_5 \left( 1 - D \frac{2m_0}{m_0} \right) \right] = -\frac{1}{2} \text{Tr} \left( \frac{H_w}{\sqrt{H_w^2}} \right) = n_+ - n_- = Q_t, \quad (8)$$

where $\text{Tr}$ denotes trace over Dirac, color, and lattice spaces.

Obviously, from (8), we have

$$\text{index}(D) = n_+ - n_- = -\frac{1}{2} \text{Tr} \left( \frac{H_w}{\sqrt{H_w^2}} \right) = \frac{1}{2} (h_- - h_+), \quad (9)$$
where \( h_+ (h_-) \) is the number of positive (negative) eigenvalues of the hermitian Wilson-Dirac operator \( H_w \). However, one does not need to obtain all eigenvalues of \( H_w \) in order to know how many of them are positive or negative. The idea is simple. Since \( H_w \) has equal number of positive and negative eigenvalues for \( m_0 \leq 0 \), then one can just focus on those low-lying (near zero) eigenmodes of \( H_w \), and see whether any of them crosses zero from positive to negative, or vice versa, when \( m_0 \) is scanned from zero up to the value used in the definition of \( D \). From the net number of crossings, one can obtain the index of \( D \). This is the spectral flow method used in Ref. [7] to obtain the index of the overlap Dirac operator. We also applied the spectral flow method to obtain the index of the overlap Dirac operator and to determine the topological susceptibility in quenched QCD [8]. In this paper, we extend our previous studies to unquenched QCD.

\[ \begin{align*}
\lambda(H) & = 0.00 \\
0.04 & \quad 0.02 \\
-0.04 & \quad -0.02
\end{align*} \]

**FIG. 1:** The spectral flow of 12 lowest-lying eigenvalues of \( H \) for the gauge configuration number 1825 in the ensemble \((m_q = 0.01, m_s = 0.04)\). There are 10 net crossings from negative to positive, so the index is \(-10\).

For the conventional domain-wall fermion [9, 10], its effective 4-dimensional Dirac oper-
ator is
\[
D = \frac{m_0(2 - m_0)}{2} \left( 1 + \gamma_5 \frac{H}{\sqrt{H^2}} \right),
\]
where
\[
H = H_w(2 + \gamma_5 H_w)^{-1}.
\]
Thus, we can obtain the topological charge of a gauge field configuration from the spectral-flow of \(H\) as a function of \(m_0\). Obviously, it is much more computationally intensive to project the low-lying eigenvalues of \(H\) than those of \(H_w\), due to the extra inverse operator \((2 + \gamma_5 H_w)^{-1}\).

In this paper, we use the spectral flow of \(H\) to determine the topological charge of the gauge configurations (http://lattices.qcdoc.bnl.gov/) generated by the RBC and UKQCD Collaborations using 2+1 flavors of domain-wall fermions on the \(16^3 \times 32\) lattice \((L \simeq 2\, \text{fm})\) with length 16 in the fifth dimension at the inverse lattice spacing \(a^{-1} \simeq 1.62(4)\, \text{GeV}\) [11]. There are three ensembles of gauge configurations with light sea quark masses \(m_q a = 0.01\), 0.02 and 0.03, and with the strange quark mass fixed at \(m_s a = 0.04\). For the ensemble with \(m_q a = 0.01\), we pick one configuration every 5 configurations, from configurations numbering from 0020 to 4015. Thus we have 800 configurations with \(m_q a = 0.01\). Similarly, for \(m_q a = 0.02\), we pick 809 configurations from configurations numbering from 0005 to 4045, and for \(m_q a = 0.03\), we pick 717 configurations from configurations numbering from 4020 to 7600.

In Fig. 1, we plot the spectral flow of 12 lowest-lying (near zero) eigenvalues of \(H(m_0)\) in the interval \(0.8 \leq m_0 \leq 1.8\), for the gauge configuration number 1825 in the ensemble with \(m_q = 0.01\) and \(m_s = 0.04\). In this case, the net crossings from negative to positive is 10, so the index is \(-10\). In general, it may happen that there are some intriguing eigenvalues lying very close to zero (e.g., the one around \(m_0 = 1.45\) in Fig. 1). Thus, with a coarse scan in \(m_0\), it may not be able to determine whether they actually cross zero or not. These ambiguities can only be resolved by tracing them closely at a finer resolution in \(m_0\). Obviously, it is a very tedious job to determine the topological charges of 2,326 gauge configurations via the spectral flow of \(H = H_w(2 + \gamma_5 H_w)^{-1}\).
II. RESULTS

In Fig. 2 we plot the histogram of topological charge distribution for $m_q a = 0.01, 0.02,$ and 0.03 respectively. Evidently, the probability distribution of $Q_t$ becomes more sharply peaked around $Q_t = 0$ as the light sea quark mass $m_q$ gets smaller. Our results of topological susceptibility $\chi_t$, and the second normalized cumulant $c_4$, together with their ratios $c_4/\chi_t$, and $c_4/(2\chi_t^2\Omega)$ are listed in Table I. The error is estimated using the jackknife method with bin size of 20 configurations for $m_q = 0.01$ and 0.02, and 13 configurations for $m_q = 0.03$, with which the statistical error saturates.

Evidently, the statistical error of the topological susceptibility is about 10%, while that of $c_4$ is very large due to low statistics. Therefore, one cannot draw any conclusions from our result of $c_4$, as well as from the ratio $c_4/\chi_t$. Interestingly, our result of $c_4/(2\chi_t^2\Omega)$ is consistent with that in Ref. [14], which is obtained from the plateaus (at large time separation) of the 2-point and 4-point time-correlation functions of the flavor-singlet pseudoscalar meson $\eta'$ in a fixed global topology with $Q_t = 0$.

In Fig 3 we plot our data of $\chi_t$ versus $m_\pi^2$, where the pion mass $m_\pi a$ and the inverse lattice spacing $a^{-1}$ are determined by the RBC and UKQCD Collaborations [11].

For three flavors with $m_u = m_d$, we may use the partial conservation of the axial current
TABLE I: The topological susceptibility $\chi_t$, the second normalized cumulant $c_4$, and their ratios $c_4/\chi_t$, and $c_4/(2\chi_t^2\Omega)$, versus the sea quark masses, for $N_f = 2 + 1$ lattice QCD with domain-wall fermions.

In order to convert $\Sigma$ to that in the $\overline{\text{MS}}$ scheme, we use the renormalization factor $Z_s^{\overline{\text{MS}}}(2\text{ GeV}) = 0.604(18)(55)$ which is determined by the RBC and UKQCD Collaborations\cite{12}, employing the non-perturbative renormalization technique through the RI/MOM scheme\cite{13}. Then the value of $\Sigma$ is transcribed to

$$\Sigma^{\overline{\text{MS}}}(2\text{ GeV}) = [259(6)(9)\text{ MeV}]^3,$$

which is in good agreement with the results extracted from $\chi_t$ in 2+1 flavors QCD\cite{14} and 2 flavors QCD\cite{15}, as well as that obtained from the low-lying eigenvalues in the $\epsilon$-regime\cite{16}. The errors represent a combined statistical error ($a^{-1}$ and $Z_s^{\overline{\text{MS}}}$) and the systematic error respectively. Since the calculation is done at a single lattice spacing, the discretization error cannot be quantified reliably, but we do not expect much larger error because the domain-wall fermion action is free from $O(a)$ discretization effects.

III. CONCLUDING REMARK

In this paper, we have obtained the topological susceptibility $\chi_t$ and the second normalized cumulant $c_4$, in 2+1 flavors lattice QCD with domain-wall fermions. The expected sea
quark mass (pion mass square) dependence of $\chi_t$ from ChPT is clearly observed. However, our statistics of $\sim 800$ configurations are insufficient to determine $c_4$ with a reasonably small error.

Finally, it is interesting to compare the topological susceptibility obtained from the global topological charge (this work) with that extracting from the plateaus (at large time separation) of the 2-point and 4-point time-correlation functions of the flavor-singlet pseudoscalar meson $\eta'$ with fixed topology [14]. We find that both methods give $\chi_t$ in agreement with the chiral effective theory. Furthermore, the chiral condensates extracted from both sets of $\chi_t$ are also in good agreement. Next, we turn to the second normalized cumulant $c_4$. If we try to measure it with the global topological charge, it would require more than 10,000 configurations in order to pin down the statistical error less than 10%. On the other hand, if we measure $c_4$ with the correlation function of topological charges in sub-volumes (with fixed global topology), we would expect that it only requires about 1,000 configurations in order to achieve a level of 10% statistical error. To conclude, it is interesting to see that there are more than one viable options to obtain the topological susceptibility and the higher normalized cumulants, in lattice QCD with exact chiral symmetry.
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