

Topological Charge in Two Flavors QCD with Optimal Domain-Wall Fermion

Tung-Han Hsieh^{*1}, Ting-Wai Chiu^{2,3}, Yao-Yuan Mao² (for the TWQCD Collaboration)

¹ *Research Center for Applied Sciences, Academia Sinica, Taipei 115, Taiwan*

E-mail: thhsieh@gate.sinica.edu.tw

² *Department of Physics, and Center for Theoretical Sciences, National Taiwan University, Taipei 10617, Taiwan*

³ *Center for Quantum Science and Engineering, National Taiwan University, Taipei 10617, Taiwan*

We measure the topological charge of the gauge configurations generated by lattice simulations of 2 flavors QCD on a $16^3 \times 32$ lattice, with Optimal Domain-Wall Fermion (ODWF) at $N_s = 16$ and plaquette gauge action at $\beta = 5.90$. Using the Adaptive Thick-Restart Lanczos algorithm, we project the low-lying modes of the 4D effective Dirac operator of ODWF, and obtain the topological charge and topological susceptibility. Our result of topological susceptibility agrees with the sea-quark mass dependence predicted by the chiral perturbation theory, and provides a determination of the chiral condensate.

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^{*}Speaker.

1. Introduction

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

$$\chi_t = \int d^4x \langle \rho(x) \rho(0) \rangle = \frac{\langle Q_t^2 \rangle}{\Omega} \quad (1.1)$$

where

$$\rho(x) = \frac{1}{32\pi^2} \epsilon_{\mu\nu\lambda\sigma} \text{tr}[F_{\mu\nu}(x) F_{\lambda\sigma}(x)], \quad Q_t \equiv \int d^4x \rho(x), \quad (1.2)$$

Q_t is the topological charge (which is an integer for QCD), $\rho(x)$ is the topological charge density, and Ω is the space-time volume. In the chiral perturbation theory (ChPT), the quark mass dependence of χ_t was derived at the tree level [1] in 1992, and it has been extended to the one-loop order recently [2]. For $N_f = 2$, these ChPT formulas can be written as

$$\chi_t/m_u = \frac{\Sigma}{1 + m_u/m_d}, \quad (1.3)$$

$$\chi_t/m_u = \frac{\Sigma}{1 + m_u/m_d} \left[1 - \left(\frac{3M_\pi^2}{32\pi^2 F_\pi^2} \right) \ln \frac{M_\pi^2}{\mu_{sub}^2} + K_6(m_u + m_d) + 2(2K_7 + K_8) \frac{m_u m_d}{m_u + m_d} \right], \quad (1.4)$$

where Σ is the chiral condensate, F_π the pion decay constant, and K_i are related to low energy constants L_i . A salient feature of χ_t is that it is suppressed in the chiral limit ($m_u \rightarrow 0$) due to the internal quark loops. Most importantly, (1.3) and (1.4) provide a viable way to extract Σ and other low energy constants.

However, one cannot determine Q_t reliably using the link variables, due to the rather strong fluctuations at short distances. Instead, we consider the Atiyah-Singer index theorem [3]

$$Q_t = n_+ - n_- = \text{index}(\mathcal{D}), \quad (1.5)$$

where n_\pm is the number of zero modes of the massless Dirac operator $\mathcal{D} \equiv \gamma_\mu(\partial_\mu + igA_\mu)$ with \pm chirality. Thus, by counting the zero modes of the massless Dirac operator, we can determine Q_t and χ_t for an ensemble of gauge configurations.

Recently, the topological susceptibility has been measured in unquenched lattice QCD with exact chiral symmetry, for $N_f = 2$ lattice QCD with overlap fermion in a fixed topology [4], and $N_f = 2 + 1$ lattice QCD with domain-wall fermion [5]. These results are in good agreement with the ChPT at the tree level (1.3).

In this work, we measure the topological charge of the gauge configurations generated by lattice simulations of 2 flavors QCD on a $16^3 \times 32$ lattice, with the Optimal Domain-Wall Fermion (ODWF) [6] at $N_s = 16$, and plaquette gauge action at $\beta = 5.90$. Mathematically, ODWF is a theoretical framework which can preserve the chiral symmetry optimally for any finite N_s . Thus the artifacts due to the chiral symmetry breaking with finite N_s can be reduced to the minimum, especially in the chiral regime. The 4D effective operator of massless ODWF is

$$D = m_0[1 + \gamma_5 S_{opt}(H_w)], \quad S_{opt}(H_w) = \frac{1 - \prod_{s=1}^{N_s} T_s}{1 + \prod_{s=1}^{N_s} T_s}, \quad T_s = \frac{1 - \omega_s H_w}{1 + \omega_s H_w}, \quad (1.6)$$

which is exactly equal to the Zolotarev optimal rational approximation of the overlap Dirac operator [7]. That is, $S_{opt}(H_w) = H_w R_Z(H_w)$, where $R_Z(H_w)$ is the optimal rational approximation of $(H_w^2)^{-1/2}$ [8].

We outline our scheme of projecting the low-lying eigenmodes of D as follows. Using $[DD^\dagger, \gamma_5] = 0$, and the representation

$$D|\theta\rangle = \lambda(\theta)|\theta\rangle, \quad \lambda(\theta) = m_0(1 + e^{i\theta}), \quad (1.7)$$

we obtain

$$S_\pm|\theta\rangle_\pm \equiv P_\pm H_w R_Z(H_w) P_\pm |\theta\rangle_\pm = \pm \cos \theta |\theta\rangle_\pm, \quad P_\pm = \frac{1 \pm \gamma_5}{2}, \quad (1.8)$$

where $|\theta\rangle = P_+|\theta\rangle + P_-|\theta\rangle = |\theta\rangle_+ + |\theta\rangle_-$. Thus, we can perform the eigenmode projection on the operator S_\pm instead of D . Moreover, $|\theta\rangle_\pm$ are related to each other through the relation

$$|\theta\rangle = \frac{1}{i \sin \theta} (\gamma_5 S - e^{-i\theta}) |\theta\rangle_\pm, \quad \theta \neq 0, \pm\pi, \pm 2\pi, \dots \quad (1.9)$$

Assuming the zero modes only residing in either $+$ or $-$ chirality, we project the low-lying modes of D as follows. First, we project the smallest eigenmodes of S_+ . If D has zero modes with positive chirality, then the smallest eigenvalues of S_+ are equal to -1 , and the corresponding full eigenvectors can be obtained using Eq. (1.9). Otherwise, we have to check whether D has zero modes with negative chirality by projecting the largest eigenmodes of S_- . If D has zero modes with negative chirality, the largest eigenvalues of S_- are equal to $+1$, and the corresponding full eigenvectors can be obtained using Eq. (1.9). Finally, for non-zero low-lying eigenmodes, we can pick either $+$ or $-$ chirality of Eq. (1.8) for projection, then obtain the full eigenvectors using Eq. (1.9).

2. The *TRLan* algorithm

In general, the low-mode projection of a large sparse matrix A can be carried out via iterative process, such as the *Lanczos algorithm* or the *Arnoldi algorithm*. The common procedure is to construct an orthonormal basis from the Krylov subspace starting from an initial vector r_0 ,

$$\mathcal{K}(A, r_0) = \text{span} \{r_0, Ar_0, A^2 r_0, \dots, A^{m-1} r_0\}. \quad (2.1)$$

The linear combinations of $\{A^i r_0, i = 0, 1, \dots, m-1\}$ form the Ritz vectors of A , which converge to the eigenvectors of A as m becomes very large.

Since H_w and S_\pm are Hermitian matrices, it is natural to use the Lanczos algorithm. The basic Lanczos process (see Fig.1-(a)) is to construct the following factorization

$$A Q_m = Q_m T_m + \beta_m q_{m+1} e_m^T, \quad (2.2)$$

where $\{q_1, q_2, \dots, q_m\}$ form an orthonormal basis, $Q_m = [q_1, q_2, \dots, q_m]$, e_m is the m -th column of the $m \times m$ identity matrix, and T_m is a tridiagonal matrix with diagonal elements α_i and sub-diagonal elements β_i . Then the Ritz pairs $(\hat{\lambda}_i, \hat{x}_i)$ can be obtained from

$$\hat{T}_m = U_m^\dagger T_m U_m, \quad X_m = Q_m U_m, \quad (2.3)$$

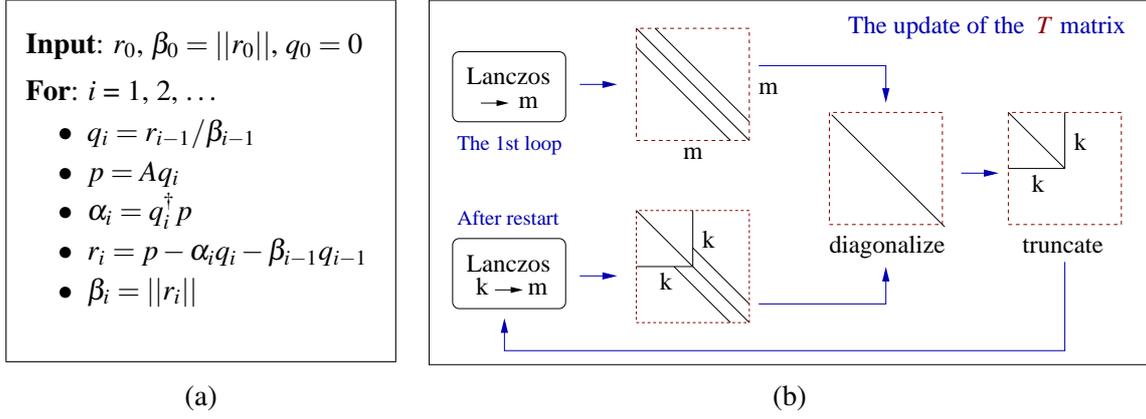


Figure 1: (a) The basic Lanczos process; (b) The Lanczos algorithm with Thick-Restart.

| method | $H_w: k' = 240, m = 340$ | | | | $S_+: k' = 100, m = 200, n_p = 240$ | | | |
|---------|--------------------------|------------------|---------|----------|-------------------------------------|------------------|---------|----------|
| | N_restarts | # of $A \cdot v$ | time(s) | speed up | N_restarts | # of $A \cdot v$ | time(s) | speed up |
| ARPACK | 388 | 35390 | 136460 | 1.00 | 13 | 1050 | 112632 | 1.00 |
| TRLan | 999 | 100140 | 572951 | 0.24 | 12 | 1300 | 105790 | 1.06 |
| v-TRLan | 383 | 59145 | 78058 | 1.75 | 11 | 1030 | 90496 | 1.24 |

Table 1: The benchmark of low-mode projection of H_w and S_+ for a non-trivial gauge configuration ($Q_t = 3$) at $\beta = 5.9$ and $m_q a = 0.01$. Here k' is the number of low-modes projected, m is the dimension of Krylov subspace, and n_p is the number of low-modes of H_w used for low-mode preconditioning in the projection of the low-modes of S_+ .

where \hat{T}_m is diagonal with eigenvalues $\hat{\lambda}_i$, U_m is a unitary matrix, and $X_m = [\hat{x}_1, \hat{x}_2, \dots, \hat{x}_m]$. As m becomes very large, the Ritz pairs $(\hat{\lambda}_i, \hat{x}_i)$ converge to the eigenmodes (λ_i, x_i) of A .

However, the Lanczos algorithm suffers from the following problems. Some spurious Ritz values may repeatedly appear when m goes to larger values. This is due to the fact that the vectors $\{q_i\}$ lose orthogonality rapidly in the finite precision arithmetics. Hence one has to apply the Gram-Schmidt procedure to re-orthogonalize them during the iteration. Also, it requires a large number of q_i to project a few Ritz pairs, consuming a large amount of memory and slowing down the computation. A way to overcome these problems is to perform a *restart*.

There are several restart schemes, in which the Thick-Restart Lanczos algorithm (TRLan) [9] turns out to be the most efficient for our purpose. The TRLan algorithm is illustrated in Fig.1-(b), where the squares in the diagram stand for the square matrix T_m , in which the non-zero matrix elements are denoted by black lines.

Obviously, the performance of the TRLan algorithm depends on the truncated dimension k and the dimension m of the Krylov subspace. Now the question is what is the optimal value of k (for a given m) such that for each restart, the reduction factor d_j of the residual of the j -th (not converged) Ritz pair is maximized, while the number of floating-point operations (FPOs) is minimized. In other words, at each restart, we try to find the optimal k by maximizing the object function [10]

$$f(k) = \frac{d_j}{\# \text{ of FPOs}}, \quad d_j \simeq \mathcal{C}_{m-k}(1 + 2\gamma), \quad \gamma = \frac{\hat{\lambda}_{k+1} - \hat{\lambda}_j}{\hat{\lambda}_m - \hat{\lambda}_{k+1}}, \quad (2.4)$$

where $\mathcal{C}_{m-k}(z)$ is the Chebyshev polynomial of degree $m - k$. For the number of FPOs, we only count the dominant parts which are directly related to the dimension m , namely, the re-orthogonalization and the update of Ritz vectors. This modified algorithm is called the *Adaptive Thick-Restart Lanczos algorithm*, which can attain substantial performance gain, with faster convergence and fewer FPOs.

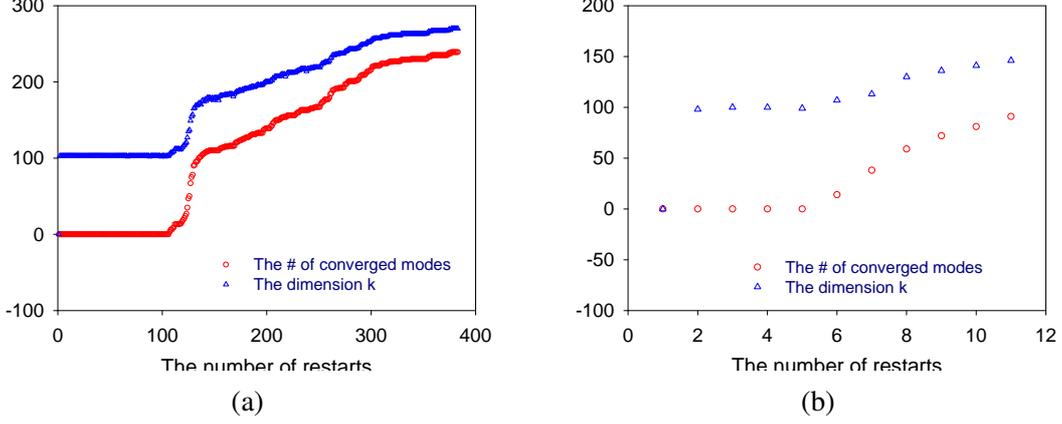


Figure 2: The number of converged Ritz pairs and the dimension k versus the number of restarts for the ν -TRLan algorithm: (a) H_w ($m = 340$); (b) S_+ of the overlap operator ($m = 240$).

For benchmarking, we project the low-lying eigenmodes of H_w and S_+ , using a nontrivial configuration ($Q_t = 3$) generated by the 2-flavor QCD simulation on a $16^3 \times 32$ lattice, with ODWF fermion at $N_s = 16$ and $m_{sea}a = 0.01$, and the plaquette gauge action at $\beta = 5.90$. In Table 1, we present our benchmark results for three different methods: ARPACK (Arnoldi algorithm with Implicit Restart), TRLan (Thick-Restart Lanczos), and ν -TRLan (Adaptive Thick-Restart Lanczos). For TRLan (by definition $k = k'$, where k' is the number of low-modes we want to project, and k is the truncated dimension at each restart), we see that its rate of convergence tends to be very slow for H_w , with a rather large condition number ($\sim 10^6$). On the other hand, for ν -TRLan, k is automatically adjusted to be an optimal value in each restart ($k' < k < m$, see Fig. 2), thus the rate of convergence is dramatically improved. It turns out that, for both H_w and S_{\pm} , ν -TRLan is faster than TRLan and ARPACK. Therefore, we use ν -TRLan to project the low-lying eigenmodes of H_w and D .

3. Lattice setup

Simulations are carried out for two flavors ($N_f = 2$) QCD on a $16^3 \times 32$ lattice at a lattice spacing $a \sim 0.11$ fm, for eight sea quark masses in the range $m_q a = 0.01, 0.02, \dots, 0.08$ [11]. For the gluon part, the plaquette action is used at $\beta = 5.90$. For the quark part, the optimal domain-wall fermion is used with $N_s = 16$. After discarding 300 trajectories for thermalization, we accumulated 3000 – 3200 trajectories in total for each sea quark mass. From the saturation of the binning error of the plaquette, as well as the evolution of the topological charge, we estimate the autocorrelation time to be around 10 trajectories. Thus we sample one configuration every 10 trajectories, then we have 270 – 290 configurations for each sea quark mass.

For each configuration, we calculate the zero modes and 80 conjugate pairs of the lowest-lying eigenmodes of the overlap Dirac operator. We outline our procedures as follows. First, we project 240 low-lying eigenmodes of H_w^2 using ν -TRLan algorithm, where each eigenmode has a residual less than 10^{-12} . Then we approximate the sign function of the overlap operator by the Zolotarev optimal rational approximation with 64 poles, where the coefficients are fixed with $\lambda_{max}^2 = (6.4)^2$, and λ_{min}^2 equal to the maximum of the 240 projected eigenvalues of H_w^2 . Then the sign function error is less than 10^{-14} . Using the 240 low-modes of H_w^2 and the Zolotarev approximation with 64 poles, we project the zero modes plus 80 conjugate pairs of the lowest-lying eigenmodes of the overlap operator with the ν -TRLan algorithm, where each eigenmode has a residual less than 10^{-12} .

4. Results

In Fig. 3, we plot the topological susceptibility $\chi_t = \langle (Q_t - \langle Q_t \rangle)^2 \rangle / \Omega$ as a function of the sea quark mass m_q . For all eight sea quark masses, our data are well fitted by a linear function $F + Gm_q$ with the intercept $F = 0.47(2.37) \times 10^{-5}$ and the slope $G = 5.50(4) \times 10^{-3}$. Evidently, the intercept is consistent with zero, in agreement with the χ PT expectation (1.3). Equating the slope to Σ/N_f , we obtain $\Sigma = 0.0110(7)$. In order to convert Σ to that in the $\overline{\text{MS}}$ scheme, we calculate the renormalization factor $Z_m^{\overline{\text{MS}}}(2 \text{ GeV})$ using the non-perturbative renormalization technique through the RI/MOM scheme [12], and obtain $Z_m^{\overline{\text{MS}}}(2 \text{ GeV}) = 0.5934(10)$ [13]. Then the value of Σ is transcribed to

$$\Sigma^{\overline{\text{MS}}}(2 \text{ GeV}) = [261(5)(7) \text{ MeV}]^3, \quad (4.1)$$

which is in agreement with our previous results : $\Sigma^{\overline{\text{MS}}}(2 \text{ GeV}) = [245(5)(12) \text{ MeV}]^3$ for $N_f = 2$ lattice QCD with overlap fermion in a fixed topology [4], and $\Sigma^{\overline{\text{MS}}}(2 \text{ GeV}) = [253(4)(6) \text{ MeV}]^3$ for $N_f = 2 + 1$ lattice QCD with domain-wall fermion [5]. The statistical error represents a combined error (including those due to a^{-1} and $Z_m^{\overline{\text{MS}}}$). The systematic error is estimated from the truncation of higher order effects and the uncertainty in the determination of lattice spacing with $r_0 = 0.49$ fm. Since our calculation is done at a single lattice spacing, the discretization error cannot be quantified reliably, but we do not expect much larger error because our lattice action is free from $O(a)$ discretization effects.

5. Concluding remarks

We have measured the topological charge of the gauge configurations generated by lattice simulations of 2 flavors QCD on a $16^3 \times 32$ lattice, with Optimal Domain-Wall Fermion (ODWF) at $N_s = 16$ and plaquette gauge action at $\beta = 5.90$. We use the Adaptive Thick-Restart Lanczos algorithm to compute the low-lying eigenmodes of H_w^2 and the overlap Dirac operator. Our result of χ_t agrees with the sea-quark mass dependence predicted by the ChPT at the tree level, and provides a good determination of the chiral condensate. Furthermore, our result of χ_t also agrees with the NLO ChPT, Eq. (1.4). We will present the details in a forthcoming paper [14].

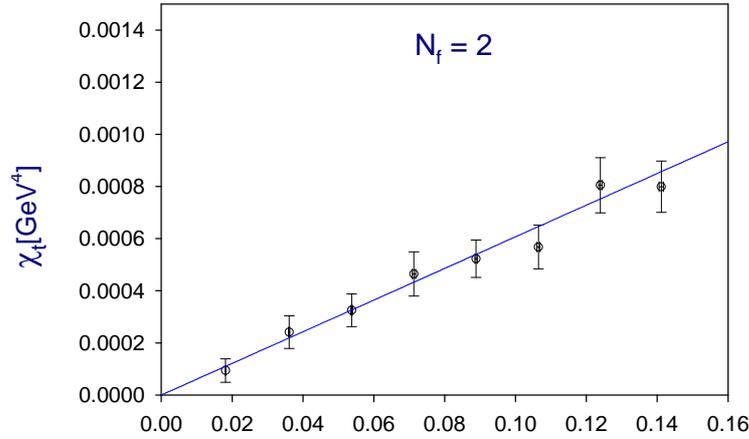


Figure 3: The topological susceptibility of two-flavors QCD with the optimal domain-wall fermion.

Acknowledgments

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