

Chiral Symmetry and the Residual Mass in Lattice QCD with the Optimal Domain-Wall Fermion

Yu-Chih Chen¹ and Ting-Wai Chiu^{1, 2, 3}

(for the TWQCD Collaboration)

¹ *Department of Physics, National Taiwan University, Taipei 10617, Taiwan*

² *Center for Quantum Science and Engineering,
National Taiwan University, Taipei 10617, Taiwan*

³ *Center for Theoretical Sciences, National Taiwan University, Taipei 10617, Taiwan*

Abstract

We derive the axial Ward identity for lattice QCD with domain-wall fermions, and from which we obtain a formula for the residual mass (45)-(46), that can be used to measure the chiral symmetry breaking due to the finite extension N_s in the fifth dimension. Furthermore, we obtain an upper bound for the residual mass in lattice QCD with the optimal domain-wall fermion.

I. INTRODUCTION

The chiral symmetry of massless fermion field plays an important role in particle physics. It forbids the additive mass renormalization which causes the fine-tuning problem associated with the scalar field. In QCD, the chiral symmetry $[SU_L(N_f) \times SU_R(N_f)]$ of N_f massless quarks is spontaneously broken to $SU_V(N_f)$, due to the strong interaction between quarks and gluons. This gives the (nearly) massless Goldstone bosons (pions) and their specific interactions. To investigate the spontaneously chiral symmetry breaking (or hadronic physics) in QCD, it requires nonperturbative methods. So far, lattice QCD is the most promising approach. However, in lattice QCD, formulating lattice fermion with exact chiral symmetry at finite lattice spacing is rather nontrivial, which is realized by the domain-wall fermion (DWF) on the (4+1)-dimensional lattice [1], and the overlap fermion on the 4-dimensional lattice [2].

For lattice QCD with DWF, in practice, one can only use a finite number N_s of sites in the fifth dimension. Thus the chiral symmetry of the massless quark fields is broken, and the emergent question is whether the chiral symmetry is preserved optimally. The answer is negative since the effective 4-dimensional Dirac operator of the conventional DWF corresponds to the overlap Dirac operator with the polar approximation of the sign function of H .

In 2002, one of us (TWC) constructed the optimal domain-wall fermion (ODWF) [3] such that the effective 4D lattice Dirac operator attains the mathematically optimal chiral symmetry for any finite N_s , exponentially-local for sufficiently smooth gauge backgrounds [4], and independent of the lattice spacing in the fifth dimension. The basic idea of ODWF is to construct a set of analytical weights, $\{\omega_s, s = 1, \dots, N_s\}$, one for each layer in the fifth dimension, such that the chiral symmetry breaking due to finite N_s can be reduced to the minimum. The 4-dimensional effective Dirac operator of massless ODWF is

$$D = \frac{1}{2r}[1 + \gamma_5 S_{opt}(H)],$$

$$S_{opt}(H) = \frac{1 - \prod_{s=1}^{N_s} T_s}{1 + \prod_{s=1}^{N_s} T_s}, \quad T_s = \frac{1 - \omega_s H}{1 + \omega_s H},$$

which is exactly equal to the Zolotarev optimal rational approximation of the overlap Dirac operator. That is, $S_{opt}(H) = H R_Z(H)$, where $R_Z(H)$ is the optimal rational approximation of $(H^2)^{-1/2}$ [5, 6].

However, in the original ODWF formulation [3], the valence quark propagator cannot be expressed in terms of the correlation function of the quark fields defined in terms of the boundary modes, unlike the conventional domain-wall fermion. In 2003, one of us (TWC) solved this problem by introduced two transparent layers with $\omega_s = 0$ [7], as boundary layers appending to the original action of ODWF such that the quark fields defined in terms of these two transparent layers obey the usual chiral projection rule in the continuum, independent of the gauge fields. Consequently any observable constructed with the quark fields manifests the symmetries exactly as those of its counterpart in the continuum. The salient feature of a transparent layer (with $\omega_s = 0$, and $T_s = 1$) is that its presence does not change the effective 4D Dirac operator.

In this paper, we derive the axial Ward identity for lattice QCD with ODWF. We find that it is necessary to extend the idea of transparent layers introduced in Ref. [7], to add another two transparent layers at the central region of the fifth dimension. With these four transparent layers, the action of lattice QCD with ODWF can be written as

$$\mathcal{A}_f = \sum_{s,s'=0}^{N_s+3} \sum_{x,x'} \bar{\psi}_s(x) \{(\rho_s D_w + \mathbb{I})_{x,x'} \delta_{s,s'} + (\sigma_s D_w - \mathbb{I})_{x,x'} (P_- \delta_{s',s+1} + P_+ \delta_{s',s-1})\} \psi_{s'}(x'), \quad (1)$$

with boundary conditions

$$\begin{aligned} P_+ \psi(x, -1) &= -rm_q P_+ \psi(x, N_s + 3), \\ P_- \psi(x, N_s + 4) &= -rm_q P_- \psi(x, 0), \end{aligned} \quad (2)$$

where $P_\pm = (1 \pm \gamma_5)/2$, D_w is the standard Wilson-Dirac operator plus a negative parameter $-m_0$ ($0 < m_0 < 2$), m_q is the bare quark mass, and r is a parameter depending on $\{\rho_s, \sigma_s\}$ and m_0 such that the valence quark propagator agrees with $(\gamma_\mu \partial_\mu + m_q)^{-1}$ in the continuum limit. The two transparent layers at the boundaries are specified by imposing $\rho_0 = \rho_{N_s+3} = \sigma_0 = \sigma_{N_s+3} = 0$. The two additional transparent layers can be located at $s = n$, and $s = n + 1$, where $n = [N_s/2]$. In other words, they have $\rho_n = \rho_{n+1} = \sigma_n = \sigma_{n+1} = 0$. In the original ODWF formulation [3], the nonzero ρ_s and σ_s are set to be ω_s (the optimal weight).

The quark fields are defined in terms of the boundary modes

$$\begin{aligned} q(x) &= \sqrt{r} [P_- \psi_0(x) + P_+ \psi_{N_s+3}(x)], \\ \bar{q}(x) &= \sqrt{r} [\bar{\psi}_0(x) P_+ + \bar{\psi}_{N_s+3}(x) P_-]. \end{aligned} \quad (3)$$

Following the derivation given in Ref. [7], it is straightforward to show (in Section III) that the valence quark propagator in a gauge background is equal to the correlation function

of the quark fields, i.e.,

$$\langle q(x)\bar{q}(y) \rangle = (D_c + m_q)^{-1}(x, y), \quad (4)$$

where

$$D_c = \frac{1}{r} \frac{1 + \gamma_5 S}{1 - \gamma_5 S}, \quad (5)$$

$$S = \frac{1 - \prod_{s=0}^{N_s+3} T_s}{1 + \prod_{s=0}^{N_s+3} T_s}, \quad (6)$$

$$T_s = \frac{1 - H_s}{1 + H_s}, \quad (7)$$

$$H_s = (\rho_s + \sigma_s) H_w [2 + (\rho_s - \sigma_s) \gamma_5 H_w]^{-1}, \quad H_w = \gamma_5 D_w. \quad (8)$$

Obviously, a transparent layer (with $\rho_s = \sigma_s = 0$) does not change S and D_c since its $T_s = 1$. Setting the nonzero weights $\rho_s = c \omega_s + d$, and $\sigma_s = c \omega_s - d$, where c and d are constants, then $H_s = \omega_s H$,

$$H = c H_w (1 + d \gamma_5 H_w)^{-1}, \quad (9)$$

and the parameter r entering the boundary conditions (2) is fixed to $r = [2m_0(1 - dm_0)]^{-1}$ such that $(D_c + m_q)^{-1}$ in the free fermion limit agrees with $(\gamma_\mu \partial_\mu + m_q)^{-1}$ in the continuum limit. Moreover, for $H_s = \omega_s H$, interchanging any two layers in the fifth dimension gives the same S , since $\{T_s\}$ commute among themselves.

For finite N_s , with the optimal weights $\{\omega_s\}$ given in Ref. [3], S is exactly equal to the Zolotarev optimal rational approximation of the sign function of H , i.e., $S = S_{opt}(H) = H R_Z(H)$, where $R_Z(H)$ is the optimal rational approximation of $(H^2)^{-1/2}$ [5, 6]. In the limit $N_s \rightarrow \infty$, $S \rightarrow H(H^2)^{-1/2}$, and D_c becomes exactly chirally symmetric, and $(D_c + m_q)^{-1}$ is well-defined for nonzero m_q , even though D_c is ill-defined for topologically nontrivial gauge background [8].

In practice, only the case $d = 0$ gives $H = c H_w$ (without the denominator), which is much easier for the projection of the low-lying eigenmodes of $D = D_c(1 + r D_c)^{-1}$ than other cases with $d \neq 0$. Since the low-lying eigenmodes of D are vital for extracting many physical observables, the original formulation [3] with $d = 0$ (and $c = 1$) seems to be a good choice.

We note in passing that setting the nonzero weights $\rho_s = c_1(\text{constant})$ and $\sigma_s = c_2(\text{constant})$ covers all variants of conventional domain-wall fermions, with S equal to the

polar approximation of the sign function of H ,

$$S_{polar}(H) = \begin{cases} H \left(\frac{1}{N_s} + \frac{2}{N_s} \sum_{l=1}^n \frac{b_l}{H^2 + d_l} \right), & N_s = 2n+1 \text{ (odd)}, \\ H \frac{2}{N_s} \sum_{l=1}^n \frac{b_l}{H^2 + d_l}, & N_s = 2n \text{ (even)}, \end{cases}$$

where

$$b_l = \sec^2 \left[\frac{\pi}{N_s} \left(l - \frac{1}{2} \right) \right], \quad d_l = \tan^2 \left[\frac{\pi}{N_s} \left(l - \frac{1}{2} \right) \right].$$

For example, setting $\rho_s = 1$ and $\sigma_s = 0$, (1) reduces to the conventional domain-wall fermion with $H = H_w(2 + \gamma_5 H_w)^{-1}$ [9], and $\rho_s = \sigma_s = 1$ to the Borici's variant with $H = H_w$ [10], and $\rho_s = c + d$ and $\sigma_s = c - d$ to the Möbius variant with $H = cH_w(1 + d\gamma_5 H_w)^{-1}$ [11].

II. AXIAL WARD IDENTITY

Now we consider N_f flavors of quarks with degenerate mass m_q , and the infinitesimal flavor non-singlet transformation

$$\begin{aligned} \delta\psi_s(x) &= i\theta_s(x)\lambda^a\psi_s(x), \\ \delta\bar{\psi}_s(x) &= -i\theta_s(x)\bar{\psi}_s(x)\lambda^a, \end{aligned} \tag{10}$$

where

$$\theta_s(x) = \begin{cases} \theta(x), & 0 \leq s \leq n \equiv [\frac{N_s}{2}], \\ -\theta(x), & n+1 \leq s \leq N_s+3. \end{cases}$$

Here λ^a is one of the flavor group generators in the fundamental representation, and the flavor indices of $\psi_s(x)$ and $\bar{\psi}_s(x)$ are suppressed. Under the transformation (10), the change of the action (1) consists of the following three parts:

$$\begin{aligned} \delta \sum_{s=0}^{N_s+3} \sum_{x,y} \rho_s [\bar{\psi}_s(x)\lambda^a D_w(x,y)\psi_s(y)] &= \sum_x i\theta(x) \sum_\mu \Delta_\mu \hat{j}_\mu^a(x), \\ \delta \sum_{s=0}^{N_s+3} [-\bar{\psi}_s(x)\lambda^a P_- \psi_{s+1}(x) - \bar{\psi}_s(x)\lambda^a P_+ \psi_{s-1}(x)] &= - \sum_x 2i\theta(x)[J_5^a(x,n) + m_q \bar{q}(x)\lambda^a \gamma_5 q(x)], \\ \delta \sum_{s=0}^{N_s+3} \sum_{x,y} \sigma_s \{ \bar{\psi}_s(x)\lambda^a D_w(x,y)[P_- \psi_{s+1}(y) + P_+ \psi_{s-1}(y)] \} &= \sum_x i\theta(x) \sum_\mu \Delta_\mu \hat{k}_\mu^a(x), \end{aligned} \tag{11}$$

where

$$\begin{aligned}
\Delta_\mu f(x, s) &\equiv f(x, s) - f(x - \mu, s), \\
\hat{j}_\mu^a(x) &\equiv \sum_{s=1}^{N_s+2} \text{sign}\left(n - s + \frac{1}{2}\right) j_\mu^a(x, s), \\
j_\mu^a(x, s) &= \frac{\rho_s}{2} [\bar{\psi}_s(x)\lambda^a(1 - \gamma_\mu)U_\mu(x)\psi_s(x + \mu) - \bar{\psi}_s(x + \mu)\lambda^a(1 + \gamma_\mu)U_\mu^\dagger(x)\psi_s(x)], \\
J_5^a(x, n) &= -\bar{\psi}_n(x)\lambda^a P_- \psi_{n+1}(x) + \bar{\psi}_{n+1}(x)\lambda^a P_+ \psi_n(x), \\
\hat{k}_\mu^a(x) &\equiv \hat{k}_\mu^{a+}(x) + \hat{k}_\mu^{a-}(x), \\
\hat{k}_\mu^{a\pm}(x) &\equiv \sum_{s=1}^{N_s+2} \text{sign}\left(n - s + \frac{1}{2}\right) k_\mu^{a\pm}(x, s), \\
k_\mu^{a\pm}(x, s) &= \frac{\sigma_s}{2} [\bar{\psi}_s(x)\lambda^a(1 - \gamma_\mu)U_\mu(x)P_\pm\psi_{s\mp 1}(x + \mu) - \bar{\psi}_s(x + \mu)\lambda^a(1 + \gamma_\mu)U_\mu^\dagger(x)P_\pm\psi_{s\mp 1}(x)].
\end{aligned} \tag{12}$$

Now the role of the two transparent layers at $s = n$ and $s = n + 1$ becomes obvious. If we want to keep J_5^a (12) not depending on D_w (similar to the J_5^a in the conventional DWF) and to express (11) in terms of the divergence of a 4-current, then it is inevitable to introduce two transparent layers in the central region of the 5th dimension. This can be seen as follows. For $1 \leq s \leq n - 1$, or $n + 2 \leq s \leq N_s + 2$, we have

$$\delta \sum_{x,y} \sigma_s \bar{\psi}_s(x)\lambda^a D_w(x, y) P_- \psi_{s+1}(y) = \mp i \sum_{x,y} \bar{\psi}_s(x)\lambda^a \sigma_s [\theta(x)D_w(x, y) - D_w(x, y)\theta(y)] P_- \psi_{s+1}(y),$$

which can be written in the form of $\sum_x \theta(x)\Delta_\mu J_\mu$. However, at $s = n$, it gives

$$\delta \sum_{x,y} \sigma_n \bar{\psi}_n(x)\lambda^a D_w(x, y) P_- \psi_{n+1}(y) = -i \sum_{x,y} \bar{\psi}_s(x)\lambda^a \sigma_n [\theta(x)D_w(x, y) + D_w(x, y)\theta(y)] P_- \psi_{n+1}(y),$$

which cannot be expressed in terms of the divergence of a 4-current unless $\sigma_n = 0$. Similarly, we also set $\sigma_{n+1} = 0$. Furthermore, for consistency, we must also set $\rho_n = \rho_{n+1} = 0$ such that $T_n = T_{n+1} = 1$.

For any observable \mathcal{O} , the variation of its vacuum expectation value with respect to (10) must vanish, i.e., $\delta^a \langle \mathcal{O} \rangle = 0$, which gives the axial Ward identity

$$\sum_\mu \Delta_\mu \langle J_\mu^a(x) \mathcal{O}(y) \rangle = 2m_q \langle \bar{q}(x)\lambda^a \gamma_5 q(x) \mathcal{O}(y) \rangle + 2 \langle J_5^a(x, n) \mathcal{O}(y) \rangle + i \langle \delta^a \mathcal{O}(y) \rangle. \tag{13}$$

where $J_\mu^a(x) \equiv \hat{k}_\mu^a(x) + \hat{j}_\mu^a(x)$. As $N_s \rightarrow \infty$, the anomalous term $\langle J_5^a(x, n) \mathcal{O}(y) \rangle$ vanishes if $\mathcal{O}(y)$ only involves the quark fields, following the same argument given in Ref. [12].

After summing over all sites x , the LHS of (13) vanishes, and its RHS gives

$$-i \sum_x \langle \delta^a \mathcal{O}(y) \rangle = 2m_q \sum_x \langle \bar{q}(x) \lambda^a \gamma_5 q(x) \mathcal{O}(y) \rangle + 2 \sum_x \langle J_5^a(x, n) \mathcal{O}(y) \rangle. \quad (14)$$

Thus, the effect of chiral symmetry breaking due to finite N_s can be regarded as an additive mass to the bare quark mass m_q , the so-called residual mass

$$m_{res}[\mathcal{O}(y)] = \frac{\sum_x \langle J_5^a(x, n) \mathcal{O}(y) \rangle}{\sum_x \langle \bar{q}(x) \lambda^a \gamma_5 q(x) \mathcal{O}(y) \rangle}, \quad (15)$$

which serves as a measure of the chiral symmetry breaking due to finite N_s . In the limit $N_s \rightarrow \infty$, $S(H) = H/\sqrt{H^2}$ and $m_{res} = 0$. Obviously, in a gauge background, the residual mass (15) depends on the observable \mathcal{O} as well as its location y . Thus it is necessary to take into account of the residual mass at all locations. This can be accomplished by summing over all lattice sites y in the axial Ward identity (14) to obtain the global residual mass

$$M_{res}[\mathcal{O}] = \frac{\sum_{x,y} \langle J_5^a(x, n) \mathcal{O}(y) \rangle}{\sum_{x,y} \langle \bar{q}(x) \lambda^a \gamma_5 q(x) \mathcal{O}(y) \rangle}. \quad (16)$$

For $\mathcal{O}(y) = \bar{q}(y) \lambda^b \gamma_5 q(y)$, (15) and (16) become

$$m_{res}(y) = \frac{\sum_x \langle J_5^a(x, n) \bar{q}(y) \lambda^b \gamma_5 q(y) \rangle}{\sum_x \langle \bar{q}(x) \lambda^a \gamma_5 q(x) \bar{q}(y) \lambda^b \gamma_5 q(y) \rangle}, \quad (17)$$

$$M_{res} = \frac{\sum_{x,y} \langle J_5^a(x, n) \bar{q}(y) \lambda^b \gamma_5 q(y) \rangle}{\sum_{x,y} \langle \bar{q}(x) \lambda^a \gamma_5 q(x) \bar{q}(y) \lambda^b \gamma_5 q(y) \rangle}, \quad (18)$$

which are usually used as a measure of the chiral symmetry breaking due to finite N_s . In the following, we will restrict our discussions to the residual mass (17), and the global residual mass (18).

III. GENERATING FUNCTIONAL FOR n -POINT GREEN'S FUNCTION

In order to express the residual mass (17) in terms of the quark propagator, we first derive the generating functional for the n -point Green's function of the fermion fields for lattice

QCD with ODWF. With four transparent layers, the action (1) can be rewritten as

$$\begin{aligned}
\mathcal{A}_f &= \sum_{s=0}^{N_s+3} \sum_{x,x'} \bar{\psi}_s(x) \gamma_5 \{ (\rho_s H_w P_+ + \rho_s H_w P_- + P_+ - P_-)_{x,x'} \psi_s(x') \\
&\quad + (\sigma_s H_w P_- + \sigma_s H_w P_+ + P_- - P_+)_{x,x'} (P_- \psi_{s+1}(x') + P_+ \psi_{s-1}(x')) \} \\
&= \sum_{s=0}^{N_s+3} \sum_{x,x'} \bar{\psi}_s(x) \gamma_5 \{ (\rho_s H_w P_- + \sigma_s H_w P_+ - 1)_{x,x'} [P_+ \psi_{s-1}(x') + P_- \psi_s(x')] \\
&\quad + (\rho_s H_w P_+ + \sigma_s H_w P_- + 1)_{x,x'} [P_+ \psi_s(x') + P_- \psi_{s+1}(x')] \} \\
&= \sum_{s=0}^{N_s+3} \sum_{x,x'} \bar{\psi}_s(x) \gamma_5 \{ Q_-^s(x, x') [P_+ \psi_{s-1}(x') + P_- \psi_s(x')] + Q_+^s(x, x') [P_+ \psi_s(x') + P_- \psi_{s+1}(x')] \},
\end{aligned}$$

where

$$Q_\pm^s \equiv \rho_s H_w P_\pm + \sigma_s H_w P_\mp \pm 1. \quad (19)$$

Defining

$$\eta_s \equiv (P_- \delta_{s',s} + P_+ \delta_{s',s-1}) \psi_{s'} \Leftrightarrow \psi_s = (P_- \delta_{s',s} + P_+ \delta_{s',s+1}) \eta_{s'}, \quad (20)$$

$$\bar{\eta}_s \equiv \bar{\psi}_s \gamma_5 Q_-^s \Leftrightarrow \bar{\psi}_s = \bar{\eta}_s (Q_-^s)^{-1} \gamma_5, \quad (21)$$

$$T_s \equiv -(Q_+^s)^{-1} Q_-^s = \frac{1 - H_s}{1 + H_s}, \quad H_s = (\rho_s + \sigma_s) H_w [2 + (\rho_s - \sigma_s) \gamma_5 H_w]^{-1}, \quad (22)$$

then the action (1) can be expressed in terms of $\eta, \bar{\eta}$ fields

$$\begin{aligned}
\mathcal{A}_f &= \bar{\eta}_0 (P_- - r m_q P_+) \eta_0 - \bar{\eta}_0 \eta_0 + \sum_{s=1}^{N_s+2} [\bar{\eta}_s \eta_s - \bar{\eta}_s T_s^{-1} \eta_{s+1}] \\
&\quad + \bar{\eta}_{N_s+3} \eta_{N_s+3} - \bar{\eta}_{N_s+3} (P_+ - r m_q P_-) \eta_0,
\end{aligned} \quad (23)$$

where the space-time indices have been suppressed.

In order to evaluate the Green's function of the fermion fields in the expression of the residual mass, we need to add the following external source terms to (23)

$$\begin{aligned}
&\bar{\eta}_n J_n + \bar{J}_{n+1} \eta_{n+1} + \bar{\eta}_{n+1} J_{n+1}, \\
&\bar{J}_q q + \bar{q} J_q = \bar{J} \eta_0 - \bar{\eta}_0 P_+ J + \bar{\eta}_{N_s+3} P_- J,
\end{aligned}$$

where

$$J \equiv \sqrt{r} J_q,$$

$$\bar{J} \equiv \sqrt{r} \bar{J}_q.$$

Then the generating functional for n -point Green's function is defined as

$$Z[J_q, \bar{J}_q, J_n, J_{n+1}, \bar{J}_{n+1}] = \mathcal{J} \int [d\bar{\eta}] [d\eta] e^{-S_J}, \quad (24)$$

where

$$S_J = \mathcal{A}_f - \bar{J}\eta_0 + \bar{\eta}_0 P_+ J - \bar{\eta}_n J_n - \bar{J}_{n+1} \eta_{n+1} - \bar{\eta}_{n+1} J_{n+1} - \bar{\eta}_{N_s+3} P_- J, \quad (25)$$

and \mathcal{J} is the Jacobian of the transformation,

$$\mathcal{J} = \prod_{s=0}^{N_s+3} \det(\rho_s H_w P_- + \sigma_s H_w P_+ - 1). \quad (26)$$

Now using the Grassman integration formula

$$\int d\bar{\chi} d\chi e^{-\bar{\chi} M \chi + \bar{v} \chi + \bar{\chi} v} = e^{\bar{v} M^{-1} v} \det M,$$

and integrating $(\eta_s, \bar{\eta}_s)$ successively from $s = N_s + 3$ to $s = 1$, (24) becomes

$$\begin{aligned} & \mathcal{J} \int [d\bar{\eta}_0] [d\eta_0] \exp \left\{ \bar{\eta}_0 \left[(P_- - rm_q P_+) - \prod_{s=1}^{N_s+2} T_s^{-1} (P_+ - rm_q P_-) \right] \eta_0 \right. \\ & - \eta_0 \left[\left(\prod_{s=1}^{N_s+2} T_s^{-1} P_- - P_+ \right) J + \prod_{s=1}^n T_s^{-1} J_n + \prod_{s=1}^n T_s^{-1} J_{n+1} \right] \\ & \left. - \left[\bar{J} + \bar{J}_{n+1} \prod_{s=n+1}^{N_s+2} T_s^{-1} (P_+ - rm_q P_-) \right] \eta_0 - \bar{J}_{n+1} \prod_{s=n+1}^{N_s+2} T_s^{-1} P_- J - \bar{J}_{n+1} J_{n+1} \right\}. \end{aligned} \quad (27)$$

Finally integrating $(\eta_0, \bar{\eta}_0)$ of (27), we obtain the generating functional

$$\begin{aligned} & Z[J_q, \bar{J}_q, J_n, J_{n+1}, \bar{J}_{n+1}] \\ &= \mathcal{J} \det \left[(P_- - rm_q P_+) - \prod_{s=1}^{N_s+2} T_s^{-1} (P_+ - rm_q P_-) \right] \exp \left\{ \bar{J}_{n+1} \prod_{s=n+1}^{N_s+2} T_s^{-1} P_- J + \bar{J}_{n+1} J_{n+1} + \right. \\ & + \left[\bar{J} + \bar{J}_{n+1} \prod_{s=n+1}^{N_s+2} T_s^{-1} (P_+ - rm_q P_-) \right] \cdot \left[(P_- - rm_q P_+) - \prod_{s=1}^{N_s+2} T_s^{-1} (P_+ - rm_q P_-) \right]^{-1} \\ & \cdot \left. \left[\left(\prod_{s=1}^{N_s+2} T_s^{-1} P_- - P_+ \right) J + \prod_{s=1}^n T_s^{-1} J_n + \prod_{s=1}^n T_s^{-1} J_{n+1} \right] \right\} \\ &= K \det[r(D_c + m_q)] \exp \left\{ \bar{J}_{n+1} T_U^{-1} P_- J + \bar{J}_{n+1} J_{n+1} + \right. \\ & \left. + [\bar{J} + \bar{J}_{n+1} T_U^{-1} (P_+ - rm_q P_-)] r^{-1} (D_c + m_q)^{-1} [J + \hat{T}^{-1} J_n + \hat{T}^{-1} J_{n+1}] \right\}, \end{aligned} \quad (28)$$

where we have used the identity

$$\left(-P_+ + \prod_{s=1}^{N_s+2} T_s^{-1} P_- \right)^{-1} \left(P_- - \prod_{s=1}^{N_s+2} T_s^{-1} P_+ \right) = \frac{1 + \gamma_5 S}{1 - \gamma_5 S} = r D_c,$$

and defined

$$\begin{aligned} T_L^{-1} &\equiv \prod_{s=1}^n T_s^{-1} \quad , \\ T_U^{-1} &\equiv \prod_{s=n+1}^{N_s+2} T_s^{-1} \quad , \\ T^{-1} &\equiv \prod_{s=1}^{N_s+2} T_s^{-1} = T_L^{-1} T_U^{-1}, \\ \hat{T}^{-1} &\equiv (-P_+ + T^{-1} P_-)^{-1} T_L^{-1}, \\ K &\equiv \mathcal{J} \det [-P_+ + T^{-1} P_-] . \end{aligned}$$

Equation (28) is one of the main results of this paper.

With the generating functional (28), we obtain the propagators in a gauge background as follows.

(I) The valence quark propagator

$$\langle q(x)\bar{q}(y) \rangle = -\frac{1}{Z} \frac{\delta^2 Z}{\delta \bar{J}_q(x) \delta J_q(y)} \Big|_0 = (D_c + m_q)^{-1}(x, y), \quad (29)$$

where the subscript 0 in the functional derivative denotes setting all J 's to zero after differentiation.

(II) The mixed correlator of the first kind

$$\begin{aligned} \langle q(x)\bar{\eta}_n(y) \rangle &= -\frac{1}{Z} \frac{\delta^2 Z}{\delta \bar{J}_q(x) \delta J_n(y)} \Big|_0 \\ &= \frac{1}{\sqrt{r}} (D_c + m_q)^{-1} (-P_+ + T^{-1} P_-)^{-1} T_L^{-1} \\ &= -\frac{1}{\sqrt{r}} D^{-1}(m_q) \gamma_5 \frac{T_L^{-1}}{T^{-1} + 1}, \end{aligned} \quad (30)$$

where

$$D^{-1}(m_q) = (1 + r D_c)(D_c + m_q)^{-1} = r + (1 - rm_q)(D_c + m_q)^{-1}, \quad (31)$$

the sea quark propagator.

(III) The mixed correlator of the second kind

$$\begin{aligned}
\langle q(x)\bar{\eta}_{n+1}(y) \rangle &= -\frac{1}{Z} \frac{\delta^2 Z}{\delta \bar{J}_q(x) \delta J_{n+1}(y)} \Big|_0 \\
&= \frac{1}{\sqrt{r}} (D_c + m_q)^{-1} (-P_+ + T^{-1} P_-)^{-1} T_L^{-1} \\
&= -\frac{1}{\sqrt{r}} D^{-1}(m_q) \gamma_5 \frac{T_L^{-1}}{T^{-1} + 1} = \langle q(x)\bar{\eta}_n(y) \rangle.
\end{aligned} \tag{32}$$

(IV) The mixed correlator of the third kind

$$\begin{aligned}
\langle \eta_{n+1}(x)\bar{q}(y) \rangle &= -\frac{1}{Z} \frac{\delta^2 Z}{\delta \bar{J}_{n+1}(x) \delta J_q(y)} \Big|_0 \\
&= T_U^{-1} (-rm_q P_- + P_+) (D_c + m_q)^{-1} \frac{1}{\sqrt{r}} + T_U^{-1} P_- \sqrt{r} \\
&= T_U^{-1} \frac{1}{2\sqrt{r}} \left(1 + \frac{1 + rm_q}{1 - rm_q} \gamma_5 \right) D^{-1}(m_q) - \frac{\sqrt{r}}{1 - rm_q} T_U^{-1} \gamma_5.
\end{aligned} \tag{33}$$

For completeness, we also consider the generating functional for n -point Green's function of fermion fields in full QCD with ODWF (satisfying the normalization condition $Z[0] = 1$)

$$Z[J_q, \bar{J}_q, J_n, J_{n+1}, \bar{J}_{n+1}] = \frac{\int e^{-\mathcal{A}_g - \mathcal{A}_f - \mathcal{A}_{PV} - \bar{J}\eta_0 + \bar{\eta}_0 P_+ J - \bar{\eta}_n J_n - \bar{J}_{n+1} \eta_{n+1} - \bar{\eta}_{n+1} J_{n+1} - \bar{\eta}_{N_s+3} P_- J}}{\int e^{-\mathcal{A}_g - \mathcal{A}_f - \mathcal{A}_{PV}}}, \tag{34}$$

where $\int \equiv \int [dU][d\psi][d\bar{\psi}][d\phi][d\bar{\phi}]$, \mathcal{A}_g is the gauge action, and \mathcal{A}_{PV} is the action of the Pauli-Villars fields $\{\bar{\phi}_s, \phi_s\}$ with $m_q = 1/r$, i.e.,

$$\mathcal{A}_{PV} = \sum_{s,s'=0}^{N_s+3} \sum_{x,x'} \bar{\phi}_s(x) \{ (\rho_s D_w + \mathbb{1})_{x,x'} \delta_{s,s'} + (\sigma_s D_w - \mathbb{1})_{x,x'} (P_- \delta_{s',s+1} + P_+ \delta_{s',s-1}) \} \phi_{s'}(x'),$$

with boundary conditions

$$\begin{aligned}
P_+ \phi(x, -1) &= -P_+ \phi(x, N_s + 3), \\
P_- \phi(x, N_s + 4) &= -P_- \phi(x, 0).
\end{aligned}$$

Since the integrals over the fermion fields have been done, we proceed to evaluate the integrals over the Pauli-Villars fields in (34). Using the Gaussian integration formula for the boson fields, and following the procedures similar to above for the fermion fields, we obtain

$$\int [d\bar{\phi}][d\phi] e^{-\mathcal{A}_{PV}} = \pi^{N_s+4} K^{-1} \det(1 + r D_c)^{-1}. \tag{35}$$

Substituting (28), and (35) into (34), we have

$$\begin{aligned}
Z[J_q, \bar{J}_q, J_n, J_{n+1}, \bar{J}_{n+1}] &= \frac{1}{\int [dU] e^{-\mathcal{A}_g} \det D(m_q)} \times \\
&\quad \int [dU] e^{-\mathcal{A}_g} \det D(m_q) \exp \left\{ \bar{J}_{n+1} T_U^{-1} P_- J + \bar{J}_{n+1} J_{n+1} + \right. \\
&\quad \left. + [\bar{J} + \bar{J}_{n+1} T_U^{-1} (P_+ - rm_q P_-)] r^{-1} (D_c + m_q)^{-1} \left[J + \hat{T}^{-1} J_n + \hat{T}^{-1} J_{n+1} \right] \right\},
\end{aligned} \tag{36}$$

where

$$\begin{aligned} D(m_q) &= (D_c + m_q)(1 + rD_c)^{-1} \\ &= m_q + \frac{1}{2} \left(\frac{1}{r} - m_q \right) (1 + \gamma_5 S), \end{aligned} \quad (37)$$

the effective 4D lattice Dirac operator, with D_c and S defined in Eqs. (5)-(8). Setting the nonzero weights $\rho_s = c\omega_s + d$, and $\sigma_s = c\omega_s - d$, where c and d are constants, then $H_s = \omega_s H$ with $H = cH_w(1 + d\gamma_5 H_w)^{-1}$. For finite N_s , with the optimal weights $\{\omega_s\}$ given in Ref. [3], S is exactly equal to the Zolotarev optimal rational approximation of the sign function of H , i.e., $S = S_{opt}(H) = HR_Z(H)$, where $R_Z(H)$ is the optimal rational approximation of $(H^2)^{-1/2}$ [5, 6]. In the limit $N_s \rightarrow \infty$, $S \rightarrow H(H^2)^{-1/2}$, and $D(0)$ is exactly equal to the overlap Dirac operator, satisfying the Ginsparg-Wilson relation [13]

$$D(0)\gamma_5 + \gamma_5 D(0) = 2rD(0)\gamma_5 D(0).$$

IV. A FORMULA FOR THE RESIDUAL MASS

Now we are ready to derive a formula for the residual mass, in terms of the quark propagator in a gauge background. The denominator of (17) can be evaluated as

$$\begin{aligned} &\sum_x \langle \bar{q}(x) \lambda^a \gamma_5 q(x) \bar{q}(y) \lambda^b \gamma_5 q(y) \rangle \\ &= -\text{tr}_F(\lambda^a \lambda^b) \text{tr}_{DC}\{[(D_c + m_q)^{-1}]^\dagger (D_c + m_q)^{-1}\}(y, y), \end{aligned} \quad (38)$$

where the subscript F denotes the flavor space, and the subscript DC the Dirac and color spaces. In the following, the subscripts F and DC will be suppressed.

Using Eqs. (12), (20), (21), and (30)-(33), we evaluate the numerator of (17) as

$$\begin{aligned} &\sum_x \langle J_5^a(x, n) \bar{q}(y) \lambda^b \gamma_5 q(y) \rangle \\ &= \text{tr}(\lambda^a \lambda^b) \left\{ \sum_x \text{tr}[\langle q(y) \bar{\psi}_n(x) \rangle P_- \langle \psi_{n+1}(x) \bar{q}(y) \rangle \gamma_5] - \sum_x \text{tr}[\langle q(y) \bar{\psi}_{n+1}(x) \rangle P_+ \langle \psi_n(x) \bar{q}(y) \rangle \gamma_5] \right\} \\ &= \text{tr}(\lambda^a \lambda^b) \left\{ - \sum_x \text{tr}[\langle q(y) \bar{\eta}_n(x) \rangle \gamma_5 P_- \langle \eta_{n+1}(x) \bar{q}(y) \rangle \gamma_5] + \sum_x \text{tr}[\langle q(y) \bar{\eta}_{n+1}(x) \rangle \gamma_5 P_+ \langle \eta_{n+1}(x) \bar{q}(y) \rangle \gamma_5] \right\} \\ &= \text{tr}(\lambda^a \lambda^b) \sum_x \text{tr}[\langle q(y) \bar{\eta}_n(x) \rangle \langle \eta_{n+1}(x) \bar{q}(y) \rangle \gamma_5] \\ &= \text{tr}(\lambda^a \lambda^b) \frac{1}{r} \text{tr}[\gamma_5 D^{-1}(m_q)(rD - P_-)\gamma_5(rD - P_+)D^{-1}(m_q)](y, y) \\ &= -\text{tr}(\lambda^a \lambda^b) \frac{1}{4r} \text{tr}\{[D^{-1}(m_q)]^\dagger (1 - S^2) D^{-1}(m_q)\}(y, y). \end{aligned} \quad (39)$$

where $D = D(0) = D_c(1 + rD_c)^{-1}$. Using (38) and (39), we can rewrite (17) as

$$m_{res}(y) = \frac{1}{4r} \frac{\text{tr}\{[D^{-1}(m_q)]^\dagger(1 - S^2)D^{-1}(m_q)\}(y, y)}{\text{tr}\{[(D_c + m_q)^{-1}]^\dagger(D_c + m_q)^{-1}\}(y, y)}, \quad (40)$$

where $D^{-1}(m_q)$ is the sea quark propagator, and $(D_c + m_q)^{-1}$ is the valence quark propagator. Therefore, (40) is well-defined only in the unitary limit, with the valence quark mass equal to the sea quark mass. We note that Eq. (40) is consistent with the form used in Refs. [11] and [14], but not in the unitary limit.

Similarly, the global residual mass (18) can be written as

$$M_{res} = \frac{1}{4r} \frac{\text{Tr}\{[D^{-1}(m_q)]^\dagger(1 - S^2)D^{-1}(m_q)\}}{\text{Tr}\{[(D_c + m_q)^{-1}]^\dagger(D_c + m_q)^{-1}\}}, \quad (41)$$

where Tr denotes the trace over the Dirac, color, and site indices.

Nevertheless, it is tedious to compute the residual mass via (40) since it involves the multiplication of $S = (1 - \prod_s T_s)(1 + \prod_s T_s)^{-1} = H \sum_{i=1}^n b_i(H^2 + d_i)^{-1}$ to the column vectors of $D^{-1}(m_q)$, requiring conjugate gradient with multi-shift.

In the following, we derive a practical formula for the residual mass, which only involves the valence quark propagator. Then the residual mass can be obtained once the valence quark propagator has been computed.

We observe that the numerator of (40) can be decomposed into two parts

$$\text{tr}\{[D^{-1}(m_q)]^\dagger D^{-1}(m_q)\}(y, y) - \text{tr}\{[SD^{-1}(m_q)]^\dagger(SD^{-1}(m_q))\}(y, y). \quad (42)$$

Using (31) and (5), we obtain

$$S = \gamma_5 \left[2r \frac{D(m_q) - m_q}{1 - rm_q} - 1 \right],$$

and

$$\begin{aligned} SD(m_q)^{-1} &= \gamma_5 \left[\frac{2r}{1 - rm_q} - \frac{1 + rm_q}{1 - rm_q} D(m_q)^{-1} \right] \\ &= \gamma_5 [r - (1 + rm_q)(D_c + m_q)^{-1}]. \end{aligned}$$

Thus the second term in (42) can be evaluated as

$$\begin{aligned} &\text{tr}\{[SD^{-1}(m_q)]^\dagger(SD^{-1}(m_q))\}(y, y) \\ &= r^2 \text{tr} \mathbb{I} - 2r(1 + rm_q) \text{Re} \text{tr}(D_c + m_q)^{-1}(y, y) \\ &\quad + (1 + rm_q)^2 \text{tr}\{[(D_c + m_q)^{-1}]^\dagger(D_c + m_q)^{-1}\}(y, y). \end{aligned} \quad (43)$$

Using (31), the first term of (42) is evaluated as

$$\begin{aligned} & \text{tr} \{ [D^{-1}(m_q)]^\dagger D^{-1}(m_q) \} (y, y) \\ &= r^2 \text{tr} \mathbb{1} + 2r(1 - rm_q) \text{Re} \text{ tr} (D_c + m_q)^{-1}(y, y) \\ &+ (1 - rm_q)^2 \text{tr} \{ [(D_c + m_q)^{-1}]^\dagger (D_c + m_q)^{-1} \} (y, y). \end{aligned} \quad (44)$$

Substituting (44) and (43) into (40), we obtain a formula for the residual mass

$$m_{res}(y) = \frac{\text{Re} \text{ tr} \{ (D_c + m_q)^{-1}(y, y) \}}{\text{tr} \{ [(D_c + m_q)^\dagger (D_c + m_q)]^{-1}(y, y) \}} - m_q, \quad (45)$$

which immediately gives the residual mass once the 12 columns of the valence quark propagator $(D_c + m_q)^{-1}(x, y)$ have been computed. Also, it is appealing from the viewpoint of exact chiral symmetry, since the first term in (45) gives m_q when D_c is exactly chirally symmetric, (i.e. $D_c \gamma_5 + \gamma_5 D_c = 0$), thus the residual mass is exactly zero.

Similarly, the global residual mass (41) can be written as

$$M_{res} = \frac{\text{Re} \text{ Tr} \{ (D_c + m_q)^{-1} \}}{\text{Tr} \{ [(D_c + m_q)^\dagger (D_c + m_q)]^{-1} \}} - m_q. \quad (46)$$

Equations (45) and (46) are two of the main results of this paper.

Now we consider an ensemble of gauge configurations generated in full QCD with n_f flavors, obeying the probability distribution

$$\prod_{f=1}^{n_f} \det D(m_f) e^{-\mathcal{A}_g},$$

then the ensemble average of the residual mass can be written as

$$\langle m_{res}(y) \rangle = \frac{\int [dU] \prod_{f=1}^{n_f} \det D(m_f) e^{-\mathcal{A}_g} m_{res}(y)}{\int [dU] \prod_{f=1}^{n_f} \det D(m_f) e^{-\mathcal{A}_g}},$$

which would be independent of y if the number of gauge configurations is sufficiently large. Obviously, the ensemble average of the global residual mass, $\langle M_{res} \rangle$, would tend to the limiting value with much less number of configurations.

V. AN UPPER BOUND FOR THE RESIDUAL MASS

For ODWF, $S(H) = S_{opt}(H)$, the Zolotarev optimal rational approximation of $\text{sgn}(H) = H(H^2)^{-1/2}$, provided that the eigenvalues of H^2 lying in the range $[\lambda_{min}^2, \lambda_{max}^2]$, where λ_{min}^2

and λ_{max}^2 are the lower and upper bounds used for computing the nonzero weights $\{\omega_s, s = 1, \dots, n-1, n+2, N_s+2\}$. Thus, for any gauge configuration yielding eigenvalues of H^2 lying in the range $[\lambda_{min}^2, \lambda_{max}^2]$, the residual mass must be bounded since it is a function of the sign function error $\|1 - S_{opt}(H)\|$ which is always less than d_Z , the maximum deviation in the Zolotarev optimal rational approximation. In the following, we obtain an upper bound for the global residual mass in lattice QCD with ODWF.

The numerator of (41) can be written as

$$\begin{aligned} \text{Tr}\{[D(m_q)^{-1}]^\dagger(1 - S^2)D^{-1}(m_q)\} &= \text{Tr}\{(1 - S^2)(D^\dagger D)^{-1}(m_q)\} \\ &\leq \left|\text{Tr}\{(1 - S^2)(D^\dagger D)^{-1}(m_q)\}\right| \leq \sum_j \alpha_j \beta_j, \end{aligned} \quad (47)$$

where the von Neumann's trace inequality has been used, and α_j and β_j are the eigenvalues of $|1 - S^2|$ and $(D^\dagger D)^{-1}(m_q)$ respectively, in the ascending order, i.e., $\alpha_1 \leq \alpha_2 \leq \dots \leq \alpha_N$, and $\beta_1 \leq \beta_2 \leq \dots \leq \beta_N$.

For ODWF, $S = S_{opt}$, $\alpha_j \leq 2d_Z$. Thus (47) gives

$$\text{Tr}\{[D(m_q)^{-1}]^\dagger(1 - S_{opt}^2)D^{-1}(m_q)\} \leq 2d_Z \text{Tr}\{(D^\dagger D)^{-1}(m_q)\}, \quad (48)$$

and (41) implies

$$M_{res} \leq \frac{d_Z}{2r} \frac{\text{Tr}\{[D(m_q)^{-1}]^\dagger D^{-1}(m_q)\}}{\text{Tr}\{[(D_c + m_q)^{-1}]^\dagger (D_c + m_q)^{-1}\}}. \quad (49)$$

From (31), the singular values of $D^{-1}(m_q)$ and $(D_c + m_q)^{-1}$ have the following relationship

$$\lambda_j = r + (1 - rm_q)\xi_j, \quad (50)$$

where ξ_j is a singular value of $(D_c + m_q)^{-1}$ and λ_j is the corresponding singular value of $D^{-1}(m_q)$. Then (50) gives

$$\frac{\sum_j |\lambda_j|^2}{\sum_j |\xi_j|^2} = (1 - rm_q)^2 + 2r(1 - rm_q) \frac{\langle \text{Re}(\xi) \rangle}{\langle |\xi|^2 \rangle} + \frac{r^2}{\langle |\xi|^2 \rangle}, \quad (51)$$

where

$$\langle |\xi|^2 \rangle = \frac{1}{N} \sum_{j=1}^N |\xi_j|^2, \quad \langle \text{Re}(\xi) \rangle = \frac{1}{N} \sum_{j=1}^N \text{Re}(\xi_j), \quad (52)$$

and N is the total number of singular values of $(D_c + m_q)^{-1}$. Therefore

$$\frac{\text{Tr}\{[D(m_q)^{-1}]^\dagger D^{-1}(m_q)\}}{\text{Tr}\{[(D_c + m_q)^{-1}]^\dagger (D_c + m_q)^{-1}\}} = (1 - rm_q)^2 + 2r(1 - rm_q) \frac{\langle \text{Re}(\xi) \rangle}{\langle |\xi|^2 \rangle} + \frac{r^2}{\langle |\xi|^2 \rangle}, \quad (53)$$

and (49) becomes

$$M_{res} \leq \frac{d_Z}{2r} \left[(1 - rm_q)^2 + 2r(1 - rm_q) \frac{\langle \text{Re}(\xi) \rangle}{\langle |\xi|^2 \rangle} + \frac{r^2}{\langle |\xi|^2 \rangle} \right]. \quad (54)$$

Thus, to obtain the upper bound of M_{res} amounts to working out an upper bound for $\langle \text{Re}(\xi) \rangle / \langle |\xi|^2 \rangle$, and a lower bound for $\langle |\xi|^2 \rangle$.

First we work out a lower bound for $\langle |\xi|^2 \rangle$. The eigenvalues of $V = \gamma_5 S$ can be expressed as $\{R_j e^{i\theta_j}, j = 1, \dots, N\}$, where R_j can be bigger or less than one since the chiral symmetry is not exact for finite N_s . Then the corresponding eigenvalues of $rD_c = (1 + V)(1 - V)^{-1}$ can be expressed as

$$x_j + iy_j = \frac{1 - R_j^2 + i2R_j \sin \theta_j}{1 + R_j^2 - 2R_j \cos \theta_j}. \quad (55)$$

Thus the eigenvalues of $(D_c + m_q)^{-1}$ are $\eta_j = r(x_j + rm_q + iy_j)^{-1}$. For finite N_s , $\langle |\eta|^2 \rangle$ is not exactly equal to $\langle |\xi|^2 \rangle$, since $[V^\dagger, V] \neq 0$, due to the eigenvalues of V not falling on a circle. However, in estimating the lower bound of $\langle |\xi|^2 \rangle$, one must fix all eigenvalues of V on a circle with a radius having the maximal deviation from one. Then, in this case, $[V^\dagger, V] = 0$, and $\langle |\eta|^2 \rangle = \langle |\xi|^2 \rangle$. Thus, we can use $\langle |\eta|^2 \rangle$ to estimate the lower bound of $\langle |\xi|^2 \rangle$. Using (55) and setting $R_j = R$, and $m \equiv rm_q$, we obtain

$$\begin{aligned} \langle |\xi|^2 \rangle &= \frac{1}{N} \sum_{j=1}^N \frac{r^2}{(x_j + m)^2 + y_j^2} = \frac{r^2}{N} \sum_{j=1}^N \frac{(1 + R^2 - 2R \cos \theta_j)}{(1 + m^2)(1 + R^2) + 2m(1 - R^2) + 2R(1 - m^2) \cos \theta_j}, \\ &= \frac{r^2}{1 + m} \left[\frac{2(1 + R^2) - (1 - m)(1 - R^2)}{(1 + m^2)(1 - R^2) + 2m(1 + R^2)} \right], \end{aligned} \quad (56)$$

where we have assumed that the distribution of the eigenvalues of V is uniform in θ , and used the formula

$$\frac{1}{2\pi} \int_0^{2\pi} \frac{d\theta}{B + A \cos \theta} = \frac{1}{\sqrt{B^2 - A^2}}.$$

For ODWF, $|1 - R^2| \leq 2d_Z$, and the lower bound of (56) is attained at $R = \sqrt{1 - 2d_Z}$, i.e.,

$$\langle |\xi|^2 \rangle \geq \frac{r^2}{1 + m} \left[\frac{2 - (3 - m)d_Z}{2m + (1 - m)^2 d_Z} \right]. \quad (57)$$

Next we work out an upper bound for $\langle \text{Re}(\xi) \rangle / \langle |\xi|^2 \rangle$. Again, using (55) and setting $R_j = R$, and $m \equiv rm_q$, we obtain

$$\begin{aligned} \langle \text{Re}(\xi) \rangle &= \frac{1}{N} \sum_{j=1}^N \frac{r(x_j + m)}{(x_j + m)^2 + y_j^2} = \frac{r}{N} \sum_{j=1}^N \frac{1 - R^2 + m(1 + R^2 - 2R \cos \theta_j)}{(1 + m^2)(1 + R^2) + 2m(1 - R^2) + 2R(1 - m^2) \cos \theta_j}, \\ &= r \frac{1 - R^2}{(1 + m^2)(1 - R^2) + 2m(1 + R^2)} + r^{-1}m \langle |\xi|^2 \rangle, \end{aligned} \quad (58)$$

and

$$\frac{\langle \text{Re}(\xi) \rangle}{\langle |\xi|^2 \rangle} = r^{-1} \left[m + \frac{(1+m)(1-R^2)}{2(1+R^2)-(1-m)(1-R^2)} \right], \quad (59)$$

where (56) has been used.

For ODWF, $|1-R^2| \leq 2d_Z$, the upper bound of (59) is attained at $R = \sqrt{1-2d_Z}$, i.e.,

$$\frac{\langle \text{Re}(\xi) \rangle}{\langle |\xi|^2 \rangle} \leq r^{-1} \left[m + \frac{(1+m)d_Z}{2-(3-m)d_Z} \right]. \quad (60)$$

Substituting (60) and (57) into (54), we obtain

$$M_{res} \leq \frac{d_Z}{2r} \left[\frac{2(1+m)}{2-(3-m)d_Z} \right], \quad (61)$$

where $m \equiv rm_q$. This is one of the main results of this paper.

In general, $0 \leq d_Z \leq 0.5$, this gives

$$(1+m) \leq \frac{2(1+m)}{2-(3-m)d_Z} \leq 4. \quad (62)$$

Thus the upper-bound of M_{res} varies in the range

$$\frac{d_Z}{2r}(1+m) \leq (M_{res})^{upper-bound} \leq \frac{2d_Z}{r}. \quad (63)$$

For ODWF, $d_Z \ll 1$ for $N_s \gg 1$, then (61) reduces to

$$M_{res} \leq \frac{d_Z}{2r} (1+rm_q) \simeq \frac{d_Z}{2r}, \quad (64)$$

where $m_q \ll m_{PV} = r^{-1}$ has been used in the last approximation.

Moreover, d_Z is an exponentially decreasing function of N_s , and it can be parametrized as [6]

$$d_Z(N_s, b) = A(b) \exp\{-C(b)N_s\}, \quad b \equiv \lambda_{max}^2/\lambda_{min}^2, \quad (65)$$

where $A(b)$ and $C(b)$ are positive definite functions of b . This immediately implies that the global residual mass for lattice QCD with ODWF is an exponentially decreasing function of N_s , regardless of the size of the lattice, at zero or finite temperatures. However, this scenario holds only when all eigenvalues of H^2 are falling inside the interval $[\lambda_{min}^2, \lambda_{max}^2]$. In general, in the simulation of full QCD with ODWF, after fixing λ_{min}^2 and λ_{max}^2 in the beginning of the simulation, it could happen that some (accepted) gauge configurations in the course of the simulation may yield eigenvalues of H^2 lying outside the interval $[\lambda_{min}^2, \lambda_{max}^2]$.

Then the global residual mass of such “unbounded” configurations could be larger than the upper bound (61), especially for those with many eigenvalues of H^2 less than λ_{min}^2 . Thus, after generating an ensemble of gauge configurations, the ensemble averaged residual mass, $\langle m_{res}(y) \rangle$ or $\langle M_{res} \rangle$, could be larger than the upper-bound (61). In the following, we discuss to what extent the low-lying eigenmodes of H^2 modify the upper-bound (61).

Consider a configuration U of which $|H|$ has N_a eigenvalues ($h_i, i = 1, \dots, N_a$) less than λ_{min} , i.e., $h_1 < h_2 < \dots < h_{N_a} < \lambda_{min}$. Here we assume $N_a \ll N = 12L^3T$. For each of these N_a eigenvalues, the corresponding eigenvalue of $|1 - S_{opt}^2(H)|$ is greater than $2d_Z$, with the maximum equal to

$$2d_a \equiv |1 - S_{opt}^2(h_1)|, \quad (66)$$

where h_1 is the smallest eigenvalue of $|H|$. Therefore (47) is modified to

$$\begin{aligned} \text{Tr}\{[D(m_q)^{-1}]^\dagger(1 - S_{opt}^2)D^{-1}(m_q)\} &\leq 2d_Z \sum_{j=1}^{N-N_a} \beta_j + 2d_a \sum_{j=N-N_a+1}^N \beta_j \\ &= [2(d_a - d_Z)Q_a + 2d_Z] \text{Tr}\{(D^\dagger D)^{-1}(m_q)\}, \end{aligned} \quad (67)$$

where

$$Q_a \equiv \frac{\sum_{j=N-N_a+1}^N \beta_j}{\sum_{j=1}^N \beta_j}, \quad (68)$$

$$\sum_{j=1}^N \beta_j = \text{Tr}\{(D^\dagger D)^{-1}(m_q)\}. \quad (69)$$

Now the upper-bound of $\text{Tr}\{(D^\dagger D)^{-1}(m_q)\}/\text{Tr}\{[(D_c + m_q)^{-1}]^\dagger(D_c + m_q)^{-1}\}$ can be evaluated as before, except replacing d_Z with d_a . Then the upper-bound of the global residual mass (61) is transcribed to

$$M_{res} \leq \left[\frac{d_Z + (d_a - d_Z)Q_a}{2r} \right] \left[\frac{2(1+m)}{2 - (3-m)d_a} \right] \equiv F(N_s, m, N_a, h), \quad (70)$$

where the factor $2(1+m)/[2 - (3-m)d_a]$ is bounded between $(1+m)$ and 4, similar to (62). Thus the most significant change due to the “unbounded” low-lying eigenmodes is to replace d_Z with $d_Z + (d_a - d_Z)Q_a$, in the first factor of (70).

Next we evaluate Q_a . Using (50), we obtain

$$Q_a = \frac{\sum_{j=N-N_a+1}^N \beta_j}{\sum_{j=1}^N \beta_j} = \frac{(N_a/N)r^2 + 2r(1-m)\lceil \text{Re}(\xi) \rceil + (1-m)^2\lceil |\xi|^2 \rceil}{r^2 + 2r(1-m)\langle \text{Re}(\xi) \rangle + (1-m)^2\langle |\xi|^2 \rangle}, \quad (71)$$

where ξ_j is a singular value of $(D_c + m_q)^{-1}$, and

$$\lfloor |\xi|^2 \rfloor = \frac{1}{N} \sum_{j=N-N_a+1}^N |\xi_j|^2, \quad \lfloor \operatorname{Re}(\xi) \rfloor = \frac{1}{N} \sum_{j=N-N_a+1}^N \operatorname{Re}(\xi_j), \quad (72)$$

$$\langle |\xi|^2 \rangle = \frac{1}{N} \sum_{j=1}^N |\xi_j|^2, \quad \langle \operatorname{Re}(\xi) \rangle = \frac{1}{N} \sum_{j=1}^N \operatorname{Re}(\xi_j). \quad (73)$$

To estimate above sums, we follow the same procedure in obtaining (56) and (58), and also assume that the distribution of the eigenvalues of $V = \gamma_5 S_{opt}$ is uniform in θ . Then we have

$$\langle |\xi|^2 \rangle = \frac{r^2}{1+m} \left[\frac{2(1+R^2) - (1-m)(1-R^2)}{(1+m^2)(1-R^2) + 2m(1+R^2)} \right], \quad (74)$$

$$\langle \operatorname{Re}(\xi) \rangle = r \frac{1-R^2}{(1+m^2)(1-R^2) + 2m(1+R^2)} + r^{-1}m \langle |\xi|^2 \rangle, \quad (75)$$

$$\lfloor |\xi|^2 \rfloor = \frac{r^2}{\pi} \int_{\theta_a}^{\pi} d\theta \frac{1+R^2 - 2R \cos \theta}{(1+m^2)(1+R^2) + 2m(1-R^2) + 2R(1-m^2) \cos \theta}, \quad (76)$$

$$\lfloor \operatorname{Re}(\xi) \rfloor = \frac{r}{\pi} \int_{\theta_a}^{\pi} d\theta \frac{1-R^2 + m(1+R^2 - 2R \cos \theta)}{(1+m^2)(1+R^2) + 2m(1-R^2) + 2R(1-m^2) \cos \theta}, \quad (77)$$

where $R = \sqrt{1-2d_a}$, and $\theta_a = (1-N_a/N)\pi$. Then the denominator of Q_a becomes

$$r^2 + 2r(1-m) \langle \operatorname{Re}(\xi) \rangle + (1-m)^2 \langle |\xi|^2 \rangle = \frac{2r^2}{2m + (1-m)^2 d_a}. \quad (78)$$

To evaluate the integrals (76) and (77), we perform the change of variable $\chi = \pi - \theta$, and obtain

$$\lfloor |\xi|^2 \rfloor = \frac{r^2}{\pi} \int_0^{N_a \pi / N} d\chi \frac{1+R^2 - 2R \cos(\pi - \chi)}{(1+m^2)(1+R^2) + 2m(1-R^2) + 2R(1-m^2) \cos(\pi - \chi)}, \quad (79)$$

$$\lfloor \operatorname{Re}(\xi) \rfloor = \frac{r}{\pi} \int_0^{N_a \pi / N} d\chi \frac{1-R^2 + m(1+R^2 - 2R \cos(\pi - \chi))}{(1+m^2)(1+R^2) + 2m(1-R^2) + 2R(1-m^2) \cos(\pi - \chi)}. \quad (80)$$

Since the upper limit of the integrals is $N_a \pi / N \ll 1$, we can use the approximation $\cos(\pi - \chi) \simeq -1 + \chi^2/2$ in the integrand, and obtain

$$\lfloor |\xi|^2 \rfloor = \frac{N_a}{N} \left(\frac{rd_a}{md_a + (1-d_a - \sqrt{1-2d_a})} \right)^2, \quad (81)$$

$$\lfloor \operatorname{Re}(\xi) \rfloor = \frac{N_a}{N} \frac{rd_a}{md_a + (1-d_a - \sqrt{1-2d_a})}, \quad (82)$$

where we have used the formula

$$\int_0^{\chi_a} d\chi \frac{A+B\chi^2}{C+D\chi^2} = \frac{B}{D} \chi_a - \frac{(BC-AD) \tan^{-1} \left(\sqrt{D/C} \chi_a \right)}{D\sqrt{CD}} \simeq \frac{A}{C} \chi_a + \mathcal{O}(\chi_a^2),$$

and suppressed the higher order terms of $\mathcal{O}((N_a/N)^2)$. Then we obtain the numerator of Q_a

$$\begin{aligned} & \left(\frac{N_a}{N} \right) r^2 + 2r(1-m)[\text{Re}(\xi)] + (1-m)^2[|\xi|^2] \\ &= \left(\frac{N_a}{N} \right) r^2 \left(\frac{1 - \sqrt{1 - 2d_a}}{1 - \sqrt{1 - 2d_a} - (1-m)d_a} \right)^2. \end{aligned} \quad (83)$$

Using (78) and (83), we get

$$\begin{aligned} Q_a &= \frac{N_a}{N} \left(m + (1-m)^2 \frac{d_a}{2} \right) \left(\frac{1 - \sqrt{1 - 2d_a}}{1 - \sqrt{1 - 2d_a} - (1-m)d_a} \right)^2 \\ &= \frac{N_a}{N} \left[\frac{(1+m) + (1-m)\sqrt{1-2d_a}}{(1+m) - (1-m)\sqrt{1-2d_a}} \right]. \end{aligned} \quad (84)$$

Since $0 \leq d_a \leq 0.5$, we have

$$\frac{N_a}{N} \leq Q_a \leq \frac{N_a}{N} \left(\frac{1}{m} \right). \quad (85)$$

In other words, Q_a is a monotonically decreasing function of d_a , which in turn is a monotonically increasing function of N_s , with the upper bound $(N_a/N)/m$.

For $N_s \gg 1$, $d_Z \ll d_a \ll 0.5$, then

$$(d_a - d_Z)Q_a \simeq d_a Q_a \simeq \frac{N_a}{N} \left(\frac{d_a}{m + d_a/2} \right), \quad (86)$$

where $m \ll 1$ has been used. If $m \ll d_a/2$, then (86) gives $(d_a - d_Z)Q_a \simeq 2N_a/N$, which is almost independent of N_s . This immediately implies that the first factor

$[d_Z + (d_a - d_Z)Q_a]/(2r)$ in the upper-bound of the residual mass (70) would look like almost “saturated” (decreasing slowly with respect to N_s) after N_s greater than some threshold value N_s^{thres} which depends on N_a (the number of eigenvalues of $|H|$ smaller than λ_{min}) and weakly on h_1 (the smallest eigenvalue of $|H|$). In other words, if there are some eigenvalues of $|H|$ smaller than λ_{min} , the exponential bound cannot be sustained for $N_s > N_s^{thres}$. This is one of the most interesting results emerging from our theoretical analysis.

In Fig. 1, we plot the upper-bounds (64) and (70) versus N_s respectively, where the integrals in Q_a are evaluated numerically. Here we set $\lambda_{min} = 0.05$, and $\lambda_{max} = 6.20$. The solid line is the upper-bound (64) of the global residual mass, for the case when all eigenvalues of $|H|$ fall inside the interval $[\lambda_{min}, \lambda_{max}]$. It decays exponentially with N_s . The dotted line is the modified upper-bound (70) of the global residual mass, for the case when some

eigenvalues of $|H|$ are smaller than λ_{min} . Here we set $N_a = 5$ (i.e., 5 eigenvalues of $|H|$ smaller than λ_{min}), and the smallest eigenvalue $h_1 = 0.005 = \lambda_{min}/10$. We see that the modified upper-bound of the global residual mass of ODWF decays exponentially up to $N_s \simeq 18$, then it decays like $1/N_s^3$ for $N_s \simeq 18-23$, and almost ‘‘saturates’’ at $\sim 10^{-5}$ for $N_s \simeq 24-33$. This agrees with our theoretical analysis of the first factor $[d_Z + (d_a - d_Z)Q_a]/(2r)$ in the upper-bound of the residual mass (70), which would become almost ‘‘saturated’’ when $N_s > N_s^{thres}$. Moreover, due to the second factor $2(1+m)/[2 - (3-m)d_a]$ in (70), the exponential bound $d_Z/(2r)$ for $N_s < N_s^{thres}$ is increased by a factor ~ 3 , as shown in Fig. 1.

Next, we turn to an ensemble of gauge configurations $\{U_i\}$. Let the smallest eigenvalue of $|H|$ with the gauge configuration U_i be $h_1^{(i)}$, and the probability distribution of $\{h_1^{(i)}\}$ satisfies

$$\int_{h_{min}}^{h_{max}} dh \rho(h) = 1,$$

where $h_{min} = \min(h_1^{(1)}, h_1^{(2)}, \dots, h_1^{(i)}, \dots)$ and $h_{max} = \max(h_1^{(1)}, h_1^{(2)}, \dots, h_1^{(i)}, \dots)$. Then the upper-bound of the global residual mass for an ensemble of gauge configurations is

$$\langle M_{res} \rangle \leq \frac{1}{h_{max} - h_{min}} \left\{ \theta(x) \int_{h_{min}}^y dh \rho(h) F(N_s, m, N_a, h) + \left(\frac{d_Z}{2r} \right) [z\theta(z) + x\theta(-x)] \right\}, \quad (87)$$

where $x = \lambda_{min} - h_{min}$, $y = \min(\lambda_{min}, h_{max})$, $z = h_{max} - \lambda_{min}$, and $F(N_s, m, N_a, h)$ is defined in (70). This is one of the main results of this paper.

VI. NUMERICAL TESTS

In this section, we test to what extent the upper-bound (87) of global residual mass for an ensemble of gauge configurations is satisfied in large-scale simulations of lattice QCD with ODWF. To this end, we perform hybrid Monte Carlo (HMC) simulations of two flavors QCD on the $16^3 \times 32$ lattice with ODWF (setting kernel $H = H_w$) at $N_s = 16$ and $\lambda_{min}/\lambda_{max} = 0.05/6.20$, plaquette gauge action at $\beta = 6.10$, and sea-quark mass $m_q a = 0.01$. We have generated 2730 trajectories. After discarding the initial 300 trajectories for thermalization, we sample one configuration every 10 trajectories. Thus we have 243 gauge configurations. For each configuration, we compute the valence quark propagator with mass $m_{val} a = m_{sea} a = 0.01$, and use the formula (45) to obtain the residual mass. We perform the same calculation for 3 different cases: $N_s = 8, 16, 32$, with the same $\lambda_{min}/\lambda_{max} = 0.05/6.20$.

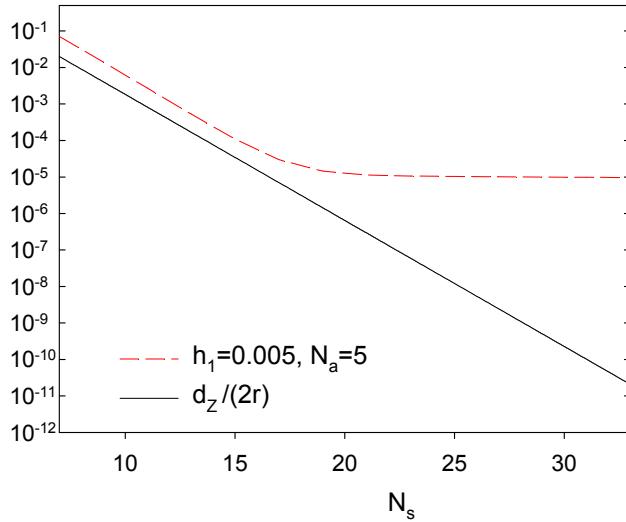


FIG. 1: The solid line is the theoretical upper-bound (64) of the global residual mass, for the case when all eigenvalues of $|H|$ fall inside the interval $[\lambda_{min}, \lambda_{max}]$. Here we set $\lambda_{min} = 0.05$, and $\lambda_{max} = 6.20$. The dotted line is the modified upper-bound (70) for the case when some of the eigenvalues of $|H|$ are smaller than λ_{min} . Here we set $N_a = 5$ (i.e., 5 eigenvalues of $|H|$ smaller than λ_{min}), and the smallest eigenvalue $h_1 = 0.005$.

Then we obtain the averaged residual mass $\langle m_{res} \rangle$ for $N_s = 8, 16, 32$, which are denoted by squares in Fig. 2. We see that for $N_s = 8$ and $N_s = 16$, $\langle m_{res} \rangle$ satisfies the exponential bound (64), $d_Z/(2r)$. However, for $N_s = 32$, $\langle m_{res} \rangle$ is much larger than the exponential bound.

Next, we compute the general upper-bound (87) to see to what extent it is satisfied by $\langle m_{res} \rangle$. For each configuration, we project 250 lowest lying eigenmodes of $|H_w|$. Then we obtain the smallest eigenvalue (h_1) of $|H_w|$, and also N_a , the number of eigenmodes of $|H_w|$ with eigenvalue smaller than λ_{min} . Among the set of 243 smallest eigenvalues $\{h_1^{(i)}, i = 1, \dots, 243\}$, the minimum is $h_{min} = 6.99106 \times 10^{-5} < \lambda_{min}$, while the maximum is $h_{max} = 0.1186 > \lambda_{min}$. The probability distribution of h_1 can be fitted by the “log-normal” function

$$\rho(h) = \rho_0 \exp \left\{ -\frac{1}{2} \left[\frac{\ln(h/h_0)}{\sigma} \right]^2 \right\}, \quad (88)$$

where $\rho_0 = 27.4326(1.2364)$, $\sigma = 0.923(43)$, and $h_0 = 0.0108(5)$. The average number of eigenvalues of $|H_w|$ smaller than λ_{min} is $\langle N_a \rangle = 1.778(85)$. The histogram of N_a is plotted

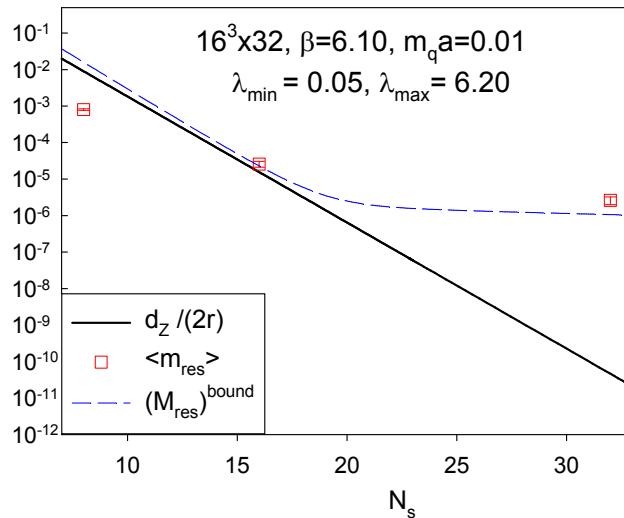


FIG. 2: The solid line is the theoretical upper-bound $d_Z/(2r)$ of the global residual mass, for the case when all eigenvalues of $|H|$ fall inside the interval $[\lambda_{min}, \lambda_{max}]$. Here we set $\lambda_{min} = 0.05$, and $\lambda_{max} = 6.20$. The dotted line is the general upper-bound (87). The squares denote the average residual mass obtained with 243 gauge configurations from simulation of 2-flavors QCD with ODWF at $\beta = 6.10$, on the $16^3 \times 32$ lattice.

in Fig. 3. Using (88) and the information of N_a , we obtain the upper-bound (87) of the global residual mass as a function of N_s , which is plotted as the dotted lines in Fig. 2. We see that the data points of $\langle m_{res} \rangle$ are in good agreement with the upper-bound (87).

A salient feature emerging from this numerical study is that the exponential bound (64) for the global residual mass holds for $N_s < 18$. However, it is difficult to sustain the exponential bound for $N_s > 20$, due to the low-lying eigenmodes of $|H|$ with eigenvalue less than λ_{min} , in agreement with our theoretical analysis of the first factor $[d_Z + (d_a - d_Z)Q_a]/(2r)$ in the upper-bound of the residual mass (70), which would become almost ‘‘saturated’’ when $N_s > N_s^{thres} \simeq 18 - 20$.

At this point, it is instructive to compare the behavior of the residual mass of the ODWF in Fig. 2 with those of the conventional DWF. For the conventional DWF, $\langle m_{res} \rangle$ behaves like $1/N_s$ for the Shamir kernel [15], and $1/N_s^2$ for the Möbius kernel with tuned parameters [16]. However, they do not possess an exponential bound for any interval of N_s , unlike the case of ODWF. Moreover, it is straightforward to generalize the theoretical analysis in the

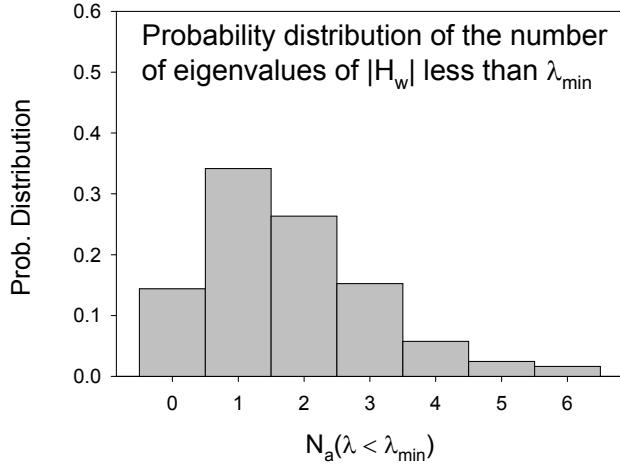


FIG. 3: The histogram of N_a , the number of eigenvalues of $|H_w|$ smaller than λ_{\min} , for 243 gauge configurations generated by HMC simulation of two flavors QCD on the $16^3 \times 32$ lattice with ODWF at $N_s = 16$ and $\lambda_{\min}/\lambda_{\max} = 0.05/6.20$, plaquette gauge action at $\beta = 6.10$, and sea-quark mass $m_q a = 0.01$.

last section to the case of conventional DWF and show that the “saturation” phenomenon at large N_s also holds for the conventional DWF.

VII. CONCLUDING REMARKS

In this paper, we have derived the axial Ward identity for lattice QCD with ODWF, by introducing two transparent layers at the central region of the fifth dimension, in addition to the two transparent layers at the boundaries for defining the quark fields [7]. From the axial Ward identity (13), we obtain (15) and (16) as the local and global residual mass, for measuring the chiral symmetry breaking due to the finite extension in the fifth dimension.

Since the global residual mass (16) depends on the observable \mathcal{O} , it is necessary to determine the residual mass of the quark for any observable \mathcal{O} . So far, the residual mass has been only studied for the the pseudoscalar $\mathcal{O}(y) = \bar{q}(y)\lambda^b\gamma_5 q(y)$, the pion interpolator. It is interesting to see how the residual mass of the quark changes with respect to the physical observable. We have derived the generating functional for the n -point Green’s function of fermion fields (28), which is essential for expressing the residual mass in terms of the quark

propagator.

For the observable $\mathcal{O}(y) = \bar{q}(y)\lambda^b\gamma_5 q(y)$, we have obtained a new formula (45) for the residual mass, which is useful in practice since it immediately gives the local residual mass once the 12 columns of the valence quark propagator $(D_c + m_q)^{-1}(x, y)$ have been computed. For the global residual mass (46), it requires all-to-all quark propagators, or the low-lying eigenmodes of $D = D_c(1 + rD_c)^{-1}$ for an estimation.

Moreover, we obtain the upper-bounds (70) and (87) of the global residual mass, for one configuration as well as an ensemble of gauge configurations in lattice QCD with ODWF. They provide a guideline for designing lattice QCD simulation with ODWF. That is, with the input values of $r = [2m_0(1 - dm_0)]^{-1}$ and m_q , how to choose the values of N_s , λ_{min} and λ_{max} such that the residual mass meets the desired tolerance, versus the cost of the simulation.

For the case when all eigenvalues of $|H|$ fall inside the interval $[\lambda_{min}, \lambda_{max}]$, only the second term in (87) contributes, then $M_{res} \leq d_Z/(2r)$, an exponentially decreasing function of N_s . However, if there are some eigenvalues of $|H|$ smaller than λ_{min} , then the first term of (87) also contributes, which makes the exponential bound only hold for $N_s < (N_s)^{thres}$, where $(N_s)^{thres}$ depends on λ_{min} and the low-lying spectrum of $|H|$. Moreover, the first term of (87) also shifts the exponential bound $d_Z/(2r)$ to a larger value $d'_Z/(2r)$, where the ratio $d'_Z/d_Z \simeq 1 - 4$, depending on m , λ_{min} and the low-lying spectrum of $|H|$. For $N_s > (N_s)^{thres}$, the upper-bound would behave like $1/N_s^3$, until it behaves like ‘‘saturated’’ (decreasing slowly with respect to N_s) at some larger N_s .

For ODWF with kernel $H = H_w$, and plaquette gauge action with $\beta = 5.95 - 6.10$, then $(N_s)^{thres} \simeq 16 - 20$ for $\lambda_{min} = 0.01 - 0.05$ and $\lambda_{max} = 6.20$. As demonstrated in Ref. [17], without fine tuning of λ_{min} , the upper bound (61) gives a reliable estimate of $\langle m_{res} \rangle$ for $N_s = 16$, with the same order of magnitude.

The existence of a range of $N_s < (N_s)^{thres}$ for which the exponential bound $d'_Z/(2r)$ holds is the salient feature of ODWF, which provides a viable way to preserve the chiral symmetry to a good precision (say, $m_{res}a < 10^{-5}$) with a modest N_s (say, $N_s \simeq 16$).

Finally, we have a few words about the efficiency of ODWF, in comparison with other variants of DWF. So far, the tests in Refs. [14, 16] have been performed with quenched gauge configurations, by measuring $\langle m_{res} \rangle$ versus the cost of computing the valence quark propagators. However, in full QCD, the cost/efficiency of HMC simulation also depends on

the acceptance rate and the rate of topological tunnelling, which have not been addressed in Refs. [14, 16]. We think it is premature to claim which lattice DWF is more efficient, only based on the cost of computing valence quark propagators versus the residual mass, without taking into account of the subtle issues (e.g., instability, topology freezing, etc.).

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