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Some remarks on the Ginsparg–Wilson fermion

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Abstract

We note that Fujikawa's proposal of generalization of the Ginsparg–Wilson relation is equivalent to setting $R = (a\gamma_5 D)^{2k}$ in the original Ginsparg–Wilson relation $D\gamma_5 + \gamma_5 D = 2aDR\gamma_5 D$. An explicit realization of D follows from the Overlap construction. The general properties of D are derived. The chiral properties of these higher-order ($k > 0$) realizations of Overlap Dirac operator are compared to those of the Neuberger–Dirac operator ($k = 0$), in terms of the fermion propagator, the axial anomaly and the fermion determinant in a background gauge field. Our present results (up to lattice size 16×16) indicate that the chiral properties of the Neuberger–Dirac operator are better than those of higher-order ones. © 2000 Elsevier Science B.V. All rights reserved.

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1. Introduction

During the last two years, it has become clear that the proper way to formulate chiral fermions on the lattice is to impose the exact chiral symmetry on the lattice, namely, the Ginsparg–Wilson relation [1]

$$D\gamma_5 + \gamma_5 D = 2aDR\gamma_5 D, \quad (1)$$

where D is the lattice Dirac operator, a is the lattice spacing, and R is a positive definite Hermitian operator which commutes with γ_5 . Equation (1) should be regarded as a generalized chiral symmetry which contains the usual chiral symmetry in the continuum limit ($a \rightarrow 0$). However, it should be noted that this exact chiral symmetry ($R = 1$) had been existing in the Overlap formalism [2–4], even before the GW relation was rediscovered. Therefore, unless one can explicitly construct a GW Dirac operator D without using the Overlap, and such a D satisfies all physical requirements; otherwise it is unlikely that the GW relation would turn out to be more fundamental than the Overlap.

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Recently, Fujikawa [5] proposed a generalization of the Ginsparg–Wilson relation as

$$\gamma_5(\gamma_5 D) + (\gamma_5 D)\gamma_5 = 2a^{2k+1}(\gamma_5 D)^{2k+2}, \quad k = 0, 1, 2, \dots \quad (2)$$

Multiplying both sides of (2) by γ_5 , we obtain

$$\gamma_5 D + D\gamma_5 = 2aD(a\gamma_5 D)^{2k}\gamma_5 D, \quad k = 0, 1, 2, \dots, \quad (3)$$

which is *equivalent* to the original GW relation (1) with

$$R = (a\gamma_5 D)^{2k}, \quad k = 0, 1, 2, \dots \quad (4)$$

It can be shown that R is hermitian and commutes with γ_5 for any D which is γ_5 -hermitian and satisfies (3) [the proof is below Eq. (16)]. The motivation of considering $k > 0$ in (4) is to improve the chiral symmetry at *small* lattice spacings. Further, Fujikawa has constructed a sequence ($k > 0$) of these GW Dirac operators based on the Neuberger–Dirac operator ($k = 0$) [3,4]. However, the price one has to pay for the improved chiral symmetry is a less localized D , since in the limit $k \rightarrow \infty$, D must tend to a chirally symmetric and nonlocal D_c , as a consequence of the Nielson–Ninomiya no-go theorem [6–8]. Therefore, it is not clear whether one may have any advantages in practice by considering $k > 0$ in (4). Nevertheless, from a theoretical viewpoint, it is interesting to see how one can construct a sequence ($k = 1, 2, \dots$) of topologically proper D satisfying the GW relation (3), in addition to the Neuberger–Dirac operator ($k = 0$).

In this paper, we examine several aspects of Fujikawa’s proposal. In Section 2, we derive the analytical properties of the GW Dirac operator satisfying (1) with $R = (a\gamma_5 D)^{2k}$. Then, in Section 3, we analyze the construction of higher-order Overlap Dirac operators, and derive their general properties. In Section 4, we compare the chiral properties of the higher-order ($k = 1, 2$) Overlap Dirac operators to those of the Neuberger–Dirac operator, by computing the fermion propagator, the axial anomaly and the fermion determinant in two-dimensional background $U(1)$ gauge fields. Finally, we discuss and conclude in Section 5.

2. General analytical properties

In this section, we begin with general considerations of the GW relation, and then derive the analytical properties of the GW Dirac operators satisfying (1) with $R = (a\gamma_5 D)^{2k}$.

In general, one can assume that the lattice Dirac operator D satisfies the Ginsparg–Wilson relation in the form

$$D\gamma_5 f(D) + g(D)\gamma_5 D = 0, \quad (5)$$

where f and g are any analytic functions. Then the fermionic action $\mathcal{A}_f = \bar{\psi} D \psi$ is invariant under the global chiral transformation

$$\psi \rightarrow \exp[\theta \gamma_5 f(D)] \psi, \quad (6)$$

$$\bar{\psi} \rightarrow \bar{\psi} \exp[\theta g(D) \gamma_5], \quad (7)$$

where θ is a global parameter.

If we set $f(D) = \mathbb{1} - aRD$ and $g(D) = \mathbb{1} - aDR$, then (5) becomes

$$D\gamma_5 + \gamma_5 D = aD(R\gamma_5 + \gamma_5 R)D, \quad (8)$$

where R is any operator.

Since the massless Dirac operator in continuum is chirally symmetric ($\mathcal{D}\gamma_5 + \gamma_5\mathcal{D} = 0$) and antihermitian ($\mathcal{D}^\dagger = -\mathcal{D}$), so it is γ_5 -hermitian ($\mathcal{D}^\dagger = \gamma_5\mathcal{D}\gamma_5$). Thus, we require that the lattice Dirac operator D also preserves this symmetry at any lattice spacing, i.e.,

$$D^\dagger = \gamma_5 D \gamma_5. \quad (9)$$

Then multiplying (8) by γ_5 and using (9), we obtain

$$D^\dagger + D = aD^\dagger(R + \gamma_5 R \gamma_5)D = aD(R + \gamma_5 R \gamma_5)D^\dagger. \quad (10)$$

Evidently, only the part of R which commutes with γ_5 can enter (10). Recall that any operator R can be decomposed into two parts as

$$R = \frac{1}{2}(R + \gamma_5 R \gamma_5) + \frac{1}{2}(R - \gamma_5 R \gamma_5),$$

where the first (second) term on r.h.s. commutes (anticommutes) with γ_5 . Therefore, without loss, one can assume that R commutes with γ_5 . Thus, (10) becomes

$$D^\dagger + D = 2aD^\dagger R D. \quad (11)$$

Taking the adjoint of (11), we immediately obtain

$$R = R^\dagger. \quad (12)$$

Then (8) becomes the usual GW relation

$$D\gamma_5 + \gamma_5 D = 2aDR\gamma_5 D, \quad (13)$$

where R is any hermitian operator which commutes with γ_5 .

Fujikawa's proposal [5] is equivalent to setting

$$R = (a\gamma_5 D)^{2k}, \quad k = 0, 1, 2, \dots, \quad (14)$$

in the usual GW relation (13). Then (13) becomes

$$D\gamma_5 + \gamma_5 D = 2aD(a\gamma_5 D)^{2k}\gamma_5 D. \quad (15)$$

It is obvious that R is hermitian since D is γ_5 -hermitian. Note that

$$\gamma_5(a\gamma_5 D)^2 = (a\gamma_5 D)^2 \gamma_5 \quad (16)$$

since

$$\begin{aligned} & \gamma_5(a\gamma_5 D)^2 \\ &= a^2 \gamma_5 (\gamma_5 D + D \gamma_5) (\gamma_5 D) - a^2 (\gamma_5 D) \gamma_5 (\gamma_5 D + D \gamma_5) + a^2 (\gamma_5 D) \gamma_5 (D \gamma_5) \\ &= 2(a\gamma_5 D)^{2k+2} - 2(a\gamma_5 D)^{2k+2} + (a\gamma_5 D)^2 \gamma_5 \\ &= (a\gamma_5 D)^2 \gamma_5, \end{aligned}$$

where (15) has been used in the second equality. Then it follows that $R = (a\gamma_5 D)^{2k}$ commutes with γ_5 .

Further, Eq. (16) gives

$$\gamma_5(\gamma_5 D)^2 \gamma_5 = (\gamma_5 D)^2, \quad (17)$$

which yields

$$DD^\dagger = D^\dagger D, \quad D \text{ is normal}, \quad (18)$$

where (9) has been used. Since D is normal, D and $D^\dagger$ have common eigenfunctions and their eigenvalues are either real or come in complex conjugate pairs,

$$D\phi_s = \lambda_s \phi_s, \quad (19)$$

$$D^\dagger \phi_s = \lambda_s^* \phi_s, \quad (20)$$

and the eigenfunctions $\{\phi_s\}$ form a complete orthonormal set. Then the general analytical properties of the eigenmodes as derived in Ref. [9] (Eqs. (37), (38) and (41) in Ref. [9]) for $R = 1/2$ also hold for the R in (14). For the sake of completeness, we outline the derivations as follows. Writing R as

$$R = (a\gamma_5 D)^{2k} = a^{2k}(\gamma_5 D\gamma_5 D)^k = a^{2k}(D^\dagger D)^k, \quad (21)$$

and applying Eq. (11) to ϕ_s , we obtain the eigenvalue equation

$$\lambda_s + \lambda_s^* = 2a^{2k+1}(\lambda_s^*)^{k+1}(\lambda_s)^{k+1}. \quad (22)$$

Multiplying both sides of (22) by $(\lambda_s)^k(\lambda_s^*)^k$, we get

$$(\lambda_s)^{k+1}(\lambda_s^*)^k + (\lambda_s)^k(\lambda_s^*)^{k+1} = 2a^{2k+1}(\lambda_s^*)^{2k+1}(\lambda_s)^{2k+1} \quad (23)$$

which can be rewritten as

$$\left| (a\lambda_s)^{k+1}(a\lambda_s^*)^k - \frac{1}{2} \right| = \frac{1}{2}. \quad (24)$$

Thus the eigenvalues in the form $z = (a\lambda_s)^{k+1}(a\lambda_s^*)^k$ fall on the circle centered at $1/2$ with radius $1/2$. The real eigenvalues (if any) of D are at $\lambda = 0$ ($z = 0$) and $\lambda = a^{-1}$ ($z = 1$). Writing $a\lambda_s = r \exp(i\theta)$, we have $z = r^{2k+1} \exp(i\theta)$. Thus, for $k = 0$, the eigenvalues of D fall on the circle centered at $1/2$ with radius $1/2$, while for $k > 0$, on the deformed circle stretched symmetrically in $\pm \hat{y}$ directions with fixed points at zero and a^{-1} , bounded inside the region $0 \leq x \leq a^{-1}$.

From (9) and (20), we obtain

$$D\gamma_5 \phi_s = \lambda_s^* \gamma_5 \phi_s. \quad (25)$$

Multiplying both sides of (25) by $\phi_s^\dagger$ and using the adjoint of (20), we get

$$\lambda_s \phi_s^\dagger \gamma_5 \phi_s = \lambda_s^* \phi_s^\dagger \gamma_5 \phi_s. \quad (26)$$

This implies that the chirality of any complex eigenmode is zero,

$$\chi_s \equiv \phi_s^\dagger \gamma_5 \phi_s = 0 \quad \text{if } \lambda_s \neq \lambda_s^*. \quad (27)$$

If λ_s is real (zero or a^{-1}), then Eqs. (25) and (19) imply that ϕ_s has definite chirality $+1$ or -1 :

$$\gamma_5 \phi_s = \pm \phi_s, \quad \text{if } \lambda_s = \lambda_s^*. \quad (28)$$

A useful property of chirality is that the total chirality of all eigenmodes must vanish,

$$\begin{aligned} \sum_s \chi_s &= \sum_s \phi_s^\dagger \gamma_5 \phi_s \\ &= \sum_s \sum_x \sum_\alpha \sum_\beta [\phi_s^\alpha(x)]^* \gamma_5^{\alpha\beta} \phi_s^\beta(x) \\ &= \sum_\alpha \sum_\beta \gamma_5^{\alpha\beta} \delta_{\alpha\beta} = 0, \end{aligned} \quad (29)$$

where the completeness relation

$$\sum_x \sum_s [\phi_s^\alpha(x)]^* \phi_s^\beta(x) = \delta^{\alpha\beta} \quad (30)$$

has been used. Since the chirality of any complex eigenmode is zero, then Eq. (29) gives the chirality sum rule [9] for real eigenmodes,

$$N_+ + n_+ = N_- + n_-, \quad (31)$$

where $n_+(n_-)$ denotes the number of zero modes of positive (negative) chirality, and $N_+(N_-)$ the number of nonzero real (a^{-1}) eigenmodes of positive (negative) chirality. Then we immediately see that any zero mode must be accompanied by a real (a^{-1}) eigenmode with opposite chirality, and the index of D is

$$\text{index}(D) \equiv n_- - n_+ = -(N_- - N_+). \quad (32)$$

It should be emphasized that the chiral properties (28), (27) and the chirality sum rule (31) hold for any normal D satisfying the γ_5 -hermiticity, as shown in Ref. [9]. However, in nontrivial gauge backgrounds, whether D possesses any zero modes or not relies on the topological characteristics [10] of D , which cannot be guaranteed by the conditions such as the locality, free of species doublings, correct continuum behavior, γ_5 -hermiticity and the GW relation.

3. Higher-order realization of Overlap Dirac operator

Now the task is to construct a topologically proper D which is local, free of species doubling, γ_5 -hermitian, having correct continuum behavior, and satisfies GW relation (3). So far, the only viable way to construct a topologically proper D is the Overlap,

$$D = \frac{1}{2a}(\mathbb{1} + \gamma_5 \epsilon), \quad \epsilon^2 = \mathbb{1} \quad (33)$$

which satisfies the GW relation (1) with $R = 1$. There are many different ways to implement the hermitian ϵ in (33). However, it is required to be able to capture the topology of the gauge background. That means, one-half of the difference of the numbers ($h_\pm$) of positive (+1) and negative (−1) eigenvalues of ϵ is equal to the background topological charge Q ,

$$\sum_x \text{tr}(a\gamma_5 D(x, x)) = \frac{1}{2} \sum_x \text{tr}(\epsilon) = \frac{1}{2}(h_+ - h_-) = Q, \quad (34)$$

where tr denotes the trace over the Dirac and color space. Otherwise, the axial anomaly of D cannot agree with the topological charge density in a nontrivial gauge background. Henceforth, we shall regard any lattice Dirac operator which is constructed through the general form of Overlap (33) as a realization of the Overlap Dirac operator.

An explicit realization of ϵ in (33) is the Neuberger–Dirac operator [3,4] with

$$\epsilon = \frac{H_w}{\sqrt{H_w^2}}, \quad (35)$$

where

$$H_w = \gamma_5(D_W - m_0 a^{-1}), \quad 0 < m_0 < 2r_w, \quad (36)$$

$$D_W = \gamma_\mu t_\mu + W, \quad D_W: \text{ massless Wilson–Dirac operator}, \quad (37)$$

$$t_\mu(x, y) = \frac{1}{2a} [U_\mu(x) \delta_{x+\hat{\mu}, y} - U_\mu^\dagger(y) \delta_{x-\hat{\mu}, y}], \quad (38)$$

$$W(x, y) = \frac{r_w}{2a} \sum_\mu [2\delta_{x, y} - U_\mu(x) \delta_{x+\hat{\mu}, y} - U_\mu^\dagger(y) \delta_{x-\hat{\mu}, y}]. \quad (39)$$

(The Wilson parameter r_w is usually set to one.)

$$\gamma_\mu = \begin{pmatrix} 0 & \sigma_\mu \\ \sigma_\mu^\dagger & 0 \end{pmatrix},$$

and

$$\sigma_\mu \sigma_\nu^\dagger + \sigma_\nu \sigma_\mu^\dagger = 2\delta_{\mu\nu}.$$

Note that the parameter m_0 plays a crucial role in detecting the topology of the gauge background.

Now the problem is how to generalize this construction to D satisfying the GW relation with $R = (a\gamma_5 D)^{2k}$ for $k > 0$. We can multiply both sides of the GW relation (1) by R and redefine $D' = RD$, then we have

$$D' \gamma_5 + \gamma_5 D' = 2D' \gamma_5 D', \quad (40)$$

where $D' = RD$ is γ_5 -hermitian since

$$D'^\dagger = D^\dagger R = \gamma_5 D \gamma_5 R = \gamma_5 D R \gamma_5 = R \gamma_5 D \gamma_5 = \gamma_5 R D \gamma_5 = \gamma_5 D' \gamma_5.$$

Now (40) is in the same form of the GW relation with $R = 1$. Thus, one can construct D' in the same way as the Overlap

$$D' = RD = \frac{1}{2a} (\mathbb{1} + \gamma_5 \epsilon), \quad \epsilon^2 = \mathbb{1}, \quad (41)$$

provided that a proper realization of ϵ can be obtained. An explicit construction based on the Neuberger–Dirac operator ($k = 0$) has been generalized to higher-orders ($k > 0$) by Fujikawa [5].

In the following, we formulate Fujikawa's construction in a more transparent way. Using $R\gamma_5 = \gamma_5 R$, we can write

$$D' = RD = (a\gamma_5 D)^{2k} D = (a\gamma_5 D)^{2k} \gamma_5 \gamma_5 D = a^{-1} \gamma_5 (a\gamma_5 D)^{2k+1}, \quad (42)$$

which yields

$$D = a^{-1} \gamma_5 (a\gamma_5 D')^{1/(2k+1)}, \quad (43)$$

where the $(2k+1)$ -th real root of the hermitian operator $a\gamma_5 D'$ is assumed.

Then (43) suggests that if the ϵ in (41) is expressed in terms of a hermitian operator H ,

$$\epsilon = \frac{H}{\sqrt{H^2}}, \quad (44)$$

then H is required to be proportional to $(\gamma_\mu \mathcal{D}_\mu)^{2k+1}$ plus higher-order terms in the continuum limit such that D behaves as $\gamma_\mu \mathcal{D}_\mu$ after taking the $(2k+1)$ -th root in (43). Thus, H must contain the term $(\gamma_\mu t_\mu)^{2k+1}$, where $\gamma_\mu t_\mu$ is the naive lattice fermion operator defined in (38). Then additional terms must be required in order to remove the species doublers in the term $(\gamma_\mu t_\mu)^{2k+1}$. So, we add the Wilson term to the $(2k+1)$ -th power, i.e., W^{2k+1} . Finally, a negative mass term $-(m_0 a^{-1})^{2k+1}$ is inserted such that ϵ is able to detect the topological charge Q of the gauge background, i.e.,

$$\frac{1}{2} \sum_x \text{tr} \left(\frac{H}{\sqrt{H^2}} \right) = Q. \quad (45)$$

Putting all these terms together, we have

$$H = \gamma_5 [(\gamma_\mu t_\mu)^{2k+1} + W^{2k+1} - (m_0 a^{-1})^{2k+1}], \quad (46)$$

which, at $k=0$, reduces to the H_w in Eq. (36). Then (43) can be rewritten as

$$D = a^{-1} \left(\frac{1}{2} \right)^{1/(2k+1)} \gamma_5 \left(\gamma_5 + \frac{H}{\sqrt{H^2}} \right)^{1/(2k+1)}, \quad (47)$$

where H is defined in (46). This is the higher-order realization of Overlap Dirac operator, as constructed by Fujikawa [5].

Next we derive some general properties of the Overlap Dirac operator D defined in (47).

The fermion propagator $S_F(x, y)$ is defined by

$$S_F(x, y) = \frac{1}{Z} \int \prod_z d\bar{\psi}(z) d\psi(z) e^{-\bar{\psi} D \psi} \psi(x) \bar{\psi}(y)$$

where

$$Z = \int \prod_z d\bar{\psi}(z) d\psi(z) e^{-\bar{\psi} D \psi}.$$

In a background gauge field of zero topological charge ($Q=0$), the fermion propagator is

$$S_F(x, y) = D^{-1}(x, y). \quad (48)$$

In the naive continuum limit with $r_w a^{-1}$ and $m_0 a^{-1}$ kept finite, the (free) fermion propagator in momentum space can be obtained after some straightforward algebras,

$$\tilde{S}_F(p) = a\gamma_5 \left[\gamma_5 \left(\mathbb{1} + \frac{1}{(\gamma_\mu t_\mu)^{2k+1}} T(p) \right) \right]^{1/(2k+1)} \quad (49)$$

where

$$t_\mu = ia^{-1} \sin(p_\mu a), \quad (50)$$

$$t^2 = a^{-2} \sum_\mu \sin^2(p_\mu a), \quad (51)$$

$$W(p) = r_w a^{-1} \sum_\mu [1 - \cos(p_\mu a)], \quad (52)$$

$$u(p) = [W(p)]^{2k+1} - (m_0 a^{-1})^{2k+1}, \quad (53)$$

$$N(p) = \sqrt{(t^2)^{2k+1} + u^2(p)}, \quad (54)$$

$$T(p) = N(p) - u(p). \quad (55)$$

Around $p \simeq 0$, $t_\mu \simeq ip_\mu$, $T(p) \simeq 2(m_0 a^{-1})^{2k+1}$, and the fermion propagator becomes

$$\tilde{S}_F(p) \simeq a\gamma_5 \left[\gamma_5 \left(\mathbb{1} + \frac{1}{(i\gamma_\mu p_\mu)^{2k+1}} 2(m_0 a^{-1})^{2k+1} \right) \right]^{1/(2k+1)} \quad (56)$$

$$\simeq 2^{1/(2k+1)} m_0 \frac{1}{i\gamma_\mu p_\mu} + a + a(1 - \delta_{k,0}) \Sigma_k(ap), \quad (57)$$

where except for $k = 0$, a momentum-dependent term denoted by $a\Sigma_k(ap)$ is present in the scalar part, which may lead to additive mass renormalization. Evidently, we have to fix the value of m_0 to

$$m_0 = \left(\frac{1}{2} \right)^{1/(2k+1)} \quad (58)$$

such that in the limit ($a \rightarrow 0$) the fermion propagator (57) agrees with the continuum propagator.

For $m_0 \in (0, 2r_w)$, on a d -dimensional lattice ($d = \text{even}$), at any one the $2^d - 1$ corners of the Brillouin zone [i.e., $ap = (\pi, 0, \dots, 0)$, $(0, \pi, \dots, 0)$, $\dots$, $(\pi, \pi, \dots, \pi)$], we have $N(p) = u(p) > 0$, thus $T(p) = u(p) - u(p) = 0$, and all doubled modes are decoupled from the fermion propagator (49).

In general, we consider an arbitrary value of m_0 . At the origin ($p = 0$) and the $2^d - 1$ corners of the Brillouin zone, we have $\sin(p_\mu a) = 0$, so $T(p)$ becomes

$$T(p) = |u(p)| - u(p), \quad (59)$$

where the possible values of $u(p)$ are:

$$\begin{aligned} u(p) &= -(m_0 a^{-1})^{2k+1} \\ &= (2r_w a^{-1})^{2k+1} - (m_0 a^{-1})^{2k+1} \\ &= (4r_w a^{-1})^{2k+1} - (m_0 a^{-1})^{2k+1} \\ &\vdots \\ &= (2dr_w a^{-1})^{2k+1} - (m_0 a^{-1})^{2k+1}. \end{aligned}$$

Here the first value of $u(p)$ corresponds to all components of p equal to zero, the second value to one of components equal to π/a , and so on, and the last value to all components equal to π/a . Note that

$$\begin{aligned} & (2nr_w a^{-1})^{2k+1} - (m_0 a^{-1})^{2k+1} \\ &= (2nr_w a^{-1} - m_0 a^{-1})[(2nr_w a^{-1})^{2k} + \cdots + (m_0 a^{-1})^{2k}], \quad n = 0, 1, \dots, d. \end{aligned}$$

Therefore, the sign of $u(p)$ is independent of the order k . From Eq. (59), we see that if $u(p) \geq 0$, then $T(p) = 0$, and this doubled mode is decoupled from the fermion propagator (49) for any order k . Since the chiral charge of a doubled mode is equal to $(-1)^n$, where n is the number of momentum components equal to π/a , then the total chiral charge Q_5 of all massless (primary and doubled) fermion modes contributing to the fermion propagator (49) can be determined. Then $\text{index}(D) = Q_5 Q$ for a gauge background with topological charge Q . Thus, in the naive continuum limit, the index of D (as a function of m_0) is independent of the order k , same as the index of the Neuberger–Dirac operator ($k = 0$), which has been determined in Ref. [11]. Explicitly,

$$\text{index}[D(m_0)] = \begin{cases} \frac{(-1)^{n+1}(d-1)!}{(d-n)!(n-1)!} Q, & 2(n-1)r_w < m_0 < 2nr_w \\ & \text{for } n = 1, \dots, d; \\ 0, & \text{otherwise.} \end{cases} \quad (60)$$

In particular, for $d = 4$,

$$\text{index}[D(m_0)] = \begin{cases} Q, & 0 < m_0 < 2r_w, \\ -3Q, & 2r_w < m_0 < 4r_w, \\ 3Q, & 4r_w < m_0 < 6r_w, \\ -Q, & 6r_w < m_0 < 8r_w, \\ 0, & \text{otherwise.} \end{cases} \quad (61)$$

For the Neuberger–Dirac operator ($k = 0$), there exists an exact discrete symmetry of the index on *any* finite lattice with even number of sites in each dimension [11]

$$\text{index}[D(m_0)] = -\text{index}[D(2dr_w - m_0)], \quad \text{for } k = 0, \quad (62)$$

which holds for any background gauge configuration. However, for higher-order Overlap Dirac operators ($k > 0$), this discrete symmetry is *not* exact on a finite lattice; only in the naive continuum limit, this discrete symmetry can be realized as in (60). Nevertheless, at $m_0 = dr_w$, it can be shown that the index is exactly zero for all k ,

$$\text{index}[D(m_0 = dr_w)] = 0, \quad \text{for all } k \geq 0, \quad (63)$$

on any finite lattice with even number of sites in each dimension, and for any background gauge configuration.

4. Tests

In this section, we compare the chiral properties of the higher-order Overlap Dirac operators ($k = 1, 2$) to those of the Neuberger–Dirac operator ($m_0 = 1$ and $R = 1/2$),

by computing the fermion propagator, the axial anomaly and the fermion determinant in two-dimensional background $U(1)$ gauge fields. Our notations for the two-dimensional background gauge field are the same as those in Ref. [9] (Eqs. (7)–(11) in Ref. [9]).

Note that the Neuberger–Dirac operator is conventionally written as

$$D = a^{-1}(\mathbb{1} + V) = a^{-1}\left(\mathbb{1} + \gamma_5 \frac{H_w}{\sqrt{H_w^2}}\right), \quad m_0 = 1; \quad (64)$$

which satisfies the GW relation with $R = 1/2$. However, the zeroth order ($k = 0$) Overlap Dirac operator is

$$D = \frac{1}{2a}\left(\mathbb{1} + \gamma_5 \frac{H_w}{\sqrt{H_w^2}}\right), \quad m_0 = 1/2; \quad (65)$$

which satisfies the GW relation with $R = 1$. In the following, we shall use the Neuberger–Dirac operator (64) in place of the zeroth order Overlap (65). All numerical results for the $k = 0$ case are obtained using the Neuberger–Dirac operator (64) rather than (65).

First of all, we checked that the eigenvalues of a higher-order ($k = 1, 2$) Overlap Dirac operator fall on the deformed circle which is stretched symmetrically in $\pm\hat{y}$ directions. In a nontrivial gauge background, the real eigenmodes (zero and a^{-1}) have definite chirality and satisfy the chirality sum rule (31), and each complex eigenmode has zero chirality (27). The Atiyah–Singer index theorem ($n_- - n_+ = Q$) is satisfied in all cases ($k = 0, 1, 2$) for gauge configurations fulfilling the topological bound [10]

$$a^2|\bar{\rho}(x)| < \epsilon_1 \simeq 0.28 \quad \forall x, \quad (66)$$

where $a^2\bar{\rho}(x)$ is the topological charge inside the unit square of area a^2 centered at x ,

$$\bar{\rho}(x) = \frac{1}{a^2} \int_{x_1-a/2}^{x_1+a/2} dy_1 \int_{x_2-a/2}^{x_2+a/2} dy_2 \frac{1}{2\pi} F_{12}(y). \quad (67)$$

The value of m_0 in the higher-order ($k > 0$) Overlap Dirac operator is fixed according to Eq. (58), $m_0 = 2^{-1/(2k+1)}$, while $m_0 = 1$ for the Neuberger–Dirac operator.

4.1. Fermion propagator

In the following, we first compute the free fermion propagator on a two-dimensional lattice, for the Neuberger–Dirac operator and higher-order ($k = 1, 2$) Overlap Dirac operators, respectively. We compare them to the exact solution of the massless fermion propagator on the torus. Then we turn on a background gauge field to examine the behaviors of the scalar part S_0 and the pseudoscalar part S_5 in the higher order ($k = 1, 2$) fermion propagators.

In general, the free fermion propagator can be written as

$$S_F(x) = S_0(x) + \gamma_\mu S_\mu(x), \quad (68)$$

where $S_0(x) = 0$ for the massless fermion in continuum; and $S_0(x) = (a/2)\delta_{x,0}$ for the Neuberger–Dirac operator.

Table 1

The free fermion propagators on a 16×16 lattice with antiperiodic boundary conditions. One of the end points of the propagator is fixed at the origin, while the other end point is at one of the sites along the diagonal ($x_1 = x_2$)

x_1	x_2	Exact	Neuberger	$k = 1$	$k = 2$
0.0	0.0	0.0000	0.0000	0.0000	0.0000
1.0	1.0	0.0796	0.0689	0.0894	0.0885
2.0	2.0	0.0396	0.0374	0.0423	0.0449
3.0	3.0	0.0259	0.0249	0.0226	0.0212
4.0	4.0	0.0184	0.0179	0.0177	0.0179
5.0	5.0	0.0131	0.0127	0.0128	0.0126
6.0	6.0	8.59×10^{-3}	8.32×10^{-3}	8.32×10^{-3}	8.38×10^{-3}
7.0	7.0	4.28×10^{-3}	4.13×10^{-3}	4.10×10^{-3}	4.17×10^{-3}
8.0	8.0	0.0000	0.0000	0.0000	0.0000
9.0	9.0	-4.28×10^{-3}	-4.13×10^{-3}	-4.10×10^{-3}	-4.17×10^{-3}
10.0	10.0	-8.59×10^{-3}	-8.32×10^{-3}	-8.32×10^{-3}	-8.38×10^{-3}
11.0	11.0	-0.0131	-0.0127	-0.0128	-0.0126
12.0	12.0	-0.0184	-0.0179	-0.0177	-0.0179
13.0	13.0	-0.0259	-0.0249	-0.0226	-0.0212
14.0	14.0	-0.0396	-0.0374	-0.0423	-0.0449
15.0	15.0	-0.0796	-0.0689	-0.0894	-0.0885

First, we examine the $S_\mu(x)$ components in (68). In Table 1, we list the component $S_1(x)$ along the diagonal ($x_1 = x_2$) of a 16×16 lattice with antiperiodic boundary conditions. One of the end points of the propagator is fixed at the origin, while the other end point is located at a site along the diagonal. Note that, by symmetry, $S_2(x) = S_1(x)$ along the diagonal. From the data in Table 1, we immediately see that in all cases (Neuberger, $k = 1, 2$), $S_1(x)$ agrees very well with the exact solution on the torus. In general, all S_μ components of the free fermion propagators are in good agreement with the exact solution for any $x = (x_1, x_2)$.

Next, we examine the scalar part $S_0(x)$ in the free fermion propagator of the higher-order ($k = 1, 2$) Overlap Dirac operators (47). In Table 2, we list $S_0(x)$ along the diagonal of the 16×16 lattice with antiperiodic boundary conditions. From the data in Table 2, we see that $S_0(x)$ is local for both $k = 1$ and $k = 2$. However, we note that $S_0(x)$ in the second order ($k = 2$) case is less localized than that of the first order ($k = 1$), as expected. It seems that $|S_0(x)|$ in both ($k = 1, 2$) orders can be fitted by an exponentially decay function for $0 < |x| < 8\sqrt{2}$.

In a background gauge field, the fermion propagator can be written as

$$S_F(x, y) = \begin{pmatrix} S_0(x, y) + S_5(x, y) & S_R(x, y) \\ S_L(x, y) & S_0(x, y) - S_5(x, y) \end{pmatrix}, \quad (69)$$

where $S_0(x, y) = S_5(x, y) = 0$ for the massless fermion in continuum; and $S_0(x, y) = (a/2)\delta_{x,y}$ and $S_5(x, y) = 0$ for the Neuberger–Dirac operator. However, for higher-order ($k > 0$) Overlap Dirac operators, both $S_0(x, y)$ and $S_5(x, y)$ are not proportional to

Table 2

The scalar part $S_0(x)$ in the free fermion propagator of the higher-order Overlap Dirac operators, along the diagonal of a 16×16 lattice with antiperiodic boundary conditions

x_1	x_2	$S_0(x), k = 1$	$S_0(x), k = 2$
0.0	0.0	0.9170	0.8950
1.0	1.0	-0.0488	-0.0630
2.0	2.0	-9.45×10^{-3}	-0.0085
3.0	3.0	-4.41×10^{-4}	3.30×10^{-3}
4.0	4.0	2.33×10^{-7}	1.56×10^{-3}
5.0	5.0	1.63×10^{-4}	5.96×10^{-4}
6.0	6.0	1.12×10^{-4}	-2.52×10^{-4}
7.0	7.0	3.47×10^{-5}	-1.72×10^{-4}
8.0	8.0	0.0000	0.0000
9.0	9.0	3.47×10^{-5}	-1.72×10^{-4}
10.0	10.0	1.12×10^{-4}	-2.52×10^{-4}
11.0	11.0	1.63×10^{-4}	5.96×10^{-4}
12.0	12.0	2.33×10^{-7}	1.56×10^{-3}
13.0	13.0	-4.41×10^{-4}	3.30×10^{-3}
14.0	14.0	-9.45×10^{-3}	-0.0085
15.0	15.0	-0.0488	-0.0630

Table 3

The scalar part $S_0(x, 0)$ and pseudoscalar part $S_5(x, 0)$ in the fermion propagator of the second order ($k = 2$) Overlap Dirac operator, in a background gauge field (see text for the parameters) on a 16×16 lattice with antiperiodic boundary conditions. One of the end points of the propagator is fixed at the origin, while the other end point is at one of the sites along the diagonal ($x_1 = x_2$)

x_1	x_2	$\text{Re}(S_0)$	$\text{Im}(S_0)$	$\text{Re}(S_5)$	$\text{Im}(S_5)$
0.0	0.0	0.8950	0.0	2.94×10^{-3}	0.00
1.0	1.0	-0.0609	0.0156	1.42×10^{-3}	-3.81×10^{-4}
2.0	2.0	-6.31×10^{-3}	5.97×10^{-3}	-2.25×10^{-4}	1.30×10^{-4}
3.0	3.0	7.24×10^{-4}	-3.08×10^{-3}	-1.08×10^{-4}	3.48×10^{-4}
4.0	4.0	-8.25×10^{-4}	-1.43×10^{-3}	6.01×10^{-5}	9.28×10^{-5}
5.0	5.0	-6.54×10^{-4}	7.07×10^{-6}	1.04×10^{-5}	-3.82×10^{-5}
6.0	6.0	3.84×10^{-4}	-1.05×10^{-4}	-1.42×10^{-5}	-1.30×10^{-5}
7.0	7.0	9.54×10^{-5}	-1.33×10^{-4}	8.16×10^{-6}	0.0
8.0	8.0	2.14×10^{-5}	1.28×10^{-4}	0.0	0.0
9.0	9.0	2.27×10^{-4}	1.36×10^{-4}	-6.21×10^{-6}	-2.31×10^{-6}
10.0	10.0	1.49×10^{-4}	2.75×10^{-4}	-4.21×10^{-6}	-1.34×10^{-5}
11.0	11.0	-2.05×10^{-4}	-7.14×10^{-4}	2.17×10^{-5}	5.83×10^{-6}
12.0	12.0	7.16×10^{-4}	-1.53×10^{-3}	-4.10×10^{-5}	9.00×10^{-5}
13.0	13.0	2.55×10^{-3}	-1.85×10^{-3}	-3.08×10^{-4}	1.76×10^{-4}
14.0	14.0	-8.30×10^{-3}	2.46×10^{-3}	-2.70×10^{-4}	1.27×10^{-5}
15.0	15.0	-0.0629	8.62×10^{-4}	1.46×10^{-3}	-2.99×10^{-5}

$\delta_{x,y}$. If $S_0(x, y)$ ($S_5(x, y)$) turns out to be nonlocal, then it would cause additive mass renormalization and the poles in the fermion propagator will be shifted accordingly.

Now we turn on a background $U(1)$ gauge field with parameters ($h_1 = 0.1$, $h_2 = 0.2$, $A_1^{(0)} = 0.3$, $A_2^{(0)} = 0.4$ and $n_1 = n_2 = 1$, as defined in Eqs. (7) and (8) in Ref. [9]). Then we examine the behaviors of $S_0(x, y)$ and $S_5(x, y)$ for the higher-order ($k = 1, 2$) Overlap Dirac operators. We find that both $S_0(x, y)$ and $S_5(x, y)$ are local in the higher-order ($k = 1, 2$) fermion propagators. In Table 3, we list the real parts and imaginary parts of $S_0(x, 0)$ and $S_5(x, 0)$ for the second order ($k = 2$) fermion propagator, along the diagonal ($x_1 = x_2$) of the 16×16 lattice.

In general, the scalar part $S_0(x, y)$ and the pseudoscalar part $S_5(x, y)$ in the higher order ($k = 1, 2$) fermion propagators seem to be local, especially for near continuum gauge configurations. However, one cannot exclude the possibility that they may cause the perturbative instability of the pole of the fermion propagator [12]. On the other hand, for the Neuberger–Dirac operator, we are sure that $S_0(x, y) = a/(2\delta_{x,y})$ and $S_5(x, y) = 0$ for any gauge configuration, as well as the perturbative stability of the pole of the fermion propagator [12]. So, from this viewpoint, the chiral properties of Neuberger–Dirac operator are better than those of higher-order Overlap Dirac operators.

4.2. Axial anomaly

The axial anomaly of GW Dirac operator D satisfying (1) is [13,14]

$$\mathcal{A}_L(x) = a \operatorname{tr}[\gamma_5(RD)(x, x)] \quad (70)$$

where the trace runs over the Dirac and color space. Substituting $R = (a\gamma_5 D)^{2k}$ into (70), we obtain

$$\mathcal{A}_L(x) = \operatorname{tr}[(a\gamma_5 D)^{2k+1}(x, x)]. \quad (71)$$

The sum of the axial anomaly over all sites is equal to the index of D ,

$$\sum_x \mathcal{A}_L(x) = n_- - n_+. \quad (72)$$

If the index of D is equal to the topological charge Q of the gauge background, then the sum of the axial anomaly is equal to Q . However, it does not necessarily imply that $\mathcal{A}_L(x)$ would agree with the topological charge density at each site. This happens only when D is local.

Since the higher-order ($k > 0$) Overlap Dirac operator (47) is also topologically proper (i.e., its index agrees with the background topological charge for any gauge background satisfying the topological bound), then it follows that its axial anomaly would agree with the topological charge density at each site if D is local (i.e., the gauge configuration satisfies the locality bound which is more restrictive than the topological bound).

In the following, we compute the axial anomaly $\mathcal{A}_L(x)$ in a two-dimensional background $U(1)$ gauge field, for the Neuberger–Dirac operator and higher-order ($k = 1, 2$) Overlap Dirac operators respectively. We compare them to the topological charge density $\bar{\rho}(x)$ (67) of the gauge background on the torus.

The deviation of the axial anomaly of a lattice Dirac operator in a gauge background can be measured in terms of

$$\delta = \frac{1}{N_s} \sum_x \frac{|\mathcal{A}_L(x) - a^2 \bar{\rho}(x)|}{a^2 |\bar{\rho}(x)|}, \quad (73)$$

where N_s is the total number of sites of the lattice, and $\bar{\rho}(x)$ is the topological charge density inside the square of area a^2 centered at x .

In a nontrivial $U(1)$ gauge background with parameters $Q = 1$, $h_1 = 0.1$, $h_2 = 0.2$, $A_1^{(0)} = 0.3$, $A_2^{(0)} = 0.4$ and $n_1 = n_2 = 1$ (as defined in Eqs. (7) and (8) in Ref. [9]) on the 12×12 lattice with $a = 1$, the axial anomaly $\mathcal{A}_L(x)$ and its deviation δ are computed for the Neuberger–Dirac operator and higher-order ($k = 1, 2$) Overlap Dirac operators, respectively. The results are:

$$\delta = \begin{cases} 0.110, & \text{Neuberger,} \\ 0.193, & k = 1, \\ 0.351, & k = 2. \end{cases} \quad (74)$$

The relatively large deviations of axial anomaly in higher-order ($k = 1, 2$) Overlap Dirac operators indicate that they are less localized than the Neuberger–Dirac operator. And the locality of D gets worse as the order k goes higher (i.e., $D_{k=2}$ is less localized than $D_{k=1}$). We have confirmed this by examining $|D(x, y)|$ versus $|x - y|$ explicitly. This implies that the ϵ in the locality bound

$$||1 - U(p)|| < \epsilon, \quad \text{for all plaquettes} \quad (75)$$

for a higher order ($k > 0$) Overlap Dirac operator is more restrictive (smaller) than that of the Neuberger–Dirac operator, and it gets smaller as the order goes higher.

For all background gauge configurations we have tested, the Neuberger–Dirac operator always gives anomaly deviation (δ) smaller than those of the higher-order ($k = 1, 2$) Overlap Dirac operators.

4.3. Fermion determinant

The fermion determinant $\det(D)$ is proportional to the exponentiation of the one-loop effective action which is the summation of any number of external sources interacting with one internal fermion loop. It is one of the most crucial quantities to be examined in any lattice fermion formulations. The determinant of D is the product of all its eigenvalues

$$\det(D) = (1 + e^{i\pi})^{(n_+ + n_-)} \det'(D) \quad (76)$$

where $\det'(D)$ is equal to the product of all non-zero eigenvalues. Since the eigenvalues of D are either real or come in complex conjugate pairs, $\det'(D)$ must be real and positive. For $Q = 0$, then $n_+ + n_- = 0$ and $\det(D) = \det'(D)$. For $Q \neq 0$, then $n_+ + n_- \neq 0$ and $\det(D) = 0$, but $\det'(D)$ still provides important information about the spectrum. In continuum, exact solutions of fermion determinants in the general background $U(1)$ gauge fields on a torus ($L_1 \times L_2$) was obtained in Ref. [15]. In the following we compute $\det'(D)$ for the Neuberger–Dirac operator and higher-order ($k = 1, 2$) Overlap Dirac operators

respectively, and then compare them with the exact solutions in continuum. For simplicity, we turn off the harmonic part ($h_1 = h_2 = 0$) and the local sinusoidal fluctuations ($A_1^{(0)} = A_2^{(0)} = 0$) and examine the change of $\det'(D)$ with respect to the topological charge Q . For such gauge configurations, the exact solution [15] is

$$\det'[D(Q)] = N \sqrt{\left(\frac{L_1 L_2}{2|Q|}\right)^{|Q|}} \quad (77)$$

Table 4

The fermion determinant versus the topological charge Q . The normalization constant is chosen such that $\det'[D(1)] = 1$. The results on the 8×8 lattice are listed in the last three columns for the Neuberger–Dirac operator and higher-order ($k = 1, 2$) Overlap Dirac operators, respectively. The exact solutions on the 8×8 torus are computed according to Eq. (77)

Q	Exact $\det'[D(Q)]_{\text{exact}}$	Neuberger $\det'[D(Q)]$	$k = 1$ $\det'[D(Q)]_{k=1}$	$k = 2$ $\det'[D(Q)]_{k=2}$
1	1.00000	1.00000	1.00000	1.00000
2	2.82843	2.77348	3.01695	3.05686
3	6.15840	5.96891	7.21380	7.51909
4	11.3137	10.7157	14.6911	15.7450
5	18.3179	16.9340	26.1688	28.2029
6	26.8177	24.2001	41.9768	44.4919
7	36.1083	32.0006	62.1673	63.6961
8	45.2548	40.2920	86.8790	85.2556
9	53.2732	45.7353	112.877	106.173
10	59.3164	50.2816	141.546	128.122

Table 5

The fermion determinant versus the topological charge Q on the 16×16 lattice. The normalization constant is chosen such that $\det'[D(1)] = 1$. The results on the lattice are listed in the last three columns for the Neuberger–Dirac operator and higher-order ($k = 1, 2$) Overlap Dirac operators, respectively. The exact solutions on the 16×16 torus are computed according to Eq. (77)

Q	Exact $\det'[D(Q)]_{\text{exact}}$	Neuberger $\det'[D(Q)]$	$k = 1$ $\det'[D(Q)]_{k=1}$	$k = 2$ $\det'[D(Q)]_{k=2}$
1	1.00000	1.00000	1.00000	1.00000
2	5.65685	5.66186	5.76472	5.78270
3	24.6336	24.0615	25.8620	26.1218
4	90.5097	90.4894	98.9598	100.627
5	293.086	286.003	337.077	346.382
6	858.166	822.664	1046.70	1092.03
7	2310.93	2170.94	3018.17	3192.52
8	5792.62	5354.28	8198.43	8786.52
9	13637.9	12309.5	20911.5	23111.2
10	30370.0	27336.6	51335.5	57563.2

where the normalization constant N is fixed by

$$N = \sqrt{\frac{2}{L_1 L_2}}$$

such that $\det'[D(1)] = 1$.

In Table 4 and Table 5, the fermion determinants $\det'(D)$ are listed for 8×8 and 16×16 lattice, respectively. It is clear that the Neuberger–Dirac operator always produces results better than those of the higher-order ($k = 1, 2$) Overlap Dirac operators. The first order ($k = 1$) Overlap Dirac operator performs better than the second order ($k = 2$) one. This is essentially due to the fact that D becomes less localized as the order (k) goes higher.

5. Discussions and conclusions

We can understand the emergence of Fujikawa's proposal by the following considerations.

If one requires that D is γ_5 -hermitian,

$$D^\dagger = \gamma_5 D \gamma_5,$$

and normal,

$$D^\dagger D = D D^\dagger$$

(note that these two conditions are sufficient to guarantee that the real eigenmodes of D have definite chirality (28) and satisfy the chirality sum rule (31), and each complex eigenmode has zero chirality (27)), then one immediately obtains

$$\gamma_5 D \gamma_5 D = D \gamma_5 D \gamma_5.$$

Multiplying above equation by γ_5 , we obtain

$$\gamma_5 \gamma_5 D \gamma_5 D = \gamma_5 D \gamma_5 D \gamma_5,$$

which can be rewritten as

$$\gamma_5 (a \gamma_5 D)^2 = (a \gamma_5 D)^2 \gamma_5.$$

Since $(a \gamma_5 D)^2$ is hermitian and commutes with γ_5 , one finds an example of $R = (a \gamma_5 D)^2$ which depends on D . Then it is straightforward to generalize this R to any powers,

$$R = (a \gamma_5 D)^{2k}, \quad k = 0, 1, 2, \dots$$

Substituting this R into the GW relation (1), we obtain (3) which is equivalent to Fujikawa's proposal (2).

It seems to us that Fujikawa's higher-order realization of the Overlap Dirac operator may not be feasible for practical computations in lattice QCD, in view of its locality, chiral properties and computational accessibility in comparison with those of the Neuberger–Dirac operator. Nevertheless, from a theoretical viewpoint, it has widened our scope and deepened our understanding of the Overlap which does capture one of the fundamental aspects of the nature.

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