Optimal Lattice Domain-Wall Fermions

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I show that the conventional formulations of lattice domain-wall fermion with any finite N_s (in the fifth dimension) do not preserve the chiral symmetry optimally and propose a new action which preserves the chiral symmetry optimally for any finite N_s.

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Currently, there are many interesting physics issues in supersymmetry, supergravity, and superstring theory that require nonperturbative (numerical) studies, in addition to those long-standing ones in QCD. A viable approach is to formulate these theories on a spacetime lattice with domain-wall fermions (DWF). The basic idea of DWF [1,2] is to use an infinite set of coupled Dirac fermion fields [$\psi_s(x)$, $s \in (-\infty, \infty)$] with masses behaving like a step function $m(s) = m\theta(s)$ such that Weyl fermion states can arise as zero modes bound to the mass defect at $s = 0$. However, if one uses a compact set of masses, then the boundary conditions of the mass (step) function must lead to the occurrence of both left-handed and right-handed chiral fermion fields, i.e., a vectorlike theory. For lattice QCD with DWF [3], in practice, one can use only a finite number (N_s) of lattice Dirac fermion fields to set up the domain wall; thus the chiral symmetry of the light fermion field is broken. Now the relevant question is how to construct the couplings between these N_s lattice Dirac fermion fields such that the exact chiral symmetry can be preserved optimally or, in other words, the residual mass of the quark field is minimal. Similarly, in numerical studies of $\mathcal{N} = 1$ supersymmetric SU(n) Yang-Mills theory with N_s domain-wall fermions, it is vital to implement the chiral symmetry of the gaugino optimally such that the supersymmetry can *most* easily emerge as an "accidental" continuum symmetry on the lattice. In this Letter, I discuss how to preserve the chiral symmetry of the light fermion fields optimally, for any finite N_s (in the fifth dimension).

First, we examine the domain-wall fermion action [In this Letter, we suppress the lattice spacings (a and a_5), as well as the Dirac and color indices, which can easily be restored. Also, it is understood that one can replace D_w with its improved lattice Dirac operator, e.g., including the cloverlike terms.] with open boundary conditions [4], in the context of lattice QCD,

$$\mathcal{A}_{dwf} = \sum_{s,s'=1}^{N_s} \sum_{x,x'} \bar{\psi}(x,s)[D_w(x,x')\delta_{s,s'} + \delta_{x,x'}D_5(s,s')]\psi(x',s'), \qquad (1)$$

where D_w is the 4D Wilson-Dirac operator with a negative parameter $-m_0$

$$D_w = \sum_{\mu=1}^{4} \gamma_\mu t_\mu + W - m_0, \qquad m_0 \in (0,2),$$

$$t_\mu(x,x') = \frac{1}{2}[U_\mu(x)\delta_{x',x+\mu} - U_\mu^\dagger(x')\delta_{x',x-\mu}],$$

$$W(x,x') = \sum_{\mu=1}^{4} \frac{1}{2}[2\delta_{x,x'} - U_\mu(x)\delta_{x',x+\mu} - U_\mu^\dagger(x')\delta_{x',x-\mu}],$$

and

$$D_5(s,s') = \delta_{s,s'} - P_-\delta_{s',s+1} - P_+\delta_{s',s-1},$$

$$P_\pm = \frac{1}{2}(1 \pm \gamma_5).$$

The boundary conditions are fixed by $P_+\psi(x,0) = P_-\psi(x,N_s+1) = 0$. The quark fields coupling to physical hadrons can be constructed from the left and right boundary modes

$$q(x) = P_-\psi(x,1) + P_+\psi(x,N_s),$$

$$\bar{q}(x) = \bar{\psi}(x,1)P_+ + \bar{\psi}(x,N_s)P_-.$$

Then the quark propagator in a background gauge field can be evaluated [5,6] as

$$\langle q(x)\bar{q}(y)\rangle = \frac{1-\gamma_5 S}{1+\gamma_5 S}, \qquad (2)$$

where

$$S = \frac{1-T}{1+T}, \qquad (3)$$

$$T = \frac{(1-H)^{N_s}}{(1+H)^{N_s}}, \qquad (4)$$

$$H = \gamma_5 \frac{D_w}{2+D_w}. \qquad (5)$$

In the limit $N_s \to \infty$, $S \to H/\sqrt{H^2}$ (the sign function of H), then the quark propagator (2) is chirally symmetric.

However, for any finite N_s, (2) does not break the chiral symmetry in the minimal way. In other words, S (3) is *not* the optimal approximation for the sign function of H. This can be shown as follows.

First, we rewrite (3) as the partial fraction

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$$S = \begin{cases} H(\frac{1}{N_s} + \frac{2}{N_s}\sum_{l=1}^{n} \frac{b_l}{H^2+d_l}) \equiv HR^{(n,n)}(H^2), & N_s = 2n+1 \text{ (odd)}, \\ H\frac{2}{N_s}\sum_{l=1}^{n} \frac{b_l}{H^2+d_l} \equiv HR^{(n-1,n)}(H^2), & N_s = 2n \text{ (even)}, \end{cases} \tag{6}$$

where

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

Here the symbol $r^{(n,m)}(x)$ denotes an irreducible rational polynomial of the form

$$r^{(n,m)}(x) = \frac{p_n x^n + p_{n-1} x^{n-1} + \cdots + p_0}{q_m x^m + q_{m-1} x^{m-1} + \cdots + q_0},$$
$$(m \geq n,\ p_i,\ q_i > 0).$$

Note that the coefficients b_l and d_l in (6) are independent of (the ratio of the maximum to the minimum) the eigenvalues of H^2. As it will become clear later, this feature already rules out the possibility that $R^{(n-1,n)}(H^2)$ or $R^{(n,n)}(H^2)$ can be the optimal rational approximation of $(H^2)^{-1/2}$.

According to de la Vallée–Poussin's theorem and Chebycheff's theorem [7], the necessary and sufficient condition for $r^{(n,m)}(x)$ to be the optimal rational polynomial of the inverse square root function $x^{-1/2}$, $0 < x_{\min} \leq x \leq x_{\max}$ is that $\delta(x) \equiv 1 - \sqrt{x} r^{(n,m)}(x)$ has an $n + m + 2$ alternate change of sign in the interval $[x_{\min}, x_{\max}]$, and attains its maxima and minima (all with equal magnitude), say,

$$\delta(x) = -\Delta, +\Delta, \ldots, (-1)^{n+m+2}\Delta$$

at consecutive points (x_i, $i = 1, \ldots, n + m + 2$)

$$x_{\min} = x_1 < x_2 < \cdots < x_{n+m+2} = x_{\max}.$$

Now, for $N_s = 2n$, $\delta(x) = 1 - xR^{(n-1,n)}(x^2)$ is nonnegative for $x > 0$. Thus $\delta(x)$ does not have any alternate change of sign for any intervals in $(0, \infty)$. Similarly, for $N_s = 2n + 1$, $\delta(x) = 1 - xR^{(n,n)}(x^2)$ is positive for $0 < x < 1$, zero at $x = 1$, and negative for $x > 1$. Thus $\delta(x)$ has only two alternate changes of sign for any $N_s = 2n + 1$. Therefore, according to de la Vallée–Poussin's theorem and Chebycheff's theorem, we conclude that both $R^{(n-1,n)}(x^2)$ and $R^{(n,n)}(x^2)$ cannot be the optimal rational approximation for $(x^2)^{-1/2}$, and (6) is *not* the optimal rational approximation for the sign function of H. In other words, for any finite N_s, the domain-wall fermion action (1) does *not* preserve the chiral symmetry optimally, which, in fact, underlies the essential difficulties encountered in lattice QCD calculations with domain-wall fermions.

Note that even if one projects out the low-lying eigenmodes of H [8] (or just the boundary term of the transfer matrix [9]), treats them exactly, and transforms H into one with narrower spectrum (i.e., with a smaller value of the ratio $\lambda_{\max}^2/\lambda_{\min}^2$) such that the chiral symmetry of (2) is improved, however, in principle, (6) still does not satisfy the criterion for the optimal rational approximation of the sign function of H, regardless of the spectrum of H.

The optimal rational approximation for the inverse square root function was first obtained by Zolotarev in 1877 [10], using Jacobian elliptic functions. A detailed discussion of Zolotarev's result can be found in Akhiezer's two books [7,11]. Unfortunately, Zolotarev's optimal rational approximation has been overlooked by the numerical algebra community until recent years.

For lattice QCD with DWF, the relevant problem is how to construct a DWF action such that the operator S in the quark propagator (2) is equal to

$$S = HR_Z(H^2),$$

where $R_Z(H^2)$ is the Zolotarev optimal rational approximation for the inverse square root of H^2. In general, we have two options for R_Z, namely,

$$R_Z^{(n,n)}(H^2) = \frac{d_0}{\lambda_{\min}} \prod_{l=1}^{n} \frac{1 + h^2/c_{2l}}{1 + h^2/c_{2l-1}}$$

and

$$R_Z^{(n-1,n)}(H^2) = \frac{d_0'}{\lambda_{\min}} \frac{\prod_{l=1}^{n-1}(1 + h^2/c_{2l}')}{\prod_{l=1}^{n}(1 + h^2/c_{2l-1}')},$$

where $h^2 = H^2/\lambda_{\min}^2$, $\lambda_{\min}^2$ ($\lambda_{\max}^2$) is the minimum (maximum) of the eigenvalues of H^2, and the coefficients d_0, d_0', c_l, and c_l' are expressed in terms of elliptic functions [11] with arguments depending on n and $\lambda_{\max}^2/\lambda_{\min}^2$.

Now if one could construct a domain-wall fermion action such that the operator T in (4) is replaced with

$$\mathcal{T} = \prod_{s=1}^{N_s} \frac{1 - \omega_s H}{1 + \omega_s H}, \tag{7}$$

then one can solve for $\{\omega_s\}$ such that the operator S (3) is equal to

$$S = \frac{1 - \mathcal{T}}{1 + \mathcal{T}} = \begin{cases} HR_Z^{(n,n)}(H^2), & N_s = 2n + 1, \\ HR_Z^{(n-1,n)}(H^2), & N_s = 2n. \end{cases} \tag{8}$$

Note that one does not have the option to put different weights for H in the numerator and the denominator of (7), since the optimal rational approximation of the sign function of H is equal to H times the optimal rational approximation of $(H^2)^{-1/2}$. Obviously, the highest degree n one can obtain with N_s flavors is only $[\frac{N_s}{2}]$.

Nevertheless, it seems to be nontrivial to implement the weights $\{\omega_s\}$ into the DWF action (1) such that (7) can be reproduced.

Instead of working with the domain-wall fermion action (1), I consider one of its variants [12], which differs from (1) by replacing $\delta_{x,x'} D_5(s,s')$ with

$$D_5(x,s;x',s') = \delta_{x,x'}\delta_{s,s'} + (D_w - 1)_{x,x'} P_- \delta_{s',s+1} + (D_w - 1)_{x,x'} P_+ \delta_{s',s-1}. \quad (9)$$

Then the quark propagator in a background gauge field can be evaluated [9] as

$$\langle q(x)\bar{q}(y)\rangle = \frac{1-\gamma_5 S_w}{1+\gamma_5 S_w}, \quad (10)$$

where S_w is the same as (3) except for substituting H with $H_w = \gamma_5 D_w$. Evidently, (10) does *not* preserve the chiral symmetry optimally, the argument is the same as the case of (2).

In view of (7) and (8), now it is clear how to construct the optimal domain-wall fermion action on the lattice. Explicitly, it reads

$$\mathcal{A} = \sum_{s,s'=1}^{N_s}\sum_{x,x'} \bar\psi(x,s)[(1+\omega_s D_w)_{x,x'}\delta_{s,s'} - (1-\omega_s D_w)_{x,x'} P_-\delta_{s',s+1} - (1-\omega_s D_w)_{x,x'} P_+\delta_{s',s-1}]\psi(x',s') \quad (11)$$

with weights

$$\omega_s = \frac{1}{\lambda_{\min}}\sqrt{1-\kappa'^2 \mathrm{sn}^2(v_s;\kappa')}, \quad (12)$$

where $\mathrm{sn}(v_s;\kappa')$ is the Jacobian elliptic function with argument v_s (13) and modulus $\kappa' = \sqrt{1-\lambda_{\min}^2/\lambda_{\max}^2}$ ($\lambda_{\max}^2$ and $\lambda_{\min}^2$ are the maximum and the minimum of the eigenvalues of H_w^2), and $\{\omega_s\}$ are obtained from the roots ($u_s = \omega_s^{-2}, s = 1,\ldots,N_s$) of the equation

$$\delta_Z(u) = \begin{cases} 1-\sqrt{u}R_Z^{(n,n)}(u) = 0, & N_s = 2n+1, \\ 1-\sqrt{u}R_Z^{(n-1,n)}(u) = 0, & N_s = 2n. \end{cases}$$

It can be shown that the argument v_s in (12) is

$$v_s = (-1)^{s-1} M\,\mathrm{sn}^{-1}\left(\sqrt{\frac{1+3\lambda}{(1+\lambda)^3}};\sqrt{1-\lambda^2}\right) + \left[\frac{s}{2}\right]\frac{2K'}{N_s}, \quad (13)$$

where

$$\lambda = \prod_{l=1}^{N_s}\frac{\Theta^2(\frac{2lK'}{N_s};\kappa')}{\Theta^2(\frac{(2l-1)K'}{N_s};\kappa')}, \quad (14)$$

$$M = \prod_{l=1}^{[\frac{N_s}{2}]}\frac{\mathrm{sn}^2(\frac{(2l-1)K'}{N_s};\kappa')}{\mathrm{sn}^2(\frac{2lK'}{N_s};\kappa')}, \quad (15)$$

K' is the complete elliptic integral of the first kind with modulus κ', and Θ is the elliptic theta function. From (12), it is clear that $\lambda_{\max}^{-1} \le \omega_s \le \lambda_{\min}^{-1}$ since $\mathrm{sn}^2(;) \le 1$.

The quark propagator in a background gauge field can be derived as

$$\langle q(x)\bar{q}(y)\rangle = \frac{1-\gamma_5 S_{\mathrm{opt}}}{1+\gamma_5 S_{\mathrm{opt}}}, \quad (16)$$

where S_{opt} is the same as (8) except substituting H with H_w.

Since the chiral symmetry of (16) is equivalent to $S_{\mathrm{opt}}^2 = 1$, its breaking due to a finite N_s can be measured in terms of the deviation

$$\Delta_Z = \max_{\forall\, Y\neq 0}\left|\frac{Y^\dagger S_{\mathrm{opt}}^2 Y}{Y^\dagger Y} - 1\right|,$$

which has a theoretical upper bound [13], $2(1-\lambda)/(1+\lambda)$, where λ is defined in (14), a function of N_s and $b = \lambda_{\max}^2/\lambda_{\min}^2$. In practice, with $N_s = 32$, one should have no difficulties to achieve $\Delta_Z < 10^{-12}$ for any gauge configurations on a finite lattice (say, $16^3\times 32$ at $\beta = 6.0$).

It is simple to incorporate the bare quark mass m_q by adding the following terms:

$$\frac{m_q}{2m_0}\sum_{x,x'}[\bar\psi(x,1)(1-\omega_1 D_w)_{x,x'}P_+\psi(x',N_s) + \bar\psi(x,N_s)(1-\omega_{N_s}D_w)_{x,x'}P_-\psi(x',1)],$$

to the optimal DWF action (11), and changing the boundary conditions to

$$P_+\psi(x,0) = -\frac{m_q}{2m_0}P_+\psi(x,N_s),$$
$$P_-\psi(x,N_s+1) = -\frac{m_q}{2m_0}P_-\psi(x,1).$$

After introducing pseudofermions (Pauli-Villars fields) with fixed mass $m_q = 2m_0$, one can derive the effective 4D lattice Dirac operator for the internal quark loops as

$$D(m_q) = r(D_c + m_q)(1 + rD_c)^{-1}, \qquad r = \frac{1}{2m_0}, \quad (17)$$

where rD_c denotes the inverse of the massless quark propagator (16) which becomes chirally symmetric in the limit $N_s \to \infty$. The exponential locality of D (17) (for any m_q and N_s) has been asserted for sufficiently smooth gauge background [14].

In the massless limit ($m_q = 0$) and $N_s \to \infty$, D (17) is exactly equal to the overlap Dirac operator [15,16], and satisfies the Ginsparg-Wilson relation [17]

$$D\gamma_5 + \gamma_5 D = 2D\gamma_5 D.$$

This implies that D is topologically proper (i.e., with the correct index and axial anomaly), similar to the case of overlap Dirac operator. For any finite N_s, D is exactly

TABLE I. The precision of chiral symmetry of the massless quark propagator in a gauge background on the 8^4 lattice at $\beta = 6.0$, for various domain-wall fermion actions with $N_s = 16$. (Note that in the limit $N_s \to \infty$, $\sigma \to 0$ for all DWF actions.)

DWF action	$\sigma(m_0 = 1.0)$	$\sigma(m_0 = 1.8)$
Shamir (1)	4.3×10^{-5}	1.9×10^{-5}
Borici (1) and (9)	5.4×10^{-4}	1.0×10^{-4}
Improved DWF (18)	2.4×10^{-6}	3.5×10^{-8}
Optimal DWF (11)	8.8×10^{-9}	3.8×10^{-10}

equal to the overlap Dirac operator with $(H_w)^{-1/2}$ approximated by Zolotarev rational polynomial.

From (17), the valence quark propagator coupling to physical hadrons can be expressed as

$$(D_c + m_q)^{-1} = r(1 - rm_q)^{-1}[D^{-1}(m_q) - 1],$$

where $D^{-1}(m_q)$ can be computed via the five-dimensional lattice Dirac operator of optimal DWF. Evidently, the valence quark propagator of optimal DWF is exactly equal to that of the overlap with Zolotarev approximation. Preliminary numerical results have demonstrated that the quark propagator of optimal DWF with $N_s = 2n$ is precisely equal to that of the overlap with $(H_w^2)^{-1/2}$ approximated by $R_Z^{(n-1,n)}(H_w^2)$. (The relative error between these two quark propagators is always less than 10^{-7} for stopping criterion 10^{-11} in the conjugate gradient loops.)

A simple way to improve the chiral symmetry of DWF action (1) is to replace D_w with $\omega_s D_w$,

$$\mathcal{A}'_{dwf} = \sum_{s,s'=1}^{N_s} \sum_{x,x'} \bar{\psi}(x,s)[\omega_s D_w(x,x')\delta_{s,s'} + \delta_{x,x'} D_5(s,s')]\psi(x',s'), \quad (18)$$

where $\{\omega_s\}$ are given in (12). It is easy to see that in the limit $a_5 \to 0$, both (11) and (18) give the same quark propagator (16) with optimal chiral symmetry. In Table I, the precision of chiral symmetry of each DWF action (with $N_s = 16$) discussed above is measured in terms of $\sigma \equiv \max_{i,j} |(\mathcal{D}^{-1}\gamma_5 + \gamma_5 \mathcal{D}^{-1})_{ij}|$, where $\mathcal{D}^{-1} = \langle q\bar{q} \rangle$ is the quenched *massless* quark propagator (with one of its end points fixed at origin) in a gauge background generated with Wilson gauge action at $\beta = 6.0$ on the 8^4 lattice, and the ranges of the indices are $1 \le i \le 12 \times 8^4$, $1 \le j \le 12$. The eigenvalues of H_w are bounded as $|\lambda(H_w)| \in [0.1848, 6.5348]$ for $m_0 = 1.0$, while $|\lambda(H_w)| \in [0.0946, 5.7484]$ for $m_0 = 1.8$. The quark propagators are computed by conjugate gradient with stopping criterion 10^{-11}. Evidently, the improved DWF action (18) preserves the chiral symmetry much better than Shamir's action and Borici's variant, and the optimal DWF (11) is the best among these DWF actions. Finally, we note that (18) can easily be implemented for machineries already geared to (1).

In summary, the problem how to construct a DWF action such that the effective 4D lattice Dirac operator can preserve the chiral symmetry optimally for any given finite N_s has been solved in (11). It provides a better understanding of exact chiral symmetry on a finite lattice, as well as the optimal way to tackle nonperturbative issues in QCD or supersymmetric QFTs.

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