Tsukuba, 1/24/03

Optimal lattice domain-wall fermions

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Abstract:

I show that the usual formulations of lattice DWF with any finite N_s (in the 5th dim.) do not preserve the chiral symmetry optimally and propose a new action which preserves the chiral symmetry optimally for any N_s.

Outlines:

1. Introduction
2. Zolotarev optimal rational approx. for $\frac{1}{\sqrt{x}}$
3. Optimal lattice DWF
4. Improved lattice DWF
5. Conclusion

References:

hep-lat/0209153, to appear in Phys. Rev. Lett.(2003).
hep-lat/0211032, Phys. Lett. B552 (2003) 97-100.

0. Basics

It is difficult to preserve the chiral symmetry

$$D\gamma_5 + \gamma_5 D = 0$$

on the lattice without violating other fundamental properties (locality, correct continuum behavior, doubler-free) of the fermion field.

But the chiral symmetry plays an important role in QCD ! It forbids an additive quark mass renormalization, and its spontaneously breaking provides (nearly) Goldstone bosons with their specific interactions.

Therefore, one needs to preserve the chiral symmetry on the lattice, otherwise, one hardly uses the lattice regularization to investigate the low energy phenomenolgy of QCD.

Note that in Wilson's formulation (1975) of lattice QCD, chiral symmetry is explicitly broken by an irrelevant term. However, it causes, $O(a)$ lattice artifacts and other undesirable effects at finite lattice spacing.

In the last few years, it has been realized that the proper way to preserve the chiral symmetry on the lattice is to require that D satisfies the Ginsparg-Wilson relation (1981),

$$D\gamma_5 + \gamma_5 D = 2raD\gamma_5 D, \quad r > 0,$$

a generalized chiral symmetry which incorporates the usual chiral symmetry in continuum.

However, a viable D (i.e, exp.-local, doubler-free, correct cont. behavior) satisfying the GW relation has not been realized until 1997. A breakthrough occurred when the overlap Dirac operator was constructed by Neuberger, in the framework of overlap formalism [Narayanan & Neuberger, 1993-1995]. The overlap Dirac operator is exactly equal to the effective 4D lattice Dirac operator of domain-wall fermions [Kaplan,'92; Shamir,'93] (after integrating out the ∞ number of heavy fermions and pseudofermions in the 5-th dim. and taking $a_5 \to 0$).

Overlap Dirac operator
[H. Neuberger, Phys. Lett. B417 ('98) 141]

$$\begin{aligned} D &= m_0 a^{-1}(1\!\!1 + V) = m_0 a^{-1}\left(1\!\!1 + \gamma_5 \frac{H_W}{\sqrt{H_W^2}}\right) \\ H_W &= \gamma_5(-m_0 + aD_W), \quad m_0 \in (0,2) \end{aligned}$$

D_W : massless Wilson-Dirac operator

The GW relation implies that $\mathcal{A}_f = \bar{\psi} D \psi$ is invariant under the chiral transformation on the lattice
[Lüscher, PLB 428 ('98) 342]

$$\begin{aligned} \psi &\rightarrow \exp\{i\theta\gamma_5(1-2arD)\}\ \psi \\ \bar{\psi} &\rightarrow \bar{\psi}\ \exp\{i\theta\gamma_5\} \end{aligned}$$

where θ is a global parameter.

Consequently the axial anomaly can be deduced from the change of the fermion measure under the chiral transformation,

$$[d\bar{\psi}d\psi]_x \rightarrow \exp\{i2\theta \mathrm{tr}[\gamma_5(\mathbb{1} - raD)(x,x)]\}\ [d\bar{\psi}d\psi]_x$$

and its sum over all sites is equal to the index of D, which is a well-defined integer
[Hasenfratz, et. al. PLB 427 (98) 125]

$$\mathrm{Index}(D) = n_+ - n_- = \sum_x \mathrm{tr}[\gamma_5(\mathbb{1} - raD)(x,x)]$$

since the zero modes (if any) of any GW Dirac operator D have definite chirality

$$D\phi = 0 \Rightarrow D\gamma_5\phi = 0,\ \ i.e.\ \gamma_5\phi = \pm\phi$$

In the continuum limit $a \rightarrow 0$,

$$\mathrm{tr}[\gamma_5(1 - arD(x,x))] \rightarrow \frac{1}{32\pi^2}\epsilon_{\mu\nu\lambda\sigma}\mathrm{tr}(F_{\mu\nu}(x)F_{\lambda\sigma}(x))$$

[Kikukawa & Yamada, Chiu, Adams, Fujikawa, Suzuki, Chiu & Hsieh]

The spectrum of GW Dirac operator

[TWC, Phys. Rev. D58 (1998) 074511]

(i) Eigenvalues of D are either real or come in complex conjugate pairs.

(ii) The eigenvalues of D fall on a circle with center at $1/2r$, and radius $1/2r$, and have the reflection symmetry with respect to the real axis.

(iii) The real eigenmodes (if any) at 0 and $1/r$ have definite chirality $+1$ or -1.

(iv) The chirality of any complex eigenmodes is zero. ($\phi_s^\dagger \gamma_5 \phi_s = 0$)

(v) Chirality sum rule : $n_+ + N_+ = n_- + N_-$

$n_\pm$: the # of zero modes of ($+/-$) chirality.

$N_\pm$: the # of $1/r$ modes of ($+/-$) chirality.

For any D satisfying $DD^\dagger = D^\dagger D$ and $D^\dagger = \gamma_5 D \gamma_5$, its spectrum also has above properties except (ii), since its eigenvalues lying on a closed contour rather than a circle.

Introduction

Currently, there are many interesting physics issues in superstring, supergravity, and supersymmetry 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 domain-wall fermions (DWF) [Rubakov'83, Callan & Harvey'86] :

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 $m(s)$ must lead to the occurrence of both LH and RH chiral fermion fields, i.e., a vector-like theory.

Lattice QCD with DWF [Kaplan'92]

In practice, one can only use 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, and so is the corresponding exact chiral symmetry on the lattice.

The relevant question :

How to construct the couplings between these N_s lattice Dirac fermion fields such that the chiral symmetry can be preserved optimally, or in other words, the residual mass of the quark field is the 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.

DWF with open boundary conditions [Shamir'93]

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

$$\begin{aligned} D_w &= \sum_{\mu=1}^{4} \gamma_\mu t_\mu + W - m_0, \quad m_0 \in (0,2) \\ t_\mu(x,x') &= \frac{1}{2}[U_\mu(x)\delta_{x',x+\mu} - U_\mu^\dagger(x')\delta_{x',x-\mu}] \\ W(x,x') &= \sum_{\mu=1}^{4} \frac{1}{2}[2\delta_{x,x'} - U_\mu(x)\delta_{x',x+\mu} - U_\mu^\dagger(x')\delta_{x',x-\mu}] \end{aligned}$$

$$\begin{aligned} D_5(s,s') &= \frac{1}{2}[\gamma_5(\delta_{s',s+1} - \delta_{s',s-1}) + 2\delta_{s,s'} - \delta_{s',s+1} - \delta_{s',s-1}] \\ &= \delta_{s,s'} - P_-\delta_{s',s+1} - P_+\delta_{s',s-1}, \quad P_\pm = \frac{1}{2}(1 \pm \gamma_5). \end{aligned}$$

The boundary conditions:

$$P_+\psi(x,0) = P_-\psi(x,N_s+1) = 0 \ .$$

The quark fields coupling to physical hadrons:

$$\begin{aligned} q(x) &= P_-\psi(x,1) + P_+\psi(x,N_s) \\ \bar{q}(x) &= \bar{\psi}(x,1)P_+ + \bar{\psi}(x,N_s)P_- \end{aligned}$$

The quark propagator can be evaluated
[Neuberger '97, Kikukawa & Noguchi '99]

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

$$\begin{aligned} S &= \frac{1-T}{1+T} \\ T &= \frac{(1-H)^{N_s}}{(1+H)^{N_s}} \\ H &= \gamma_5 \frac{D_w}{2+D_w} \end{aligned}$$

In the limit $N_s \to \infty$, S becomes the sign fn. of the Hermitian operator H,

$$\lim_{N_s\to\infty} S = \frac{H}{\sqrt{H^2}} \ ,$$

then D^{-1} is chirally symmetric.

However, for any finite N_s, D^{-1} does not break the chiral symmetry in the minimal way. In other words, S is *not* the optimal approx. for the sign function of H.

Physical picture:

The coupling between the LH fields (at $s = 1$) and the RH fields (at $s = N_s$) goes to zero only at $N_s \to \infty$.

However, at any finite N_s, the conventional DWF does not provide the optimal blocking between the boundary fields. In other words, the product of these N_s transfer matrices does not constitute the optimal filter to block the transmission of chiral zero modes coupling the LH and RH boundary fields.

$$\begin{aligned} S &= \frac{1-T}{1+T} \\ T &= \frac{(1-H)^{N_s}}{(1+H)^{N_s}} \\ H &= \gamma_5 \frac{D_w}{2+D_w} \end{aligned}$$

According to de la Vallée-Poussin's theorem and Chebycheff's theorem:

The necessary and sufficient condition for an irreducible rational polynomial

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

to be the optimal rational polynomial of

$$\frac{1}{\sqrt{x}},\quad 0 < x_{min} \leq x \leq x_{max}$$

is that $\delta(x) \equiv 1 - \sqrt{x}r^{(n,m)}(x)$ has $n+m+2$ alternate change of sign in $[x_{min}, x_{max}]$, and attains its maxima and minima (all with equal magnitude), say,

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

at consecutive points

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

de la Vallée-Poussin's theorem

Given any two positive and continuous fns. $f(x), g(x) > 0,\ x \in [1, b]$, the problem is to find the irreducible rational polynomial of degree n with positive real coefficients,

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

such that the deviation

$$d(r) = \max_{x \in [1,b]} |f(x) - g(x) r(x)|$$

is the minimum.

Now if there exists $r(x)$ such that

$$\delta(x) = f(x) - g(x) r(x)$$

changes sign alternatively $2n + 2$ times within the interval $[1, b]$, and attains its maxima and minima, say,

$$\delta(x) = \delta_1, -\delta_2, \cdots, +\delta_{2n+1}, -\delta_{2n+2} \quad (\delta_i > 0)$$

at consecutive points,

$$x_1 < x_2 < \cdots < x_{2n+2} \ ,$$

then it can be shown that

$$d(r) \geq \min\{\delta_1, \delta_2, \cdots, \delta_{2n+2}\} \equiv d_{min} \quad \forall \ r(x).$$

Proof:

Suppose there exists an irreducible rational polynomial $R(x)$ of degree n, such that

$$d(R) = \max_{x\in[1,b]} |f(x) - g(x)R(x)| < d_{min}$$

Then

$$\begin{aligned} D(x) &\equiv g(x)R(x) - g(x)r(x) \\ &= f(x) - g(x)r(x) - [f(x) - g(x)R(x)] \\ &= \delta(x) - \Delta(x) \end{aligned}$$

is a continuous function, and it also changes sign alternatively at least $2n+2$ times in $[1, b]$, since $|\Delta(x)| \leq d(R) < d_{min}$. Thus $D(x)$ has at least $2n+1$ zeros in $(1, b)$. On the other hand,

$$D(x) = g(x)[R(x) - r(x)] \equiv g(x)\frac{u(x)}{v(x)}$$

where $u(x)$ and $v(x)$ are polynomials of degree $2n$. Therefore $D(x)$ cannot have more than $2n$ zeros, i.e., a contradiction. This completes the proof.

In general, de la Vallée-Poussin's thm. asserts that if there exists an irreducible rational polynomial of the form

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

such that

$$\delta(x) = f(x) - g(x)r^{(n,m)}(x)$$

has $n + m + 2$ alternate change of sign in the interval $[1, b]$, and attains its maxima and minima, say,

$$\delta(x) = \delta_1, -\delta_2, \cdots, (-1)^{n+m+1}\delta_{n+m+2} \quad (\delta_i > 0)$$

at consecutive points,

$$x_1 < x_2 < \cdots < x_{n+m+2} \ ,$$

then

$$d(r) \geq \min\{\delta_1, \delta_2, \cdots, \delta_{n+m+2}\} \equiv d_{min}$$

for all irreducible rational polynomial $r^{(n,m)}(x)$.

Chebycheff's theorem

It asserts that the optimal irreducible rational polynomial $r^{(n,m)}(x)$ must satisfy the criterion that the difference $\delta(x) = f(x) - g(x)r^{(n,m)}(x)$ has $n + m + 2$ alternate change of sign in the interval $[1, b]$.

For DWF with open boundary conditions

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

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

For $N_s = 2n$,

$$\delta(x) = 1 - xR^{(n-1,n)}(x^2) \geq 0 \quad \forall\ x > 0$$

For $N_s = 2n+1$,

$$\delta(x) = 1 - xR^{(n,n)}(x^2) \begin{cases} > 0, & 0 < x < 1 \\ = 0, & x = 1 \\ < 0, & x > 1 \end{cases}$$

Therefore, both $R^{(n-1,n)}(x^2)$ and $R^{(n,n)}(x^2)$ cannot be the optimal approx. for $(x^2)^{-1/2}$, and S is not the optimal approx. for sign(H). Thus, for any finite N_s, the DWF action does not preserve the chiral symmetry optimally, which in fact underlies the essential difficulties encountered in lattice QCD calculations with DWF.

Zolotarev optimal rational polynomial

The optimal rational approximation for $1/\sqrt{x}$ was first obtained by Zolotarev in 1877, using Jacobian elliptic functions.

For lattice QCD with DWF, the relevant prob. is how to construct a DWF action such that the operator S in the quark propagator for any finite N_s is equal to

$$S = H(H^2)_Z^{-1/2}$$

where $(H^2)_Z^{-1/2}$ can be either

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

or

$$R_Z^{(n-1,n)}(H^2) = \frac{d'_0}{\lambda_{min}} \frac{\prod_{l=1}^{n-1}(1 + h^2/c'_{2l})}{\prod_{l=1}^{n}(1 + h^2/c'_{2l-1})}$$

where $h^2 = H^2/\lambda^2_{min}$, and λ^2_{min} and λ^2_{max} are the minimum and the 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.

$$
\begin{aligned}
c_l &= \frac{\mathrm{sn}^2(\frac{lK'}{2n+1};\kappa')}{1-\mathrm{sn}^2(\frac{lK'}{2n+1};\kappa')}, \quad \kappa' = \sqrt{1-\lambda_{min}^2/\lambda_{max}^2} \\
d_0 &= \frac{2\lambda}{1+\lambda}\prod_{l=1}^{n}\frac{1+c_{2l-1}}{1+c_{2l}} \\
\lambda &= \prod_{l=1}^{2n+1}\frac{\Theta^2\left(\frac{2lK'}{2n+1};\kappa'\right)}{\Theta^2\left(\frac{(2l-1)K'}{2n+1};\kappa'\right)} \\
c_l' &= \frac{\mathrm{sn}^2(\frac{lK'}{2n};\kappa')}{1-\mathrm{sn}^2(\frac{lK'}{2n};\kappa')} \\
d_0' &= \frac{2\lambda'}{1+\lambda'}\frac{\prod_{l=1}^{n}(1+c_{2l-1}')}{\prod_{l=1}^{n-1}(1+c_{2l}')}, \quad \lambda' = \prod_{l=1}^{2n}\frac{\Theta^2\left(\frac{2lK'}{2n};\kappa'\right)}{\Theta^2\left(\frac{(2l-1)K'}{2n};\kappa'\right)}
\end{aligned}
$$

Θ is the elliptic theta function, and the Jacobian elliptic function $\mathrm{sn}(u;\kappa')$ is defined by the elliptic integral

$$
u = \int_0^{\mathrm{sn}} \frac{dt}{\sqrt{(1-t^2)(1-\kappa'^2t^2)}} \ ,
$$

and K' is the complete elliptic integral of the first kind with modulus κ',

$$
K' = \int_0^1 \frac{dt}{\sqrt{(1-t^2)(1-\kappa'^2t^2)}} \ ,
$$

How to construct optimal lattice DWF

If one can construct a DWF action such that the operator T is replaced with

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

then $\{\omega_s\}$ can be solved exactly in terms of elliptic functions such that the operator S is equal to the optimal rational approx. of sign(H)

$$\begin{aligned} \mathcal{S} &= \frac{1-\mathcal{T}}{1+\mathcal{T}} = \frac{\prod_{s=1}^{N_s}(1+\omega_s H) - \prod_{s=1}^{N_s}(1-\omega_s H)}{\prod_{s=1}^{N_s}(1+\omega_s H) + \prod_{s=1}^{N_s}(1-\omega_s H)} \\ &= \begin{cases} H R_Z^{(n,n)}(H^2), & N_s = 2n+1 \\ H R_Z^{(n-1,n)}(H^2), & N_s = 2n \end{cases} \end{aligned}$$

since it amounts to solving N_s roots of

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

which give $\omega_s = 1/\sqrt{u_s}, s = 1, \cdots, N_s$.

Recall that $\delta_Z(u)$ has $N_s + 1$ alternate change of sign in the interval $[1, \lambda_{max}^2/\lambda_{min}^2]$, the salient feature of the optimal rational polynomial R_Z.

Obviously, the highest deg. n of R_Z is $[\frac{N_s}{2}]$.

Instead of working with Shamir's DWF action, I consider one of its variants [Borici'99], which differs from Shamir DWF by replacing $\delta_{x,x'} D_5(s,s')$ with

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

Then the quark propagator can be evaluated [Edwards & Heller, 2000] as

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

$$\begin{aligned} \mathcal{S} &= \frac{1-\mathcal{T}}{1+\mathcal{T}} \\ \mathcal{T} &= \frac{(1-H_w)^{N_s}}{(1+H_w)^{N_s}}, \quad H_w = \gamma_5 D_w \end{aligned}$$

In the limit $N_s \to \infty$, $\mathcal{S}$ becomes sign(H_w),

$$\lim_{N_s \to \infty} \mathcal{S} = \frac{H_w}{\sqrt{H_w^2}} \ ,$$

then D^{-1} is chirally-symmetric.

Evidently, $\mathcal{S}$ is *not* the optimal approximation for the sign function of H_w for any finite N_s, the argument is same as the case of S. Therefore D^{-1} does *not* break the exact chiral symmetry in the minimal way.

Optimal Domain Wall Fermions

[TWC, hep-lat/0209153]

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

with

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

where $\mathrm{sn}(v_s;\kappa')$ is the Jacobian elliptic fn. with argument v_s and modulus $\kappa' = \sqrt{1-\lambda_{min}^2/\lambda_{max}^2}$ (λ_{max}^2 and λ_{min}^2 are the max. and the min. of the eigenvalues of H_w^2), and ω_s are obtained from the roots $(u_s = \omega_s^{-2}, s = 1,\cdots,N_s)$ of

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

Note that $\delta_Z(u)$ has N_s+1 alternate change of sign in $[1, \lambda_{max}^2/\lambda_{min}^2]$, the salient feature of optimal rational polynomial.

The argument v_s reads

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

where

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

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

K' is the complete elliptic integral of the first kind with modulus κ', and Θ is the elliptic theta function.

For the optimal DWF, the quark propagator can be evaluated as

$$r^{-1} D_c^{-1}(x,y) \equiv \langle q(x)\bar{q}(y)\rangle = \frac{1-\gamma_5 \mathcal{S}_{opt}}{1+\gamma_5 \mathcal{S}_{opt}}, \qquad r = \frac{1}{2m_0}$$

$$\begin{aligned} \mathcal{S}_{opt} &= \frac{1-\mathcal{T}}{1+\mathcal{T}} \\ &= \frac{\prod_{s=1}^{N_s}(1+\omega_s H_w) - \prod_{s=1}^{N_s}(1-\omega_s H_w)}{\prod_{s=1}^{N_s}(1+\omega_s H_w) + \prod_{s=1}^{N_s}(1-\omega_s H_w)} \\ &= \begin{cases} H_w R_Z^{(n,n)}(H_w^2), & N_s = 2n+1 \\ H_w R_Z^{(n-1,n)}(H_w^2), & N_s = 2n \end{cases} \end{aligned}$$

Since the chiral symmetry of D_c^{-1} is equivalent to $\mathcal{S}_{opt}^2 = 1$, its breaking due to a finite N_s can be measured in terms of the deviation Δ_Z which has a theoretical upper bound [TWC et. al., hep-lat/0206007],

$$\Delta_Z = \max_{\forall\ Y \neq 0} \left| \frac{Y^\dagger \mathcal{S}_{opt}^2 Y}{Y^\dagger Y} - 1 \right| < \frac{2(1-\lambda)}{1+\lambda}$$

Since λ is a function of N_s and $b = \lambda_{max}^2/\lambda_{min}^2$, thus for any given gauge configuration, one can determine what values of N_s and b (i.e., how many low-lying eigenmodes of H_w^2 should be projected out) are required to attain one's desired accuracy in preserving the exact chiral symmetry. 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

$$-rm_q \sum_{x,x'} [\bar{\psi}(x,1)(\omega_1 D_w(x,x') - 1)P_+\psi(x',N_s)$$

$$+\bar{\psi}(x,N_s)(\omega_{N_s} D_w(x,x') - 1)P_-\psi(x',1)], \quad r = \frac{1}{2m_0}$$

to the optimal DWF action, and changing the boundary conditions to

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

After introducing pseudofermions (Pauli-Villars fields) with fixed mass $m_q = 1/r = 2m_0$, one can derive the effective 4D lattice Dirac op. for the internal quark loops

$$\begin{aligned} D(m_q) &= r(D_c + m_q)(1 + rD_c)^{-1} = rm_q + (1 - rm_q)D \\ D &= \frac{1}{2}(1 + \gamma_5 S_{opt}) \end{aligned}$$

which, in the limit $N_s \to \infty$ and $m_q = 0$, is exactly equal to the overlap Dirac operator [Neuberger'97]

$$D_o = \frac{1}{2}\left(1 + \gamma_5 \frac{H_w}{\sqrt{H_w^2}}\right)$$

At finite N_s, D is exactly equal to the overlap Dirac operator with $(H_w^2)^{-1/2}$ approximated by Zolotarev rational polynomial.

At finite N_s, D is exponentially-local for sufficiently smooth gauge background, and is more localized than itself at $N_s = \infty$.
[TWC, hep-lat/0211032]

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 5-dimensional lattice Dirac operator of optimal DWF.

Numerical studies 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 CG loops.)

Improved Lattice DWF [TWC, hep-lat/0209153]

A simple way to improve the chiral symmetry of Shamir action is to replace D_w with $\omega_s D_w$,

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

(Note that mass terms enter through the b.c.)
The generating functional $W[\bar{J},J]$ for connected n-point Green's function:

$$e^{-W[\bar{J},J]} = \frac{\int [d\psi][d\bar{\psi}] e^{-\mathcal{A}_I + \sum_x \{\bar{J}(x)q(x) + \bar{q}(x)J(x)\}}}{\int [d\psi][d\bar{\psi}] e^{-\mathcal{A}_I}}$$

where $\bar{J}(x)$ and $J(x)$ are Grassman sources of the quark fields. Explicitly,

$$W[\bar{J},J] = \bar{J}\left[\left(\frac{1+\gamma_5 S}{1-\gamma_5 S}\right) + r m_q\right]^{-1} \rho^{-1} J$$

where

$$\begin{aligned} S &= \frac{1-\mathcal{T}}{1+\mathcal{T}}, \quad \mathcal{T} = \prod_{s=1}^{N_s} T_s = \prod_{s=1}^{N_s} \frac{1-\omega_s H_s}{1+\omega_s H_s} \\ H_s &= H_w(2\rho + \omega_s \gamma_5 H_w)^{-1} \end{aligned}$$

Then the quark propagator $\langle q(x)\bar{q}(y)\rangle$ is

$$\frac{\delta^2 W[\bar{J},J]}{\delta\bar{J}(x)\delta J(y)} = \left[\left(\frac{1+\gamma_5 S}{1-\gamma_5 S}\right) + r m_q\right]^{-1} \rho^{-1} \equiv r^{-1}(D_c + m_q)^{-1}$$

Thus the deviation from optimal chiral sym. is due to the fact that $2\rho - 1 + \omega_s \gamma_5 H_w \neq 0$. One can tune ρ to minimize $(2\rho - 1 + \omega_s \gamma_5 H_w)$ for a given set of gauge configurations. Note that one can use a set of parameters $\{\rho_s\}$, but the tunings would be too tedious to be practical.

TESTS : with $N_s = 16$, measure

$$\sigma \equiv \max_{i,j} |(D_c^{-1}\gamma_5 + \gamma_5 D_c^{-1})_{ij}|$$

where $D_c^{-1} = r\langle q\bar{q}\rangle$ is the quenched massless quark propagator (with one of its endpoints fixed at origin) on the 8^4 lattice at $\beta = 6.0$ (Wilson gauge action). The CG stopping criterion is 10^{-11}.

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

Conclusion

The theoretical problem how to construct a DWF action such that the effective 4D lattice Dirac operator preserves the chiral symmetry optimally for any given finite N_s in the 5-th dimension, has been completely solved.

The optimal lattice domain-wall fermions 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.