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Recent Development of Domain-Wall/Overlap Fermions for Lattice QCD

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IAC & LOC: "to cover results on your recent proposal of the optimal domain-wall fermions and related developments of domain-wall/overlap fermions for QCD by other groups"

Plan:

- Review the formulations of lattice QCD with DWF, and show that it is possible
  (i) to preserve the chiral symmetry optimally for any N_s (sites in the 5-th dim)
  (ii) to replace its non-ultralocal $H = H_w/(2+a_5\gamma_5 H_w)$ with ultralocal H_w, in the transfer matrix as well as the effective 4D lattice Dirac operator

- Neuberger's double pass algorithm for computing the quark propagator in optimal DWF/overlap

- Related developments

Introduction

The basic idea of domain-wall fermions (DWF) [Rubakov & Shaposhnikov '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

Exact chiral symmetry on the lattice was pioneered by Kaplan (1992) with his proposal of DWF on the 5-dim. lattice, in which the fifth dim. (internal flavor space) is discretized with N_s sites (flavors) and lattice spacing a_5

Although Kaplan's initial motivation was to provide a nonperturbative formulation of chiral gauge theories, the idea turned out to be natural and well-defined for vector-like gauge theories (e.g. QCD), with quark fields constructed from the boundary modes [Shamir '93, Shamir & Furman '94]

Soon after Kaplan proposed DWF for chiral gauge theories, Narayanan and Neuberger ('93) observed that the chiral determinant can be written as the inner-product ("overlap") of two fermionic many body states of two bilinear H. For vector gauge theories like QCD, the fermion determinant is the product of a complex conjugate pair of chiral determinants, thus it is gauge invariant, real, non-negative, and the corresponding lattice (overlap) Dirac operator for massless quarks [Neuberger,'97] can be rep. by a finite matrix of fixed shape regardless of the topology of the background gauge field, without undesired doubling or any fine-tuning.

Mathematically, the overlap Dirac operator is exactly equal to the effective 4D lattice Dirac operator of DWF (for internal fermions dressed with pseudofermions [Frolov & Slavnov '93]), in the limit $N_s \to \infty$ followed by $a_5 \to 0$.

$$D = m_0 \left(1 + \gamma_5 \frac{H_w}{\sqrt{H_w^2}} \right) , \quad H_w = \gamma_5 D_w$$

D_w is the standard Wilson operator plus $-m_0$ $(0 < m_0 < 2)$.

However, at finite N_s and a_5, DWF suffers:
(i) The chiral symmetry of quark propagator is not optimal for any N_s,
(ii) Due to the $H = \gamma_5 D_w/(2 + a_5 D_w)$ in the transfer matrix, the quark det. and propagator might be sensitive to a_5, even for $N_s \to \infty$. Nonperturbative renormalizations are required.

A relevant question:
How to construct a DWF action such that the chiral symmetry can be preserved optimally, and the non-ultralocal H is replaced with H_w.

Lattice QCD with conventional DWF

[Kaplan '92, Shamir '93, Shamir & Furman '94]

$$\mathcal{A}_F = \sum_{s,s'=1}^{N_s} \sum_{x,x'} \bar{\psi}(x,s)[a_5 D_w(x,x')\delta_{s,s'} + \delta_{x,x'} D_5(s,s')]\psi(x',s')$$

D_w is 4D Wilson-Dirac operator plus $-m_0$
$(0 < m_0 < 2,\ 0 < a_5 m_0 < 2)$

$$D_5(s,s') = \delta_{s,s'} - P_-\delta_{s',s+1} - P_+\delta_{s',s-1}, \quad P_\pm = \frac{1}{2}(1 \pm \gamma_5).$$

The boundary conditions:

$$\begin{aligned} P_+\psi(x,0) &= -rm_q P_+\psi(x,N_s),\ r = \frac{1}{m_0(2-a_5 m_0)} \\ P_-\psi(x,N_s+1) &= -rm_q P_-\psi(x,1) \end{aligned}$$

The quark fields are:

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

To regularize the fermion determinant, Pauli-Villars (pseudofermion) fields $\{\phi(x,s), \bar{\phi}(x,s)\}$ carrying the same (flavor, color, Dirac) indices of $\{\psi(x,s), \bar{\psi}(x,s)\}$ but obeying the Bose stat. are introduced. [Frolov & Slavnov '93]

$$\mathcal{A}_{PF} = \sum_{s,s'=1}^{N_s} \sum_{x,x'} \bar{\phi}(x,s)[a_5 D_w(x,x')\delta_{s,s'} + \delta_{x,x'} D_5(s,s')]\phi(x',s')$$

with the boundary conditions:

$$\begin{aligned} P_+\phi(x,0) &= -P_+\phi(x,N_s), \quad (m_q = 1/r) \\ P_-\phi(x,N_s+1) &= -P_-\psi(x,1) \ . \end{aligned}$$

The action of the system is

$$\mathcal{A} = \mathcal{A}_G + \mathcal{A}_F + \mathcal{A}_{PF}$$

where $\mathcal{A}_G$ is the gluon action.

The generating functional for n-point Green's function of quark fields q and $\bar{q}$ can be derived as [TWC, hep-lat/0303008]

$$Z[J,\bar{J}] = \frac{\int [dU] e^{-\mathcal{A}_G[U]} \; \mathrm{det} D(m_q) \; e^{\bar{J}(D_c+m_q)^{-1}J}}{\int [dU] e^{-\mathcal{A}_G[U]} \; \mathrm{det} D(m_q)}$$

where

$$\begin{aligned}
D(m_q) &= (D_c + m_q)(1 + rD_c)^{-1} \\
&= m_q + (1/r - m_q)[1 + \gamma_5 S(H)]/2 \\
(D_c + m_q)^{-1} &= (1 - rm_q)^{-1}[D(m_q)^{-1} - r] \\
rD_c &= \frac{1 + \gamma_5 S(H)}{1 - \gamma_5 S(H)} \\
S(H) &= \frac{1 - T^{N_s}}{1 + T^{N_s}} \equiv HR(H) \;, \quad T = \frac{1 - a_5 H}{1 + a_5 H} \\
H &= \gamma_5 \frac{D_w}{2 + a_5 D_w}
\end{aligned}$$

In the limit $N_s \to \infty$, $S(H) \to \frac{H}{\sqrt{H^2}} \equiv \mathrm{sgn}(H)$, then D_c is chirally symmetric

$$D_c \gamma_5 + \gamma_5 D_c = 0$$

and $D \equiv D(0) = [1 + \gamma_5 S(H)]/2r$ satisfies the Ginsparg-Wilson relation

$$D\gamma_5 + \gamma_5 D = 2r D \gamma_5 D$$

Further, at $a_5 = 0$, H becomes $H_w = \gamma_5 D_w$, then D is exactly equal to the overlap Dirac operator [Neuberger '97]

$$D_{ov} = m_0 \left(1 + \gamma_5 \frac{H_w}{\sqrt{H_w^2}} \right)$$

Remarks:

1. The axial anomaly is recovered through the Chern-Simmons current [Golterman et al. '92, Shamir '93]

2. In the limit $N_s \longrightarrow \infty$, the non-singlet flavor symmetry $SU_L(N_f) \times SU_R(N_f)$ of N_f massless quarks is exact for finite lattice spacing a [Shamir '93]

3. The effective 4D lattice Dirac operator $D(m_q)$ is exponentially-local for sufficiently smooth background gauge fields. [Hernandez et. al '98, Kikukawa '00]

4. Any quark observable in QCD can be obtained from $Z[J, \bar{J}]$ by differentiation, and it has the usual discrete symmetries (C, T, P).

Quark propagator

$$\langle q(x)\bar{q}(y)\rangle = -\left.\frac{\delta^2 Z[J,\bar{J}]}{\delta\bar{J}(x)\delta J(y)}\right|_{J=\bar{J}=0}$$
$$= \frac{\int[dU]e^{-\mathcal{A}_G}\prod_f \mathrm{det}D(m_f)\ (D_c+m_q)^{-1}_{x,y}}{\int[dU]e^{-\mathcal{A}_G}\prod_f \mathrm{det}D(m_f)}$$

Current-current correlator

$$-\langle\bar{d}(x)\gamma_4 P_- s(x)\bar{s}(0)\gamma_4 P_- d(0)\rangle \qquad P_\pm = \frac{1}{2}(1\pm\gamma_5)$$
$$= -\left.\frac{\delta}{\delta J_d(x)}\gamma_4 P_- \frac{\delta}{\delta\bar{J}_s(x)}\frac{\delta}{\delta J_s(0)}\gamma_4 P_-\frac{\delta}{\delta\bar{J}_d(0)} Z[\{J_f,\bar{J}_f\}]\right|_{J=\bar{J}=0}$$
$$= \frac{\int[dU]e^{-\mathcal{A}_g}\prod \mathrm{det}D(m_f)\mathrm{tr}[(D_c+m_d)^{-1}_{0,x}\gamma_4 P_-(D_c+m_s)^{-1}_{x,0}\gamma_4 P_-]}{\int[dU]e^{-\mathcal{A}_G}\prod \mathrm{det}D(m_f)}$$

Note that the V-A structure of the left-handed quark currents is preserved exactly.

5. If the effective 4D lattice Dirac operator $D(m_q)$ (or any GW Dirac operator) is used to define the quark action, then subtleties could emerge. (recall that CP in χGT with GW Dirac operator is broken by $O(a)$ effect) [Lüscher '98, Hasenfratz, Lattice 2001]

Consider the massless ($m_q = 0$) case,

$$\begin{aligned} \mathcal{A}_F &= \sum_{x,y} \bar{q}(x) D_{x,y} q(y) \\ &= \sum_{x,y} [\bar{q}(x) P_+ D_{x,y} \hat{P}_- q(y) + \bar{q}(x) P_- D_{x,y} \hat{P}_+ q(y)] \end{aligned}$$

where

$$\begin{aligned} \hat{P}_\pm &= \frac{1}{2}[1 \pm \gamma_5(1 - 2raD)] \ , \quad \hat{P}_\pm^2 = \hat{P}_\pm \\ P_\pm &= \frac{1}{2}(1 \pm \gamma_5) \ , \quad P_\pm^2 = P_\pm \end{aligned}$$

Then its left-handed quark current does not manifest the V-A structure.

$$\bar{d}(x)\gamma_\mu \hat{P}_- s(x) \neq \bar{d}(x) P_+ \gamma_\mu s(x)$$

Consequently, the effective weak Hamiltonian constructed from these quark currents would break the $SU_L(2)$ gauge symmetry of the EW interactions, by the $O(a)$ effect. [Fujikawa, Ishibashi & Suzuki, '02]

This dilemma cannot be resolved by re-defining the quark field as $\widehat{q} = (1 - raD)q = (1 + raD_c)^{-1} q$

$$\mathcal{A}_F = \bar{q} D q = \bar{q} P_+ D_c P_- \widehat{q} + \bar{q} P_- D_c P_+ \widehat{q} = \bar{q} D_c \widehat{q}$$

Note that D_c becomes nonlocal in the limit $N_s \to \infty$

It seems that quark fields have to be defined by the boundary modes of DWF, even though one can compute the quark propagator via the 4D effective $D(m_q)$.

Is the fifth dimension physical or unphysical ?

Problems of the conventional DWF:

1. For any finite N_s, $S(H)$ is not the optimal approx. for sgn(H). [TWC '02]

2. Even at $N_s \to \infty$, $S(H) = H/\sqrt{H^2}$ still depends on a_5 through the non-ultralocal $H = H_w/(2 + a_5\gamma_5 H_w)$.

It turns out that both problems can be solved by constructing a DWF action such that $S(H)$ is replaced with

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

where $\{\omega_s\}$ are weights which depend on N_s, λ_{max} and λ_{min} (max. and min. of the eigenvalues of $|H_w|$).

Borici's variant of DWF [Borici '00, Edwards, Heller,'01]

$$\mathcal{A}_F = \sum_{s,s'=1}^{N_s} \sum_{x,x'} \bar{\psi}(x,s)\{(a_5 D_w(x,x') + \delta_{x,x'})\delta_{s,s'}$$
$$-(\delta_{x,x'} - a_5 D_w(x,x'))(P_+\delta_{s',s-1} + P_-\delta_{s',s+1})\}\psi(x',s')$$
$$\equiv \quad \bar{\Psi}\mathcal{D}_F\Psi$$

with boundary conditions and quark fields same as the conventional DWF. After introducing pseudofermion fields (with $m_q = 2m_0$), the fermion determinant is

$$\det(\mathcal{D}_F \mathcal{D}_{PF}^{-1}) = \det\{m_q + (m_0 - m_q/2)[1 + \gamma_5 S(H_w)]\}$$
$$S(H_w) = \frac{(1 + a_5 H_w)^{N_s} - (1 - a_5 H_w)^{N_s}}{(1 + a_5 H_w)^{N_s} + (1 - a_5 H_w)^{N_s}} \xrightarrow{N_s \to \infty} \frac{H_w}{\sqrt{H_w^2}}$$

Problems:

$$\langle q(x)\bar{q}(y)\rangle \neq (D_c + m_q)^{-1}_{x,y} \ , \quad D_c = 2m_0 \frac{1 + \gamma_5 S(H_w)}{1 - \gamma_5 S(H_w)}$$

$S(H_w)$ is not the optimal rational approx. for $\mathrm{sgn}(H_w)$

The deviation of $S(H)$ from $\mathrm{sgn}(H) = \frac{H}{\sqrt{H^2}}$

$$\begin{aligned}\sigma(S) &= \max_{\forall\ Y\neq 0} \left| \frac{Y^\dagger\{\mathrm{sgn}(H) - S(H)\}Y}{Y^\dagger Y} \right| \\ &\leq \max_{\{x\}} |\mathrm{sgn}(x) - S(x)| \ ,\end{aligned}$$

where $\{x\}$ are eigenvalues of H.
Using the identity

$$|\mathrm{sgn}(x) - S(x)| = \left| 1 - \sqrt{x^2} R(x^2) \right| \ , \quad S(x) = xR(x^2)$$

which holds for any $x \neq 0$, one obtains

$$\sigma(S) \leq \max_{\{x^2\}} \left| 1 - \sqrt{x^2} R(x^2) \right|$$

where $\{x^2\}$ are eigenvalues of H^2.

So the problem of finding $S_{opt}(x) = xR_{opt}(x^2)$ of $\mathrm{sgn}(x)$ with $x \in [-x_{max}, -x_{min}] \cup [x_{min}, x_{max}]$ is equivalent to finding $R_{opt}(x^2)$ of $(x^2)^{-1/2}$ with $x^2 \in [x^2_{min}, x^2_{max}]$.

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

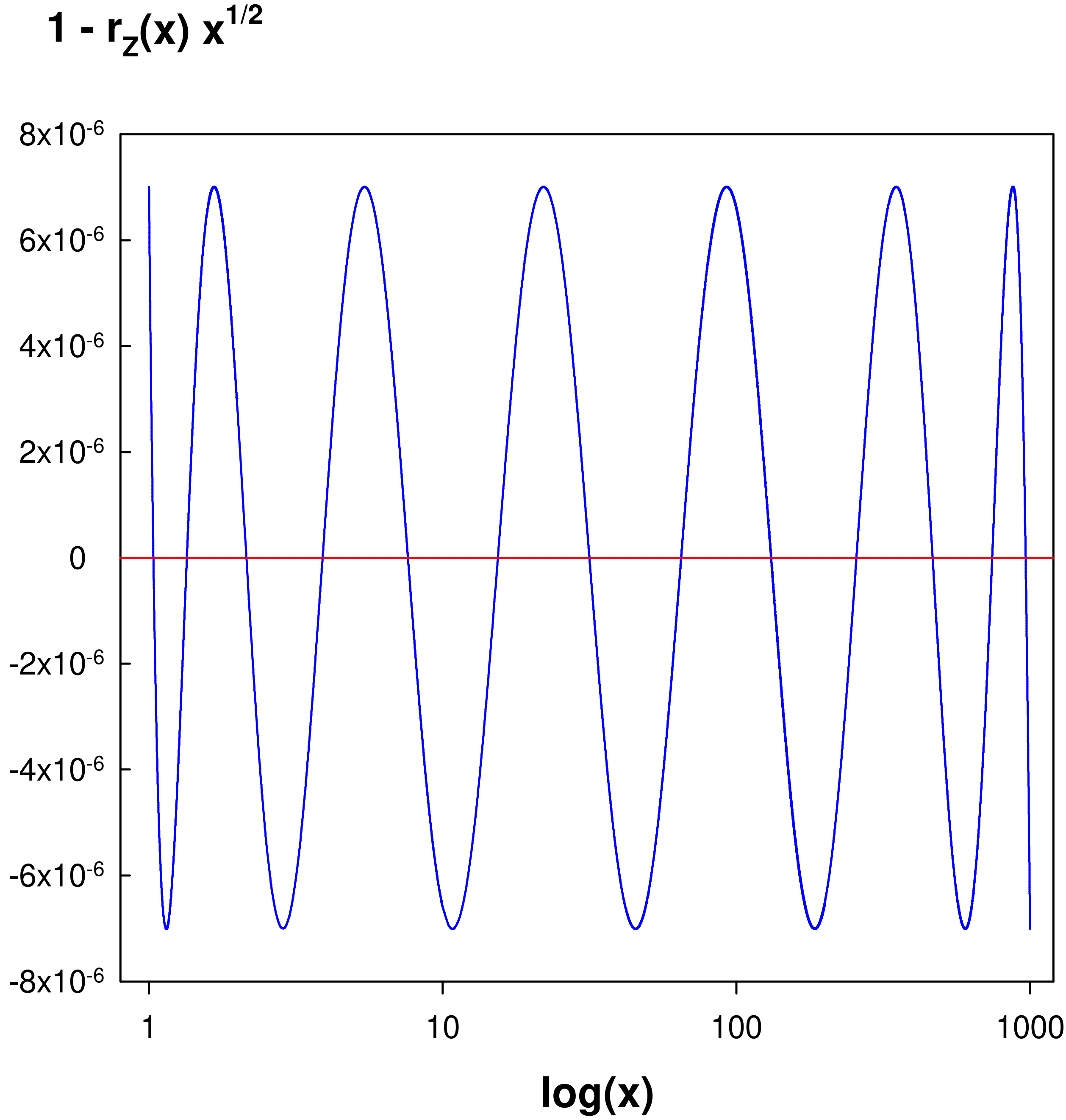
$$\frac{1}{\sqrt{x}}, \quad 0 < x_{min} \leq x \leq x_{max}$$

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

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



1 - r_Z(x) x^1/2
8x10^-6
6x10^-6
4x10^-6
2x10^-6
0
-2x10^-6
-4x10^-6
-6x10^-6
-8x10^-6
1
10
100
1000
log(x)

For the conventional DWF

$$S(x) = \frac{(1+x)^{N_s} - (1-x)^{N_s}}{(1+x)^{N_s} + (1-x)^{N_s}} \equiv xR(x^2)$$

(i) $N_s = 2n$,

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

(ii) $N_s = 2n + 1$,

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

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 $S(H)$ is not the optimal approx. for $\mathrm{sgn}(H)$. Thus, for any finite N_s, the conventional DWF does not preserve chiral symmetry optimally. [TWC '02]

Note that one can project out the low-lying eigenmodes of H [Hernandez et al.'00, Jansen & Nagai'03], or the boundary term of transfer matrix [Edwards & Heller,'00], treats them exactly, and transforms H into one with narrower spectrum such that the error of $S(H)$ could be reduced, however, in principle, $S(H)$ still does not satisfy the criterion for the optimal rational approx. of $\mathrm{sgn}(H)$, regardless of the spectrum of H.

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

$$S_{opt}(H_w) = \begin{cases} H_w R_Z^{(n,n)}(H_w^2), & N_s = 2n+1, \\ H_w R_Z^{(n-1,n)}(H_w^2), & N_s = 2n. \end{cases}$$

$$\begin{aligned} R_Z^{(n,n)}(H_w^2) &= \frac{d_0}{\lambda_{min}} \prod_{l=1}^{n} \frac{1 + h_w^2/c_{2l}}{1 + h_w^2/c_{2l-1}} \\ R_Z^{(n-1,n)}(H_w^2) &= \frac{d_0'}{\lambda_{min}} \frac{\prod_{l=1}^{n-1}(1 + h_w^2/c_{2l}')}{\prod_{l=1}^{n}(1 + h_w^2/c_{2l-1}')} \end{aligned}$$

where $h_w^2 = H_w^2/\lambda_{min}^2$, and the coefficients d_0, d_0', c_l and c_l' are expressed in terms of elliptic functions.

$$c_l = \frac{\mathrm{sn}^2(\frac{lK'}{2n+1};\kappa')}{1-\mathrm{sn}^2(\frac{lK'}{2n+1};\kappa')}, \quad c'_l = \frac{\mathrm{sn}^2(\frac{lK'}{2n};\kappa')}{1-\mathrm{sn}^2(\frac{lK'}{2n};\kappa')}$$

$$d_0 = \frac{2\lambda}{1+\lambda}\prod_{l=1}^{n}\frac{1+c_{2l-1}}{1+c_{2l}}, \quad d'_0 = \frac{2\lambda'}{1+\lambda'}\frac{\prod_{l=1}^{n}(1+c'_{2l-1})}{\prod_{l=1}^{n-1}(1+c'_{2l})}$$

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

$\kappa' = \sqrt{1-\lambda_{min}^2/\lambda_{max}^2}$, Θ is the elliptic theta function, and the Jacobian elliptic fn $\mathrm{sn}(u;\kappa')$ is defined by

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

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 $S(H)$ is replaced with

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

then one can solve for $\{\omega_s\}$ such that

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

which amounts to solving N_s roots of

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

It turned out that these N_s roots can be solved exactly in terms of elliptic functions. [TWC '02]

Optimal DWF [TWC '02, hep-lat/0303008]

$$\mathcal{A}_f = \sum_{s,s'=0}^{N_s+1} \sum_{x,x'} \bar{\psi}(x,s)[(1+\omega_s D_w)_{x,x'}\delta_{s,s'}$$
$$-(1-\omega_s D_w)_{x,x'}(P_-\delta_{s',s+1} + P_+\delta_{s',s-1})]\psi(x',s')$$

with boundary conditions

$$\begin{aligned} P_+\psi(x,-1) &= -rm_q P_+\psi(x,N_s+1), \quad r = \frac{1}{2m_0} \\ P_-\psi(x,N_s+2) &= -rm_q P_-\psi(x,0) \end{aligned}$$

The quark fields:

$$q(x) = \sqrt{r}[P_-\psi(x,0) + P_+\psi(x,N_s+1)]$$
$$\bar{q}(x) = \sqrt{r}[\bar{\psi}(x,0)P_+ + \bar{\psi}(x,N_s+1)P_-]$$

The weights are : $\omega_0 = \omega_{N_s+1} = 0$,

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

where $\mathrm{sn}(v_s;\kappa')$ is the Jacobian elliptic fn.

The weights $\{\omega_s\}$ are obtained from the roots $[u_s = \omega_s^{-2}, s = 1, \cdots, N_s]$ of

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

The argument v_s reads

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

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

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

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

After introducing the pseudofermions ($m_q = 2m_0$), the generating function for n-point function of q and $\bar{q}$ can be derived as [TWC, hep-lat/0303008]

$$Z[J,\bar{J}] = \frac{\int [dU] e^{-\mathcal{A}_G[U]} \ \mathrm{det} D(m_q) \ e^{\bar{J}(D_c+m_q)^{-1}J}}{\int [dU] e^{-\mathcal{A}_G[U]} \ \mathrm{det} D(m_q)}$$

where

$$\begin{aligned}
D_c &= 2m_0 \frac{1+\gamma_5 S_{opt}(H_w)}{1-\gamma_5 S_{opt}(H_w)} \\
D(m_q) &= (D_c + m_q)(1 + rD_c)^{-1} \\
&= m_q + (m_0 - m_q/2)[1 + \gamma_5 S_{opt}(H_w)] \\
S_{opt}(H_w) &= \begin{cases} H_w R_Z^{(n,n)}(H_w^2), & N_s = 2n+1, \\ H_w R_Z^{(n-1,n)}(H_w^2), & N_s = 2n. \end{cases}
\end{aligned}$$

$D(m_q)$ (for any N_s and m_q) is exponentially local for sufficiently smooth gauge background [TWC '02]

Since $S_{opt}(H_w)$ is the optimal rational approximation to $\text{sgn}(H_w)$, the bound of $\sigma(S_{opt})$ is the minimum

$$
\begin{aligned}
\sigma(S_{opt}) &= \max_{\forall\ Y \neq 0} \left| \frac{Y^\dagger \{\text{sgn}(H_w) - S_{opt}(H_w)\} Y}{Y^\dagger Y} \right| \\
&\leq \frac{1-\lambda}{1+\lambda} \simeq A(b) e^{-c(b) N_s}
\end{aligned}
$$

where $b = \lambda_{max}^2 / \lambda_{min}^2$

$$
\begin{aligned}
A(b) &\simeq 4.06(1) b^{-0.0091(1)} \ln(b)^{0.0042(3)} \\
c(b) &\simeq 4.27(45) \ln(b)^{-0.746(5)}
\end{aligned}
$$

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.

Quenched quark propagators in ODWF

$$\langle q(x)\bar{q}(y)\rangle = (D_c + m_q)^{-1}_{x,y} = (1 - rm_q)[D^{-1}_{x,y}(m_q) - r]$$
$$= \sum_{s,s'}(P_-\delta_{s,0} + P_+\delta_{s,N_s+1})\mathcal{D}^{-1}_{odw}(x,s;y,s')(P_+\delta_{s',0} + P_-\delta_{s',N_s+1})$$

(1) To solve the linear system of 5D optimal DWF

$$\mathcal{D}_{odw}(x,s;y,s')Y$$
$$= [(1+\omega_s D_w)\delta_{s,s'} - (1-\omega_s D_w)(P_-\delta_{s',s+1} + P_+\delta_{s',s-1})]Y$$
$$= (P_+\delta_{s,0} + P_-\delta_{s,N_s+1}) \cdot 1\!\!1$$

(2) To solve the system of effective 4D Dirac op.

$$D(m_q)D^\dagger(m_q)Y$$
$$= \left\{m_q^2 + (m_0^2 - m_q^2/4)\,[2 + (\gamma_5 \pm 1)S_{opt}(H_w)]\right\} Y = 1\!\!1$$

with nested conjugate gradient, where the inner CG is iterated with Neuberger's double pass algorithm (1998). For quenched QCD, see [Hsieh, TWC, hep-lat/0305016]

Neuberger's double pass algorithm (1998)

Consider the matrix-vector product:

$$R^{(n-1,n)}(H^2) \cdot Y = \sum_{l=1}^{n} \frac{b_l}{H^2 + d_l} Y = \sum_{l=1}^{n} b_l Z^{(l)}$$

$$(H^2 + d_l) Z^{(l)} = Y$$

where $\{Z^{(l)}\}$ are obtained by multi-shift CG.

Problem: memory storage of $2n + 3$ large vectors.

Neuberger's observation: individual $Z^{(l)}$ is not required but the sum $\sum b_l Z^{(l)}$. Since $\{Z_i^{(l)}, P_i^{(l)}\}$ at the i-th iter. are linear combinations of their preceedents in the iter. process, thus it is possible to obtain their updating coefficients $\{\alpha_i^{(l)}, \beta_i^{(l)}\}$ in the first pass, and then use them to update $\sum b_l Z^{(l)}$ successively in the second pass, with memory storage of only 5 vectors, for any degree n of R.

Salient features of 2-pass algorithm

The number of floating point operations for Neuberger's 2-pass algorithm is independent of the degree n of R, provided N_{sites} is much larger than the number of iteration L_i in the conjugate gradient. This implies that $(H^2)^{-1/2}Y \simeq R^{(n-1,n)}(H^2) \cdot Y$ can be approximated to very high precision with sufficiently large n, without noticeably extra costs. [Hsieh, TWC, hep-lat/0306025]

1-pass: $F_1 \simeq N_{site}L_i[3552 + 120(n-1)p]$
$(n-1)p$ = effective number of $\{Z^{(l)}, P^{(l)}, l = 2, \cdots, n\}$ being updated, before $Z^{(l)}$ converges.

2-pass: $F_2 \simeq 6888 N_{site}L_i$

For $n > n_Z$, $F_1 > F_2$

$$n_Z \simeq \begin{cases} 34 \;, & p = 0.83 \text{ (polar)} \\ 59 \;, & p = 0.48 \text{ (Zolotarev)} \end{cases}$$

In practice, for $n \geq 16$, 2-pass is faster than 1-pass.

Conclusions

(1) A new lattice DWF action has been constructed such that its effective 4D lattice Dirac operator has optimal chiral symmetry for any N_s and gauge background.

(2) Quenched quark propagators for many quark masses can be computed efficiently (almost the same cost for any N_s) with Neuberger's double pass algorithm. Large scale computations (e.g., $20^3 \times 60$) are feasible even for PC clusters.

(3) Lattice QCD with dynamical quarks can be implemented similar to dynamical Wilson quarks.

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