OPTIMAL LATTICE DOMAIN-WALL FERMIONS WITH FINITE $N_s$*

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I review the lattice formulations of vector-like gauge theories (e.g. QCD) with domain-wall fermions, and discuss how to optimize the chiral symmetry for any finite $N_s$ (in the fifth dimension), as well as to eliminate its dependence on $a_5$.

1. Introduction

A viable approach to study strongly-coupled gauge theories (e.g. QCD) is to formulate these theories on a spacetime lattice with domain-wall fermions. The basic idea of domain-wall fermions (DWF) 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 vector-like theory. For lattice QCD with DWF 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 quark fields (in the massless limit) is broken. Obviously, the discretization in the fifth dimension also introduces the lattice spacing $a_5$ into the theory. Presumably, only in the limit $N_s \to \infty$ and $a_5 \to 0$, the correct effective 4D theory with exact chiral symmetry can be recovered. Now the relevant question is how to minimize its dependence on $N_s$ and $a_5$. Since, in general,

*Invited talk given at 2002 International Workshop on Strong Coupling Gauge Theories and Effective Field Theories (SCGT02), Nagoya, Japan, 10-13 Dec 2002.
†Work partially supported by grants NSC91-2112-M002-025 and NSC-40004F of the National Science Council, ROC.
they are independent parameters, it may happen that even in the limit $N_s \to \infty$, the massless quark propagator is exactly chirally symmetric but still has a strong dependence on $a_5(\neq 0)$. If this is the case, then the limit ($a_5 \to 0$) has to be taken before one can measure physical observables at any finite lattice spacing $a$, which of course, is difficult for any practical computations.

It turns out that the conventional DWF action with open boundary conditions\footnote{1} suffers from: (i) The chiral symmetry of the quark propagator is not optimal for any finite $N_s$; (ii) The quark determinant and propagator are sensitive to the lattice spacing $a_5$, even for very large $N_s$.

In this talk, I present a formulation\footnote{5} of lattice QCD with DWF, in which the quark propagator is $a_5$-invariant and has optimal chiral symmetry for any $N_s$ and background gauge field.

2. Problems of the conventional domain-wall fermions

First, we outline the basic features of DWF on the lattice. In general, given DWF action $A_f[\bar{\psi}, \psi]$ with fermion fields $\{\psi(x, s), \bar{\psi}(x, s); s = 1, \cdots, N_s\}$, one can construct the quark fields $q(x), \bar{q}(x)$ from the boundary modes, and obtain the quark propagator in a background gauge field as

\[
\langle q(x)\bar{q}(y) \rangle = \frac{\int [d\bar{\psi}] [d\psi] q(x)\bar{q}(y) e^{-A_f}}{\int [d\bar{\psi}] [d\psi] e^{-A_f}} = (D_c + m_q)^{-1}_{x,y}
\]

where $m_q$ is the bare quark mass,

\[
D_c = \frac{1 + \gamma_5 S}{1 - \gamma_5 S}, \quad S = \prod_{s=1}^{N_s} \frac{(1 + a_5 H_s) - \prod_{s=1}^{N_s} (1 - a_5 H_s)}{1 + a_5 H_s + \prod_{s=1}^{N_s} (1 - a_5 H_s)},
\]

and $\{H_s, s = 1, \cdots, N_s\}$ are Hermitian operators which depend on $A_f$.

For the conventional DWF, $H_s$ is the same for all $s$, and is equal to

\[
H = H_w(2 + \gamma_5 a_5 H_w)^{-1}, \quad H_w = \gamma_5 D_w,
\]

where $D_w$ is the standard Wilson-Dirac operator plus a negative parameter $-m_0$ ($0 \leq m_0 \leq 2$). In the limit $N_s \to \infty$, $S$ becomes $\text{sgn}(H)$,

\[
\lim_{N_s \to \infty} S = \frac{a_5 H}{\sqrt{a_5^2 H^2}^2} = \frac{H}{\sqrt{H^2}},
\]

and the quark propagator possesses exact chiral symmetry

\[
\lim_{N_s \to \infty, m_q \to 0} \left[(D_c + m_q)^{-1} \gamma_5 + \gamma_5 (D_c + m_q)^{-1}\right] = 0.
\]

\footnote{Here the color and Dirac indices are suppressed.}
However, for the conventional DWF, the quark propagator still depends on \( a_5 \) through \( H \). It turns out that the effects of \( a_5 \) cannot be neglected even for very large \( N_s \). This is the essential difficulty encountered in lattice QCD calculations with the conventional DWF. So the relevant problem for lattice QCD with DWF is how to construct a DWF action such that its \( S \) operator is independent of \( a_5 \), for any \( N_s \), and gauge background.

Another difficulty of the conventional DWF is that it does not preserve the chiral symmetry optimally for any finite \( N_s \). In other words, its \( S \) operator

\[
S(a_5 H) = \frac{(1 + a_5 H)^{N_s} - (1 - a_5 H)^{N_s}}{(1 + a_5 H)^{N_s} + (1 - a_5 H)^{N_s}} = a_5 HR(a_5^2 H^2)
\] (6)

is not the optimal rational approximation of \( \text{sgn}(H) \). The deviation of \( S(a_5 H) \) from \( \text{sgn}(H) \) can be measured in terms of

\[
\sigma(S) = \max_{\{\eta\}} \frac{Y^{-1}(\text{sgn}(H) - S(a_5 H)Y) \leq \max_{\{\eta\}} |\text{sgn}(\eta) - S(\eta)| ,
\]

where \( \{\eta\} \) are eigenvalues of \( a_5 H \). Using the simple identity

\[
|\text{sgn}(x) - S(x)| = |1 - \sqrt{x^2 R(x^2)}| , \quad S(x) = xR(x^2)
\] (8)

which holds for any \( x \neq 0 \) and \( S(x) = xR(x^2) \), we can rewrite as

\[
\sigma(S) \leq \max_{\{\eta^2\}} \left| 1 - \sqrt{\eta^2 R(\eta^2)} \right|
\] (9)

where \( \{\eta^2\} \) are eigenvalues of \( a_5^2 H^2 \). For the conventional DWF, the r.h.s. of (9) is not the minimum for any given \( N_s \), i.e., \( R(x^2) \) is not the optimal rational approximation of \((x^2)^{-1/2}\). Obviously, the problem of finding the optimal rational approximation \( S_{opt}(x) = xR_{opt}(x^2) \) of \( \text{sgn}(x) \) with \( x \in [x_{\text{min}}, x_{\text{max}}] \) is equivalent to finding the optimal rational approximation \( R_{opt}(x^2) \) of \((x^2)^{-1/2}\) with \( x^2 \in [x_{\text{min}}^2, x_{\text{max}}^2] \).

According to de la Vallée-Poussin’s theorem and Chebycheff’s theorem, the necessary and sufficient condition for an irreducible rational polynomial

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

to be the optimal rational polynomial of the inverse square root function \((x^{-1/2})\), \( 0 < x_{\text{min}} \leq x \leq x_{\text{max}} \) is that \( \delta(x) = 1 - \sqrt{x} r^{(n,m)}(x) \) has \( n + m + 2 \) alternate change of sign in the interval \([x_{\text{min}}, x_{\text{max}}]\), and attains its maxima and minima (all with equal magnitude), say,

\[
\delta(x) = -\Delta, +\Delta, \cdots, (-1)^{n+m+2} \Delta
\]
at consecutive points \((x_i, i = 1, \cdots, n + m + 2)\)

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

In other words, if \(r^{(n,m)}\) satisfies the above condition, then its error

\[
\sigma(r^{(n,m)}) = \max_{x \in [x_{\text{min}}, x_{\text{max}}]} \left| 1 - \sqrt{x} r^{(n,m)}(x) \right|
\]

is the minimum among all irreducible rational polynomials of degree \((n, m)\).

It is easy to show \(^5\) that \(R(x^2)\) \(^6\) of the conventional DWF is not the optimal rational approximation for \((x^2)^{-1/2}\). The optimal rational approximation for the inverse square root function was first obtained by Zolotarev\(^8\) in 1877, using Jacobian elliptic functions. A detailed discussion of Zolotarev’s result can be found in Akhiezer’s two books \(^7\).

Thus the relevant problem for lattice QCD with DWF is to construct a DWF action such that the operator \(S\) in the quark propagator (1) is equal to

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

(10)

where \(R_Z(H_w^2)\) is the Zolotarev optimal rational polynomial \(^8\) \(^9\) \(^10\)

\[
R_Z^{(n,n)}(H_w^2) = \frac{d_0}{\lambda_{\text{min}}} \prod_{l=1}^{n} \frac{1 + h_w^2/c_{2l}}{1 + h_w^2/c_{2l-1}}, \quad h_w^2 = H_w^2/\lambda_{\text{min}}^2
\]

(11)

and

\[
R_Z^{(n-1,n)}(H_w^2) = \frac{d'_0}{\lambda_{\text{min}}} \frac{\prod_{l=1}^{n-1} (1 + h_w^2/c'_{2l})}{\prod_{l=1}^{n-2} (1 + h_w^2/c'_{2l-1})},
\]

(12)

and the coefficients \(d_0, d'_0, c_l\) and \(c'_l\) are expressed in terms of elliptic functions \(^4\) with arguments depending only on \(N_s\) and \(b = \lambda_{\text{max}}^2/\lambda_{\text{min}}^2\) \((\lambda_{\text{min}}\) and \(\lambda_{\text{max}}\) are the minimum and the maximum of the eigenvalues of \(|H_w|\)).

3. The optimal domain-wall fermions

Recently, I have constructed a new lattice DWF action \(^5\) \(^6\), \(^9\) \(^11\) such that the quark propagator is \(a_5\)-invariant and preserves the chiral symmetry optimally for any \(N_s\) and background gauge field. Further, its effective 4D lattice Dirac operator for the internal fermion loops is shown to be exponentially-local for sufficiently smooth gauge backgrounds \(^9\).
Explicitly, the optimal lattice domain-wall fermion action reads
\[ A_f = \sum_{s,s'=0}^{N_s+1} \sum_{x,x'} \bar{\psi}(x,s) \{ (\omega_s a_5 D_w(x,x') + \delta_{x,x'}) \delta_{s,s'} \]
\[ - (\delta_{x,x'} - \omega_s a_5 D_w(x,x')) (P_- \delta_{s',s+1} + P_+ \delta_{s',s-1}) \} \psi(x',s') \] (13)
with boundary conditions
\[ P_+ \psi(x,-1) = -r m_q P_+ \psi(x,N_s+1), \quad r = \frac{1}{2m_0} \] (14)
\[ P_- \psi(x,N_s+2) = -r m_q P_- \psi(x,0), \] (15)
and the quark fields constructed from the left and right boundary modes
\[ q(x) = \sqrt{T} [P_- \psi(x,0) + P_+ \psi(x,N_s+1)] \] , (16)
\[ \bar{q}(x) = \sqrt{T} [\bar{\psi}(x,0) P_+ + \bar{\psi}(x,N_s+1) P_-] \] , (17)
where the weights \( \{ \omega_s \} \) are given by
\[ \omega_0 = \omega_{N_s+1} = 0 \]
\[ \omega_s a_5 = \frac{1}{\lambda_{\text{min}}} \sqrt{1 - \kappa'^2 \text{sn}^2 (v_s; \kappa')}, \quad s = 1, \cdots, N_s \] (18)
Here \( \text{sn}(v_s; \kappa') \) is the Jacobian elliptic function with argument \( v_s \) and modulus \( \kappa' = \sqrt{1 - 1/b} \), where \( b = \lambda_{\text{max}}^2 / \lambda_{\text{min}}^2 \).

For the optimal DWF, \( H_s = \omega_s H_w \) in the operator \( S \) (2), and the weights in (19) are obtained from the roots \( u_s = (\omega_s a_5)^{-2}, s = 1, \cdots, N_s \) of the equation
\[ \delta_Z(u) = \begin{cases} 1 - \sqrt{uR_n^2(u)} = 0, & N_s = 2n + 1 \\ 1 - \sqrt{uR_{n-1}^2(u)} = 0, & N_s = 2n \end{cases} \]
such that \( S \) is equal to \( S_{\text{opt}} \) (10), the optimal rational approximation of \( \text{sgn}(H_w) \), and the quark propagator (11) has the optimal chiral symmetry for any \( N_s \) and \( b = \lambda_{\text{max}}^2 / \lambda_{\text{min}}^2 \).

The argument \( v_s \) in (19) is
\[ v_s = (-1)^{s-1} M \text{sn}^{-1} \left( \frac{1 + 3\lambda}{(1 + \lambda)^3}; \sqrt{1 - \lambda^2} \right) + \frac{s}{2} \frac{2K'}{N_s} \] (20)

\footnote{In this paper, we suppress the lattice spacing \( a \), as well as the Dirac and color indices, which can be restored easily.}
\begin{equation}
\lambda = \prod_{l=1}^{N_s} \Theta^2 \left( \frac{2lK'}{N_s}; \kappa' \right), \quad M = \prod_{l=1}^{N_s} \frac{\sn^2 \left( \frac{(2l-1)K'}{N_s}; \kappa' \right)}{\sn^2 \left( \frac{2lK'}{N_s}; \kappa' \right)},
\end{equation}

where $K'$ is the complete elliptic integral of the first kind with modulus $\kappa'$, and $\Theta$ is the elliptic theta function. From (19), it is clear that $\lambda_{\text{max}}^{-1} \leq \omega_a a_5 \leq \lambda_{\text{min}}^{-1}$, since $\sn^2(\cdot) \leq 1$.

Obviously, the optimal domain-wall fermion action (13) is invariant for any $a_5$, since its dependence on $a_5$ is only through the product $\omega_a a_5$ (19), which only depends on $N_s$, $\lambda_{\text{min}}$ and $\lambda_{\text{max}}^2/\lambda_{\text{min}}^2$. Therefore, $a_5$ is a redundant parameter in the optimal domain-wall fermion action (13).

The generating functional for $n$-point Green’s function of quark fields $q$ and $\bar{q}$ is defined as

\begin{equation}
Z[J, \bar{J}] = \frac{\int [dU][d\bar{\psi}][d\psi][d\phi][d\bar{\phi}] e^{-A_s - A_f - A_{\psi} + \sum_x \{\bar{J}(x)q(x) + \bar{q}(x)J(x)\}}}{\int [dU][d\bar{\psi}][d\psi][d\phi][d\bar{\phi}] e^{-A_s - A_f - A_{\psi}}},
\end{equation}

where $A_s$ is the gauge field action, $A_f$ is the domain-wall fermion action, $A_{\psi}$ is the corresponding pseudofermion action with $m_q = 2m_0$, and $\bar{J}$ and $J$ are the Grassman sources of $q$ and $\bar{q}$ respectively. The purpose of introducing the pseudofermion fields (which carry all attributes of the fermion fields but obey the Bose statistics) is to provide the denominator $(1 + rD_c)^{-1}$ in the effective 4D lattice Dirac operator

\begin{equation}
D(m_q) = (D_c + m_q)(1 + rD_c)^{-1}, \quad D_c = 2m_0 \left( \frac{1 + \gamma_5 S_{\text{opt}}}{1 - \gamma_5 S_{\text{opt}}} \right)
\end{equation}

for internal fermion loops such that $D(m_q)$ is exponentially-local (21) (for any $N_s$ and $m_q$), and its fermion determinant ratio (in the limit $N_s \to \infty$ and $a \to 0$) is equal to the corresponding ratio of $\det[\gamma_{\mu}(\partial_{\mu} + iA_{\mu}) + m_q]$.

Evaluating the integrations over $\{\psi, \bar{\psi}\}$ and $\{\phi, \bar{\phi}\}$ in (22), one obtains

\begin{equation}
Z[J, \bar{J}] = \frac{\int [dU]e^{-A_s[U]}\det[D(m_q)]e^{\bar{J}(D_c + m_q)^{-1}J}}{\int [dU]e^{-A_s[U]}\det[D(m_q)]}.
\end{equation}

Then any $n$-point Green’s function can be obtained by differentiating $Z[J, \bar{J}]$ with respect to $J$ and $\bar{J}$ successively. In particular, the quark propagator is

\begin{equation}
\langle q(x)\bar{q}(y) \rangle = \frac{\delta^2 Z[J, \bar{J}]}{\delta J(x)\delta J(y)} \bigg|_{J=\bar{J}=0} = \frac{\int [dU]e^{-A_s[U]}\det[D(m_q)](D_c + m_q)^{-1}_{x,y}}{\int [dU]e^{-A_s[U]}\det[D(m_q)]}.
\end{equation}
which, in a background gauge field, becomes
\[ \langle q(x)\bar{q}(y) \rangle = (D_c + m_q)^{-1}_{x,y}, \]
and it goes to \[ [\gamma^\mu(\partial^\mu + iA^\mu) + m_q]^{-1} \] in the limit \( N_s \to \infty \) and \( a \to 0 \).

For any gauge background and \( N_s \), \( D_c \) has the optimal chiral symmetry since the error \( \sigma(S_{opt}) \) is the minimum, and \( \sigma(S_{opt}) \leq (1 - \lambda)/(1 + \lambda) \approx A(b)e^{-c(b)\lambda} \), where \( \lambda \) is defined in (21), \( A(b) \) and \( c(b) \) can be estimated as \( A(b) \approx 4.06(1)b^{-0.0091(1)}\ln(b)^{0.0042(3)} \), \( c(b) \approx 4.27(45)\ln(b)^{-0.746(5)} \), \( b = \lambda^{2}_{max}/\lambda^{2}_{min} \).

Finally, we note that \( D(0) (N_s \to \infty) \) times a factor \( r = 1/2m_0 \) is exactly equal to the overlap Dirac operator, \( D_o = [1 + (H^2_{w})^{-1/2}] / 2 \). 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 \( N_s \), \( r \) times \( D(0) \) is exactly equal to the overlap Dirac operator with \( (H^2_{w})^{-1/2} \) approximated by Zolotarev optimal rational polynomial, \( (N_s = \text{odd}) \), or \( (N_s = \text{even}) \). Further discussions can be found in Ref. [6].

Acknowledgments
I am grateful to Koichi Yamawaki and Yoshio Kikukawa for inviting me to this interesting workshop and to all organizers of SCGT02 for their kind hospitality.

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