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This work is dedicated to the late Professor
 James S. Ball

ABSTRACT

We present the domain-wall fermion operator which is reflection symmetric in the fifth dimension, with the approximate sign function $S(H)$ of the effective 4-dimensional Dirac operator satisfying the bound $|1 - S(\lambda)| \leq 2d_Z$ for $\lambda^2 \in [\lambda_{min}^2, \lambda_{max}^2]$, where d_Z is the maximum deviation $|1 - \sqrt{x}R_Z(x)|_{max}$ of the Zolotarev optimal rational polynomial $R_Z(x)$ of $1/\sqrt{x}$ for $x \in [1, \lambda_{max}^2/\lambda_{min}^2]$, with degrees $(n-1, n)$ for $N_s = 2n$, and (n, n) for $N_s = 2n + 1$.

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1. Introduction

In lattice QCD with exact chiral symmetry [1–3], the overlap Dirac operator with bare quark mass m_q in general can be written as

$$D(m_q) = m_q + \frac{(1 - rm_q)}{2r} \left[1 + \gamma_5 \frac{H}{\sqrt{H^2}} \right],$$

$$r = 1/[2m_0(1 - dm_0)], \quad m_0 \in (0, 2), \quad (1)$$

where $H = cH_w(1 + d\gamma_5 H_w)^{-1}$, and c and d are constants. Here $H_w = \gamma_5 D_w$, and D_w is the standard Wilson-Dirac operator minus the parameter $m_0 \in (0, 2)$.

The eigenmodes of (1) consist of complex conjugate pairs, and (for topologically non-trivial gauge field) real eigenmodes with definite chiralities at m_q and $1/r$ satisfying the chirality sum rule [4], $n_+ - n_- + N_+ - N_- = 0$, where n_{\pm} (N_{\pm}) denote the number of eigenmodes at m_q ($1/r$) with \pm chirality. Empirically, the real eigenmodes always satisfy either $(n_- = N_+ = 0, n_+ = N_-)$ or $(n_+ = N_- = 0, n_- = N_+)$. Thus, we have

$$\det D(m_q) = \begin{cases} (rm_q)^{n_+} \det \mathcal{H}_-^2 = (rm_q)^{-n_+} \det \mathcal{H}_+^2, & n_+ \geq 0, \\ (rm_q)^{n_-} \det \mathcal{H}_+^2 = (rm_q)^{-n_-} \det \mathcal{H}_-^2, & n_- \geq 0, \end{cases}$$

where $\mathcal{H}_{\pm}^2 = P_{\pm}(D^{\dagger}D)$, and $P_{\pm} = (1 \pm \gamma_5)/2$. It follows that the pseudofermion action for any number of flavors of overlap fermion can be expressed in terms of n_{\pm} and \mathcal{H}_{\pm}^2 (Hermitian and positive-definite), thus it is amenable to the hybrid Monte Carlo simulation

(HMC) [5]. However, this approach requires the computation of the change of n_{\pm} at each step of the molecular dynamics in HMC, which is prohibitively expensive for large lattices [6,7]. Moreover, the discontinuity of the fermion determinant at the topological boundary highly suppresses the crossing rate between different topological sectors, and thus renders HMC failing to sample all topological sectors ergodically.

These difficulties can be circumvented by using domain-wall fermion (DWF) with finite N_s in the fifth dimension. Then HMC of lattice QCD with DWF on the 5-dimensional lattice can sample all topological sectors ergodically and also keep the chiral symmetry at a good precision. This has been demonstrated for 2-flavor QCD [8,9], and (1+1)-flavor QCD [10]. For DWF with finite N_s , it is vital to preserve the chiral symmetry maximally, or equivalently, the approximate sign function $S(H)$ of the effective 4-dimensional Dirac operator satisfies the bound, $|1 - S(\lambda)| \leq d_Z$ for $\lambda^2 \in [\lambda_{min}^2, \lambda_{max}^2]$, where d_Z is the maximum deviation $|1 - \sqrt{x}R_Z(x)|_{max}$ of the Zolotarev optimal rational approximation $R_Z(x)$ of $1/\sqrt{x}$ for $x \in [1, \lambda_{max}^2/\lambda_{min}^2]$, with degrees (n, n) for $N_s = 2n + 1$, and $(n-1, n)$ for $N_s = 2n$. This can be attained by assigning a weight to each layer (along the fifth dimension) of the DWF, according to the formula [11]

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

where $\text{sn}(v_s; \kappa')$ is the Jacobian elliptic function with argument v_s (see Eq. (13) of Ref. [11]) and modulus $\kappa' = \sqrt{1 - 1/b}$, $b = \lambda_{max}^2/\lambda_{min}^2$. Here λ_{max}^2 and λ_{min}^2 are the upper bound and lower bound for the eigenvalues of H^2 . It should be emphasized that λ_{min} and λ_{max} have to be fixed properly for each set of simulations, depending on the parameters $\beta = 6/g^2$, quark masses, and

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lattice size, such that the desired precision of chiral symmetry can be attained with the minimal cost of the simulation.

Nevertheless, (2) breaks the R_5 (reflection) symmetry in the fifth dimension, which is essential for obtaining the exact pseudofermion action for hybrid Monte Carlo simulation of one-flavor DWF [10], as well as other applications. In this paper, we obtain the weights satisfying the R_5 symmetry ($\omega_s = \omega_{N_s-s+1}$, $s = 1, \dots, N_s$) such that the approximate sign function $S(H)$ of the effective 4-dimensional Dirac operator satisfies the bound, $|1 - S(\lambda)| \leq 2d_Z$, which is twice of that of the optimal DWF without R_5 symmetry [11]. In other words, if one imposes the R_5 symmetry, this is the optimal chiral symmetry one can have.

2. Optimal domain-wall fermion

In general, the 5-dimensional lattice operator of DWF can be written as [12]

$$[\mathcal{D}(m)]_{xx';ss'} = (\rho_s D_w + 1)_{xx'} \delta_{ss'} + (\sigma_s D_w - 1)_{xx'} L_{ss'}, \quad (3)$$

where $\rho_s = c\omega_s + d$, $\sigma_s = c\omega_s - d$, and c, d are constants. The indices x and x' denote the sites on the 4-dimensional space-time lattice, and s and s' the indices in the fifth dimension, while the lattice spacing a and the Dirac and color indices have been suppressed. The operator L is independent of the gauge field, and it can be written as

$$L = P_+ L_+ + P_- L_-, \quad P_{\pm} = (1 \pm \gamma_5)/2,$$

and

$$(L_+)_{ss'} = (L_-)_{s's} = \begin{cases} -m\delta_{N_s, s'}, & s = 1, \\ \delta_{s-1, s'}, & 1 < s \leq N_s, \end{cases}$$

where N_s is the number of sites in the fifth dimension, $m \equiv rm_q$, m_q is the bare quark mass, and $r = 1/[2m_0(1 - dm_0)]$. Including the action of the Pauli-Villars fields (with bare mass $m_{PV} = 1/r$), the partition function of DWF in a gauge background can be integrated successively to obtain the fermion determinant of the effective 4-dimensional Dirac operator,

$$Z = \int [d\Psi][d\bar{\Psi}][d\Phi][d\Phi^\dagger] \exp \left\{ -\bar{\Psi} \mathcal{D}(m) \Psi - \Phi^\dagger \mathcal{D}(1) \Phi \right\} \\ = \det D(m_q),$$

where

$$D(m_q) = (D_c + m_q)(1 + rD_c)^{-1} \\ = m_q + \frac{(1 - rm_q)}{2r} [1 + \gamma_5 S(H)], \quad (4) \\ D_c = \frac{1}{r} \frac{1 + \gamma_5 S(H)}{1 - \gamma_5 S(H)}, \\ S(H) = \frac{1 - \prod_{s=1}^{N_s} T_s}{1 + \prod_{s=1}^{N_s} T_s}, \quad T_s = \frac{1 - \omega_s H}{1 + \omega_s H}, \\ H = cH_w(1 + d\gamma_5 H_w)^{-1}, \quad H_w = \gamma_5 D_w. \quad (5)$$

For the optimal DWF without R_5 symmetry [11], the weights $\{\omega_s\}$ are fixed according to the formula (2), then $S(H)$ is equal to the Zolotarev optimal rational approximation of the sign function of H , i.e., $S(H) = HR_Z(H^2)$, satisfying the bound, $|1 - S(\lambda)| \leq d_Z$ for $\lambda^2 \in [\lambda_{\min}^2, \lambda_{\max}^2]$, where d_Z is the maximum deviation $|1 - \sqrt{x}R_Z(x)|_{\max}$ of the Zolotarev optimal rational approximation $R_Z(x)$ of $1/\sqrt{x}$ for $x \in [1, \lambda_{\max}^2/\lambda_{\min}^2]$, with degrees (n, n) for $N_s = 2n + 1$, and $(n - 1, n)$ for $N_s = 2n$. However, it breaks the R_5 symmetry, i.e., $R_5 \mathcal{D}(0) R_5 \neq \mathcal{D}(0)$, where $(R_5)_{s, s'} = \delta_{s', N_s+1-s}$. In the following, we construct the optimal DWF satisfying the R_5 symmetry.

3. Optimal domain-wall fermion with R_5 symmetry

First we recall the basic features of the optimal rational approximation of the ratio of two positive and continuous functions $f(x)/g(x)$ for $x \in [1, b]$. Let $R^{(m, n)}(x)$ denote an irreducible rational polynomial of the form

$$R^{(m, n)}(x) = \frac{p_m x^m + p_{m-1} x^{m-1} + \dots + p_0}{q_n x^n + q_{n-1} x^{n-1} + \dots + q_0} \quad (n \geq m, p_i, q_i > 0).$$

According to de la Vallée-Poussin's theorem and Chebycheff's theorem, the necessary and sufficient condition for $R^{(m, n)}(x)$ to be the optimal rational approximation of $f(x)/g(x)$ for $x \in [1, b]$ is that $\delta(x) \equiv f(x) - g(x)R^{(m, n)}(x)$ has $(m + n + 2)$ alternate changes of sign in the interval $[1, b]$, and attains its maxima and minima (all with equal magnitude), say,

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

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

$$1 = x_1 < x_2 < \dots < x_{m+n+2} = b.$$

For $f(x)/g(x) = 1/\sqrt{x}$, Zolotarev obtained two optimal rational polynomials in 1877, $R_Z^{(n-1, n)}(x)$ and $R_Z^{(n, n)}(x)$ [13], in terms of the Jacobian elliptic functions. The basic formulas of Zolotarev optimal rational polynomial are collected in Appendix A. (See also Refs. [14, 15].)

For the optimal DWF without R_5 symmetry [11], the approximate sign function $S(H)$ of the effective 4-dimensional lattice Dirac operator is exactly equal to $HR_Z^{(n-1, n)}(H^2)$ for $N_s = 2n$, and $HR_Z^{(n, n)}(H^2)$ for $N_s = 2n + 1$.

In Fig. 1, we plot the deviation $\delta_Z^{(m, n)}(x) = 1 - \sqrt{x}R_Z^{(m, n)}(x)$ of the Zolotarev optimal rational polynomials $R_Z^{(7, 8)}(x)$ and $R_Z^{(8, 8)}(x)$ for $x \in [1, b]$, $b = \lambda_{\max}^2/\lambda_{\min}^2 = (6.20/0.05)^2 = 15376$. In both cases, $\delta(x)$ has $(m + n + 2)$ alternate changes of sign in the interval $[1, b]$, with $(m + 1)$ minima and $(n + 1)$ maxima, all of the same magnitude, thus satisfying the necessary and sufficient condition for the optimal rational approximation of $1/\sqrt{x}$ in the interval $[1, b]$, according to de la Vallée-Poussin's theorem and Chebycheff's theorem. Note that $d_Z \simeq 1.19447 \times 10^{-5}$ in the left figure (a), which is about 2.2 times of $d_Z \simeq 5.39351 \times 10^{-6}$ in the right figure (b), i.e., $d_Z^{(n-1, n)} \simeq 2.2d_Z^{(n, n)}$, as pointed out in Ref. [15].

3.1. $N_s = 2n$ (even)

For the case $N_s = 2n$ (even), the requirement of R_5 symmetry implies that $\omega_s = \omega_{N_s+1-s}$, and

$$\delta(\lambda) = 1 - S(\lambda) = \frac{2 \prod_{s=1}^n (1 - \omega_s \lambda)^2}{\prod_{s=1}^n (1 - \omega_s \lambda)^2 + \prod_{s=1}^n (1 + \omega_s \lambda)^2} \geq 0, \quad (6)$$

unlike the $\delta_Z^{(n-1, n)}(x)$ (shown in Fig. 1(a)) which varies alternately between $+d_Z$ and $-d_Z$. Nevertheless, one can shift $\delta_Z(x)$ by a constant $+d_Z$, simply by changing the overall coefficient D_0 of $R_Z^{(n-1, n)}$ (18) to D'_0 ,

$$D'_0 = \frac{1}{\sqrt{\xi}} \frac{\prod_{l=1}^n (\xi + C_{2l-1})}{\prod_{l=1}^{n-1} (\xi + C_{2l})}, \quad \xi = \frac{1}{1 - \kappa'^2 \text{sn}^2 \left(\frac{\kappa'}{2n}; \kappa' \right)}. \quad (7)$$

Then the maximal deviation becomes $2d_Z$, which is twice of that of the Zolotarev optimal rational polynomial. Obviously, this is the optimal chiral symmetry one can have for DWF with R_5 symmetry. This can be attained by requiring $\delta(\lambda)$ to have $2n + 1$ alternative maxima and minima for $\lambda \in [\lambda_{\min}, \lambda_{\max}]$,

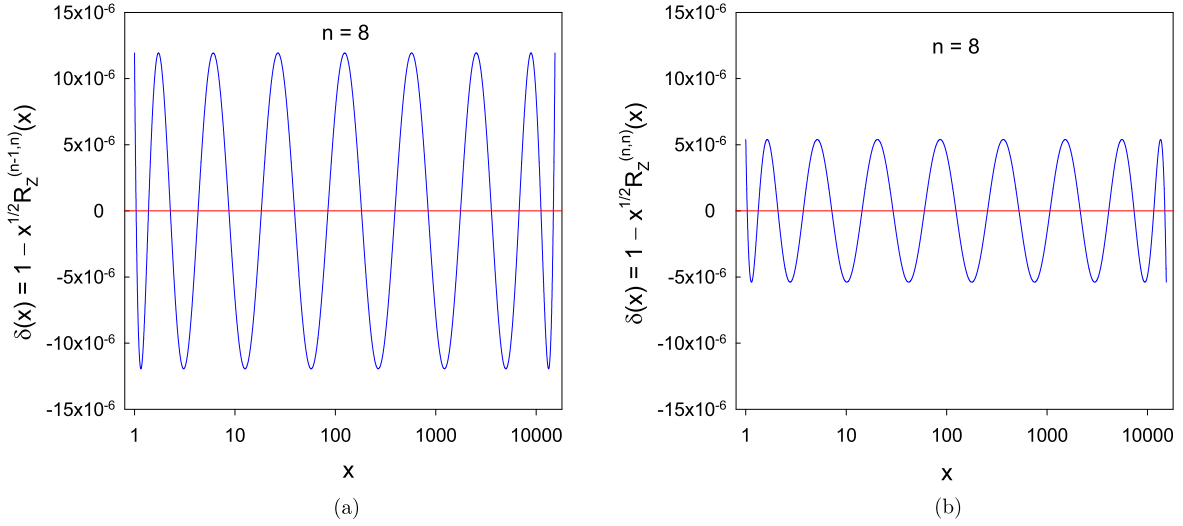


Fig. 1. The deviation $\delta(x) = 1 - \sqrt{x}R_Z^{(m,n)}(x)$ of the Zolotarev optimal rational polynomial $R_Z^{(m,n)}(x)$ for $x \in [1, b]$, $b = \lambda_{\max}^2/\lambda_{\min}^2 = (6.20/0.05)^2 = 15376$. In the left figure (a), $(m, n) = (n - 1, n) = (7, 8)$, while in the right figure (b), $(m, n) = (n, n) = (8, 8)$. In both cases, $\delta(x)$ has $(m + n + 2)$ alternate changes of sign in the interval $[1, b]$, with $(m + 1)$ minima and $(n + 1)$ maxima, all of the same magnitude, satisfying the necessary and sufficient condition of the optimal rational approximation of $1/\sqrt{x}$ for $x \in [1, b]$, according to de la Vallée-Poussin’s theorem and Chebycheff’s theorem.

$$\delta(\lambda) = 2d_Z, 0, \dots, 2d_Z, 0, 2d_Z, \quad d_Z = \frac{1 - \Lambda}{1 + \Lambda}, \quad (8)$$

at the consecutive points $(\lambda_{\min} = \lambda_1 < \lambda_2 < \dots < \lambda_{2n+1} = \lambda_{\max})$, where d_Z is the maximum deviation $|1 - \sqrt{x}R_Z^{(n-1,n)}(x)|_{\max}$ of the Zolotarev optimal rational polynomial $R_Z^{(n-1,n)}(x)$ for $1/\sqrt{x}$, $x \in [1, b]$. This immediately implies that the weights in (3) can be fixed by the positions of the minima of $\delta(x)$,

$$\omega_s = \omega_{N_s+1-s} = \frac{1}{\lambda_{\min}} \sqrt{1 - \kappa'^2 \operatorname{sn}^2\left(\frac{(2s-1)K'}{N_s}; \kappa'\right)}, \quad (9)$$

$$s = 1, \dots, N_s/2,$$

where $\operatorname{sn}(u; \kappa')$ is the Jacobian elliptic function with modulus $\kappa' = \sqrt{1 - 1/b}$, and K' is the complete elliptic function of the first kind with modulus κ' . Then the approximate sign function $S(H)$ of the effective 4-dimensional Dirac operator (4) becomes

$$S(H) = hD'_0 \frac{\prod_{l=1}^{n-1} (h^2 + C_{2l})}{\prod_{l=1}^n (h^2 + C_{2l-1})}, \quad h = \frac{H}{\lambda_{\min}}, \quad (10)$$

which is exactly the same as the Zolotarev optimal rational approximation of the sign function (see Eq. (18)) except replacing D_0 by D'_0 . Note that if we replace D_0 by D''_0 ,

$$D''_0 = \frac{\prod_{l=1}^n (1 + C_{2l-1})}{\prod_{l=1}^{n-1} (1 + C_{2l})}, \quad (11)$$

then $\delta(x)$ is shifted by a constant $-d_Z$, thus its maxima become 0, and minima $-2d_Z$. However, this cannot be realized by DWF with even N_s and R_5 symmetry, due to the constraint (6), $\delta(\lambda) \geq 0$.

In Fig. 2, we plot $1 - S(\lambda)$ of the optimal DWF with R_5 symmetry, for $N_s = 16$, $\lambda_{\max}/\lambda_{\min} = 6.20/0.05$, and the weights according to (9). We see that $1 - S(\lambda)$ has $2n + 1 = 17$ alternate maxima and minima in the interval $[\lambda_{\min}, \lambda_{\max}]$, with 8 minima and 9 maxima, and $|1 - S(\lambda)|_{\max} = 2d_Z$, where d_Z is the maximum deviation $|1 - \sqrt{x}R_Z^{(7,8)}(x)|_{\max}$ of the Zolotarev optimal rational polynomial, as shown in Fig. 1(a).

3.2. $N_s = 2n + 1$ (odd)

For the case $N_s = 2n + 1$, the requirement of R_5 symmetry implies that $\omega_s = \omega_{N_s+1-s}$, and

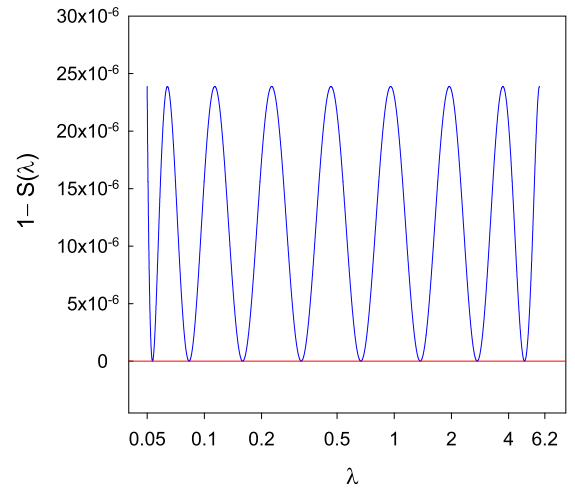


Fig. 2. The deviation $1 - S(\lambda)$ of the optimal DWF with R_5 symmetry, for $N_s = 16$, $\lambda_{\max}/\lambda_{\min} = 6.20/0.05$, where the weights are computed according to (9).

$$\delta(\lambda) = 1 - S(\lambda) = \frac{2(1 - \omega_{n+1}\lambda) \prod_{s=1}^n (1 - \omega_s \lambda)^2}{(1 - \omega_{n+1}\lambda) \prod_{s=1}^n (1 - \omega_s \lambda)^2 + (1 + \omega_{n+1}\lambda) \prod_{s=1}^n (1 + \omega_s \lambda)^2},$$

which can be positive, zero, or negative. Thus, we have two options to attain the optimal chiral symmetry with R_5 symmetry, i.e., to shift $\delta(\lambda)$ by a constant $+d_Z$, or $-d_Z$.

The first option is to require $\delta(\lambda)$ to have $2n + 2$ alternative maxima and minima in the interval $[\lambda_{\min}, \lambda_{\max}]$,

$$\delta(\lambda) = 2d_Z, 0, \dots, 2d_Z, 0, \quad d_Z = \frac{1 - \sigma}{1 + \sigma},$$

at consecutive points $(\lambda_{\min} = \lambda_1 < \lambda_2 < \dots < \lambda_{2n+2} = \lambda_{\max})$, where d_Z is the maximum deviation $|1 - \sqrt{x}R_Z^{(n,n)}(x)|_{\max}$ of the Zolotarev optimal rational polynomial $R_Z^{(n,n)}(x)$ for $1/\sqrt{x}$ in the interval $[1, b]$. Thus the weights in (3) can be fixed by the positions of the minima of $\delta(x)$,

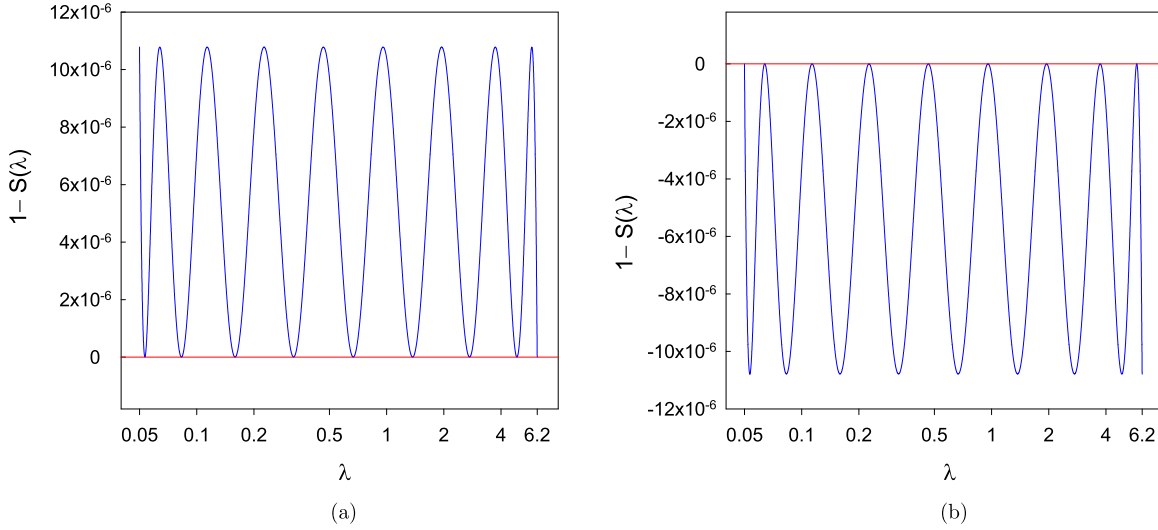


Fig. 3. The deviation $1 - S(\lambda)$ of the optimal DWF with R_5 symmetry, for $N_s = 17$, $\lambda_{\min} = 0.05$, and $\lambda_{\max} = 6.20$. In (a), the weights are computed according to (12), while in (b), according to (15).

$$\omega_s = \omega_{N_s+1-s} = \frac{1}{\lambda_{\min}} \sqrt{1 - \kappa'^2 \text{sn}^2 \left(\frac{(2s-1)K'}{N_s}; \kappa' \right)},$$

$$s = 1, \dots, (N_s + 1)/2. \quad (12)$$

Note that the smallest weight ω_{n+1} is chosen to be the unpaired one at the center of the fifth dimension, such that $\delta(\lambda)$ does not change sign for all $\lambda \in [\lambda_{\min}, \lambda_{\max}]$. Then the approximate sign function $S(H)$ of the effective 4-dimensional Dirac operator (4) becomes

$$S(H) = h d'_0 \frac{\prod_{l=1}^n (h^2 + c_{2l})}{\prod_{l=1}^n (h^2 + c_{2l-1})}, \quad h = \frac{H}{\lambda_{\min}}, \quad (13)$$

which is exactly the same as the Zolotarev optimal rational approximation of the sign function (see Eq. (19)) except for the overall coefficient d'_0 ,

$$d'_0 = \frac{1}{\sqrt{\xi}} \prod_{l=1}^n \frac{(\xi + c_{2l-1})}{(\xi + c_{2l})}, \quad \xi = \frac{1}{1 - \kappa'^2 \text{sn}^2 \left(\frac{K'}{2n+1}; \kappa' \right)}. \quad (14)$$

The second option is to require $\delta(\lambda)$ to have $2n + 2$ alternative maxima and minima in the interval $[\lambda_{\min}, \lambda_{\max}]$,

$$\delta(\lambda) = 0, -2d_z, \dots, 0, -2d_z, \quad d_z = \frac{1 - \sigma}{1 + \sigma},$$

at consecutive points ($\lambda_{\min} = \lambda_1 < \lambda_2 < \dots < \lambda_{2n+2} = \lambda_{\max}$). This immediately implies that the weights in (3) can be fixed by the positions of the maxima of $\delta(x)$,

$$\omega_s = \omega_{N_s+1-s} = \frac{1}{\lambda_{\min}} \sqrt{1 - \kappa'^2 \text{sn}^2 \left(\frac{(N_s + 3 - 2s)K'}{2N_s}; \kappa' \right)},$$

$$s = 1, \dots, (N_s + 1)/2. \quad (15)$$

Note that the largest weight ω_{n+1} is chosen to be the unpaired one at the center of the fifth dimension, such that $\delta(\lambda)$ does not change sign for all $\lambda \in [\lambda_{\min}, \lambda_{\max}]$. Then the approximate sign function $S(H)$ of the effective 4-dimensional Dirac operator (4) becomes

$$S(H) = h d''_0 \prod_{l=1}^n \frac{(h^2 + c_{2l})}{(h^2 + c_{2l-1})}, \quad h = \frac{H}{\lambda_{\min}}, \quad (16)$$

which is exactly the same as the Zolotarev optimal rational approximation of the sign function (see Eq. (19)) except for the overall coefficient d''_0 ,

$$d''_0 = \prod_{l=1}^n \frac{(1 + c_{2l-1})}{(1 + c_{2l})}. \quad (17)$$

In Fig. 3, we plot $1 - S(\lambda)$ of the optimal DWF with R_5 symmetry, for $N_s = 17$, and $\lambda_{\max}/\lambda_{\min} = 6.20/0.05$. In Fig. 3(a), the weights are computed according to (12), while in Fig. 3(b), according to (15). In both cases, $1 - S(\lambda)$ has $2n + 2 = 18$ alternate maxima and minima in the interval $[\lambda_{\min}, \lambda_{\max}]$, with 9 minima and 9 maxima. The maximum deviation $|1 - S(\lambda)|_{\max} = 2d_z$, where d_z is the maximum deviation $|1 - \sqrt{x}R_Z^{(8,8)}|_{\max}$ of the Zolotarev optimal rational polynomial, as shown in Fig. 1(b).

4. Numerical test

Theoretically, the sign function error $|1 - S(H)|$ of the optimal DWF with R_5 symmetry is twice of that without R_5 symmetry. Nevertheless, it is interesting to check their difference in large-scale simulations of lattice QCD, by computing the residual mass [12]

$$m_{\text{res}} = \frac{1}{4r} \frac{\langle \text{tr} \{ [D^{-1}(m_q)]^\dagger (1 - S^2) D^{-1}(m_q) \}_{0,0} \rangle_U}{\langle \text{tr} \{ [(D_c + m_q)^{-1}]^\dagger (D_c + m_q)^{-1} \}_{0,0} \rangle_U}$$

$$= \frac{\langle \text{tr} (D_c + m_q)^{-1} \rangle_U}{\langle \text{tr} [\gamma_5 (D_c + m_q) \gamma_5 (D_c + m_q)^{-1}] \rangle_U} - m_q,$$

where $(D_c + m_q)^{-1}$ denotes the valence quark propagator, tr denotes the trace running over the color and Dirac indices, and the brackets $\langle \dots \rangle_U$ denote averaging over an ensemble of gauge configurations.

To generate the gauge ensemble, we perform the hybrid Monte Carlo simulation of $(2 + 1)$ -flavor QCD on the $24^3 \times 48$ lattice with the Wilson gauge action at $\beta = 6/g^2 = 6.10$ (lattice spacing $a \sim 0.06$ fm), for the sea-quark masses $m_u a = m_d a = 0.005$ and $m_s a = 0.04$, with pion mass ~ 260 MeV. For the quark part, we use optimal DWF with R_5 symmetry for u , d and s quarks, with $c = 1$, $d = 0$ (i.e., $H = H_w$), $N_s = 16$, and $\lambda_{\max}/\lambda_{\min} = 6.20/0.05$. The weights are computed according to the formula (9). The strange

quark is simulated with the exact pseudofermion action for one-flavor DWF [10], and the up and down quarks are simulated with the 2-flavor algorithm as outlined in [9]. We generate the initial 400 trajectories with 2 Nvidia GTX-TITAN GPUs working together. After discarding the initial 240 trajectories for thermalization, we sample one configuration every 5 trajectories, resulting 32 “seed” configurations. Then we use these 32 seed configurations as the initial configurations for 32 independent simulations on 32 Nvidia GTX-TITAN GPUs. Each GPU generates 100–110 trajectories, and we accumulate a total of 3300 trajectories. From the saturation of the binning error of the plaquette, as well as the evolution of the topological charge, we estimate the autocorrelation time to be around 10 trajectories. Thus we sample one configuration every 10 trajectories, and obtain 330 configurations for this ensemble.

Then we compute two sets of quark propagators with point source at the origin and $m_q a = 0.005$, one set with the $\{\omega_s\}$ exactly the same as the sea-quarks (with R_5 symmetry), and the other set with the $\{\omega_s\}$ (2) without R_5 symmetry. The residual mass of the set with R_5 symmetry is $(m_{res} a)^{R_5} = 0.00024(1)$, while that of the set without R_5 symmetry is $m_{res} a = 0.00014(1)$. Thus the ratio $(m_{res})^{R_5} / m_{res} \simeq 1.71(14)$, consistent with the theoretical expectation.

5. Concluding remarks

With the weights (9), (12) and (15) for optimal DWF with R_5 symmetry, together with those (2) for optimal DWF without R_5 symmetry [11], this completes the study of DWF with the approximate sign function $S(H)$ in the effective 4-dimensional lattice Dirac operator satisfying $|1 - S(\lambda)| \leq 2d_Z$ (with R_5 symmetry) or $|1 - S(\lambda)| \leq d_Z$ (without R_5 symmetry) for $\lambda^2 \in [\lambda_{min}^2, \lambda_{max}^2]$, where d_Z is the maximum deviation $|1 - \sqrt{x}R_Z(x)|_{max}$ of the Zolotarev optimal rational polynomial $R_Z(x)$ of $1/\sqrt{x}$ for $x \in [1, \lambda_{max}^2/\lambda_{min}^2]$, with degrees $(n-1, n)$ for $N_s = 2n$, and (n, n) for $N_s = 2n+1$.

The correspondence between the approximate sign function $S(H)$ of the optimal DWF and the Zolotarev optimal rational polynomial gives the optimal rational approximation a more general viewpoint. In general, the deviation $\delta(x) = 1 - \sqrt{x}R_Z(x)$ can be shifted by a constant ϵ , simply by adjusting the overall coefficient D_0 in (18) or d_0 in (19). In particular, for $R_Z^{(n-1, n)}$, if D_0 is replaced by D'_0 (7), then $\epsilon = +d_Z$, $\delta_{max} = 2d_Z$ and $\delta_{min} = 0$; while by D''_0 (11), $\epsilon = -d_Z$, $\delta_{max} = 0$ and $\delta_{min} = -2d_Z$. Similarly, for $R_Z^{(n, n)}$, if d_0 is replaced by d'_0 (14), $\epsilon = +d_Z$, $\delta_{max} = 2d_Z$ and $\delta_{min} = 0$; while by d''_0 (14), $\epsilon = -d_Z$, $\delta_{max} = 0$ and $\delta_{min} = -2d_Z$. Even though this does not satisfy the criterion that the maxima and the minima of $\delta(x)$ all have the same magnitude and $\delta_{min} = -\delta_{max}$, the most salient features of the optimal rational approximation are preserved, namely, the number of alternate maxima and minima is $(m+n+2)$, with $(n+1)$ maxima and $(m+1)$ minima, as well as all maxima (minima) are equal. We can regard this as the generalized optimal rational approximation (with a constant shift ϵ). For $\epsilon > 0$, this can be realized by DWF with/without R_5 symmetry. However, for $\epsilon < 0$, it cannot be realized by DWF with R_5 symmetry and $N_s = 2n$ (even), due to the constraint (6), $\delta(\lambda) \geq 0$.

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Appendix A

In this appendix, we collect the basic formulas of the Zolotarev optimal rational polynomials $R_Z^{(n-1, n)}(x)$ and $R_Z^{(n, n)}(x)$ for the inverse square root function $1/\sqrt{x}$, $x \in [1, b]$.

$$R_Z^{(n-1, n)}(x) = D_0 \frac{\prod_{l=1}^{n-1} (x + C_{2l})}{\prod_{l=1}^n (x + C_{2l-1})} = \sum_{l=1}^n \frac{B_l}{x + C_{2l-1}}, \quad (18)$$

$$R_Z^{(n, n)}(x) = d_0 \prod_{l=1}^n \frac{x + C_{2l}}{x + C_{2l-1}} = (x + c_{2n}) \sum_{l=1}^n \frac{b_l}{x + C_{2l-1}}, \quad (19)$$

where

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

$$B_l = D_0 \frac{\prod_{i=1}^{n-1} (C_{2i} - C_{2l-1})}{\prod_{i=1, i \neq l}^n (C_{2i-1} - C_{2l-1})},$$

$$b_l = d_0 \frac{\prod_{i=1}^{n-1} (c_{2i} - c_{2l-1})}{\prod_{i=1, i \neq l}^n (c_{2i-1} - c_{2l-1})},$$

$$D_0 = \frac{2\Lambda}{1 + \Lambda} \frac{\prod_{l=1}^n (1 + C_{2l-1})}{\prod_{l=1}^{n-1} (1 + C_{2l})}, \quad d_0 = \frac{2\sigma}{1 + \sigma} \prod_{l=1}^n \frac{1 + c_{2l-1}}{1 + c_{2l}},$$

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

Here $\text{sn}(u; \kappa') = \eta$ is the Jacobian elliptic function with modulus $\kappa' = \sqrt{1 - 1/b}$, as defined by the integral

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

$K' = u(1)$ is the complete elliptic function of the first kind with modulus κ' , and Θ is the elliptic theta function.

For $R_Z^{(n-1, n)}$, the deviation $\delta(x) = 1 - \sqrt{x}R_Z^{(n-1, n)}(x)$ has $2n+1$ alternate changes of sign in the interval $[1, b]$, and attains its maxima and minima,

$$\delta(x) = d_Z, -d_Z, \dots, d_Z, -d_Z, d_Z, \quad d_Z = \frac{1 - \Lambda}{1 + \Lambda},$$

at consecutive points $(1 = x_1 < x_2 < \dots < x_{2n+1} = b)$,

$$x_i = \frac{1}{1 - \kappa'^2 \text{sn}^2(\frac{(i-1)K'}{2n}; \kappa')}, \quad i = 1, \dots, 2n+1.$$

For $R_Z^{(n, n)}$, the deviation $\delta(x) = 1 - \sqrt{x}R_Z^{(n, n)}(x)$ has $2n+2$ alternate changes of sign in the interval $[1, b]$, and attains its maxima and minima,

$$\delta(x) = d_Z, -d_Z, \dots, d_Z, -d_Z, \quad d_Z = \frac{1 - \sigma}{1 + \sigma},$$

at consecutive points $(1 = x_1 < x_2 < \dots < x_{2n+2} = b)$,

$$x_i = \frac{1}{1 - \kappa'^2 \text{sn}^2(\frac{(i-1)K'}{2n+1}; \kappa')}, \quad i = 1, \dots, 2n+2.$$

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