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Spectrum of Preconditioned Moebius Domain-wall Operators

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The convergence property of iterative solvers strongly depends on the spectrum of the Dirac operator. For most standard algorithms to work, the real part of the spectrum should be positive. The domain-wall operator does not satisfy this condition, which is one of the reasons for the difficulty in applying the multi-grid algorithms. In this presentation, we examine several preconditioning operators for the Möbius domain-wall operator and investigate their spectra.

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1. Introduction

Among major fermion operators, the domain-wall operator belongs to a difficult class to solve. The real part of the spectrum is negative due to the large negative mass called the domain-wall height. In Fig. 1, we plot the eigenvalues of a free Möbius domain-wall operator [1] with the scale factor, $b_s + c_s$ in eq. (2) below, set to 2. Because of this feature, standard iterative methods like Conjugate Gradient (CG) or BiCGstab for the operator itself, D, do not work. We therefore usually apply the CG method to positive definite operators, such as $D^\dagger D$. As $D^\dagger D$ has a larger condition number than the original D, however, this algorithm is not an ideal one.

A standard recipe to accelerate the solver is to apply a preconditioner. The multigrid preconditioner is very successful for Wilson fermion. A lot of efforts have also been made to multigrid algorithms for the domain-wall fermion [2–6]. Compared with the Wilson fermion case, however, it is still developing and sub-optimal. Among the works mentioned above, Brower et al. [4] noted the fact that it is not the operator D but a one divided by the Pauli-Villars operator, $D(m = M_{\rm PV})^{-1}D(m = m_q)$, represents the physical degrees of freedom. Here, $M_{\rm PV}$ is the Pauli-Villars' mass which is taken unity in the lattice unit, and m_q is the target quark mass. It is an approximate operator of the overlap operator and gives a positive definite spectrum. As $D(m = M_{\rm PV})^{-1}$ is a rather expensive operator, they instead used $D(m = M_{\rm PV})^\dagger$ to build their multigrid preconditioner.

Inspired by their work, in this work, we apply several preconditioners to the Möbius domain-wall operators and investigate the spectra.

Because we are motivated by an application to the multigrid algorithm, we investigate local preconditioners that avoid complicated coarse operators. We introduce a domain decomposed operator whose domain would correspond to a site on the coarse grid. Such an operator and domain decomposed preconditioner are also beneficial in the performance on parallel computers as they can reduce the neighboring communication.

We describe our preconditioning in the next section. Section 3 shows the result of the spectra. The last section is for summary.

2. Preconditioned Operators

We start with the following domain-wall operator [1]:

$$D(m) = \begin{pmatrix} D_+^{(1)} & D_-^{(1)}P_- & 0 & \cdots & 0 & -mD_-^{(1)}P_+ \\ D_-^{(2)}P_+ & D_+^{(2)} & D_-^{(2)}P_- & 0 & \cdots & 0 \\ 0 & D_-^{(3)}P_+ & D_+^{(3)} & D_-^{(3)}P_- & & 0 \\ \vdots & & \ddots & \ddots & \ddots & \vdots \\ 0 & & & D_-^{(N_s-1)}P_+ & D_+^{(N_s-1)} & D_-^{(N_s-1)}P_- \\ -mD_-^{(N_s)}P_- & 0 & \cdots & 0 & D_-^{(N_s)}P_+ & D_+^{(N_s)} \end{pmatrix}, \quad (1)$$

where

$$D_+^{(s)} = b_s D_{\rm W}(-M_0) + 1, \qquad D_-^{(s)} = c_s D_{\rm W}(-M_0) - 1. \quad (2)$$

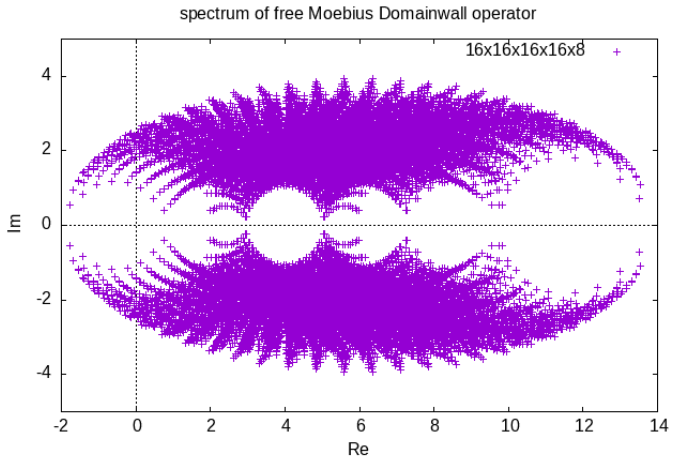

Figure 1: Spectrum of a free Möbius domain-wall operator. The lattice size is $16^4 \times 8$ and the quark mass is 0.01. We set parameters $b = 1.5$ and $c = 0.5$, and the domain-wall height $M_0 = -1$ (see eqs. (1), (2), and the explanation there).

$D_{\rm W}$ is the Wilson Dirac operator of which mass is set to $-M_0$, where $M_0 > 0$ is the domain-wall height. m is the quark mass, N_s the extent of the fifth coordinate, and $P_\pm = \frac{1}{2}(1 \pm \gamma_5)$. We adopt the Möbius domain-wall setup, b_s and c_s independent of the "fifth" coordinate s, and thus denote $b = b_s$ and $c = c_s$ in the following.

We first factor out the diagonal part with respect to the four-dimensional sites. By using the even-odd decomposition of 4D sites, the Dirac operator can be written as

$$D = \begin{pmatrix} D_{\rm ee} & D_{\rm eo} \\ D_{\rm oe} & D_{\rm oo} \end{pmatrix} = C \begin{pmatrix} 1 & D_{\rm ee}^{-1} D_{\rm eo} \\ D_{\rm oo}^{-1} D_{\rm oe} & 1 \end{pmatrix} = \begin{pmatrix} 1 & D_{\rm eo} D_{\rm ee}^{-1} \\ D_{\rm oe} D_{\rm oo}^{-1} & 1 \end{pmatrix} C. \tag{3}$$

Here, the diagonal part,

$$C \equiv \begin{pmatrix} D_{\rm ee} & 0 \\ 0 & D_{\rm oo} \end{pmatrix}, \tag{4}$$

is easy to invert and C^{-1} can be calculated site-by-site. In fact, as it does not depend on the gauge field so it is a constant matrix over the lattice sites. We use C^{-1} as a preconditioner. Note that solving an even-odd preconditioned system, $1 - D_{\rm ee}^{-1} D_{\rm eo} D_{\rm oo}^{-1} D_{\rm oe}$, is equivalent to apply C^{-1}. As emphasized in [5], even-odd preconditioning accelerates the solver significantly for the domain-wall operator[1], we expect that C^{-1} can be a good preconditioner even without even-odd decomposition.

Next, we consider a domain decomposed operator, which uses even-odd decomposition against the blocks of sites [7]. Applying a multigrid method, we assume each block corresponds to a site on the coarse grid. In practice we choose the size of each block 4^4 as displayed in Fig. 2. They are divided into even blocks (E) and odd blocks (O). We denote the decomposed operator as

$$D = \begin{pmatrix} D_{\rm EE} & D_{\rm EO} \\ D_{\rm OE} & D_{\rm OO} \end{pmatrix} = B \begin{pmatrix} 1 & D_{\rm EE}^{-1} D_{\rm EO} \\ D_{\rm OO}^{-1} D_{\rm OE} & 1 \end{pmatrix}, \quad B \equiv \begin{pmatrix} D_{\rm EE} & 0 \\ 0 & D_{\rm OO} \end{pmatrix}. \tag{5}$$

[1] Ref. [5] also mentions that $D_{\rm ee} - D_{\rm eo} D_{\rm oo}^{-1} D_{\rm oe}$ is better than $1 - D_{\rm ee}^{-1} D_{\rm eo} D_{\rm oo}^{-1} D_{\rm oe}$.

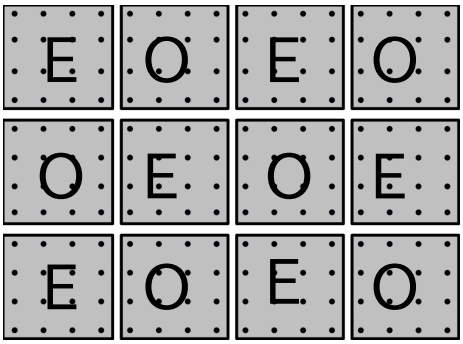

Figure 2: Two-dimensional sketch of even-odd block decomposition. $D_{\rm EE}$ operates on only "E" region, $D_{\rm OO}$ on "O" region, and $D_{\rm EO}$ and $D_{\rm OE}$ connect these two regions.

The matrix $D_{\rm EE}$ and $D_{\rm OO}$ do not have hops between the blocks. $D_{\rm EO}$ and $D_{\rm OE}$ contain only the hops between the nearest neighbor blocks.

We note that the Pauli-Villars operator has a mass of the cutoff scale and expect that the low frequency modes which spread over several blocks would be suppressed. We therefore use B as an approximation of the Pauli-Villars operator.

3. Spectrum of the Preconditioned Operators

We use Bridge++ code set [8–10] to measure the spectra of the domain-wall operator and various preconditioned operators. For each operator, we calculate low- and high- end of the spectrum, by using the implicitly restarted Arnoldi method [11]. The measurement is performed on the Supercomputer Fugaku at RIKEN R-CCS. Bridge++ contains a branch that is well-optimized to the Fugaku's architecture, A64FX [12].

The configuration is provided by JLQCD collaboration, which is a 2+1 flavor finite temperature configuration in the confined phase. The lattice size is $48^3 \times 16$ and $N_s = 12$ and the quark masses are set to the physical point.

Let us start with the spectrum without preconditioning. Figure 3 shows the spectrum of the Möbius domain-wall operator combined with various preconditioners. The original operator is displayed in the top-left panel. The real part is not positive definite. Its preconditioned version with C^{-1} (middle-left) is not positive definite either, while the extent of the spectrum becomes smaller. The bottom-left panel in Fig. 3 is a positive definite squared version, $(C^{-1}D)^\dagger C^{-1}D$.

Next, we examine the preconditioning with the Pauli-Villars operator. The top-right panel of Fig. 3 shows that preconditioning with $D_{\rm PV}^\dagger = D(m = M_{\rm PV})^\dagger$ provides a positive spectrum. The low modes almost align along the imaginary axis with a positive shift of order of the quark mass. It implies that $D_{\rm PV}^\dagger D$ is a good approximation of $D_{\rm PV}^{-1}D$ and overlap operator for small eigenmodes as pointed out in [4]. The figure shows that the high-end of the spectrum of this operator is rather different from the expected behavior for the approximate overlap operator that would not develop such large eigenvalues. Changing $D_{\rm PV}$ to the block diagonal operator $B_{\rm PV}$ affects the spectrum drastically as in the middle-right panel. The real part of the low-lying eigenvalues spread to the negative region. We also examine $B_{\rm PV}^{-1}$ as a preconditioner in the bottom-right panel of Fig. 3. We invert $B_{\rm PV}$ loosely by applying a fixed number of iterations of the minimal residual algorithm in

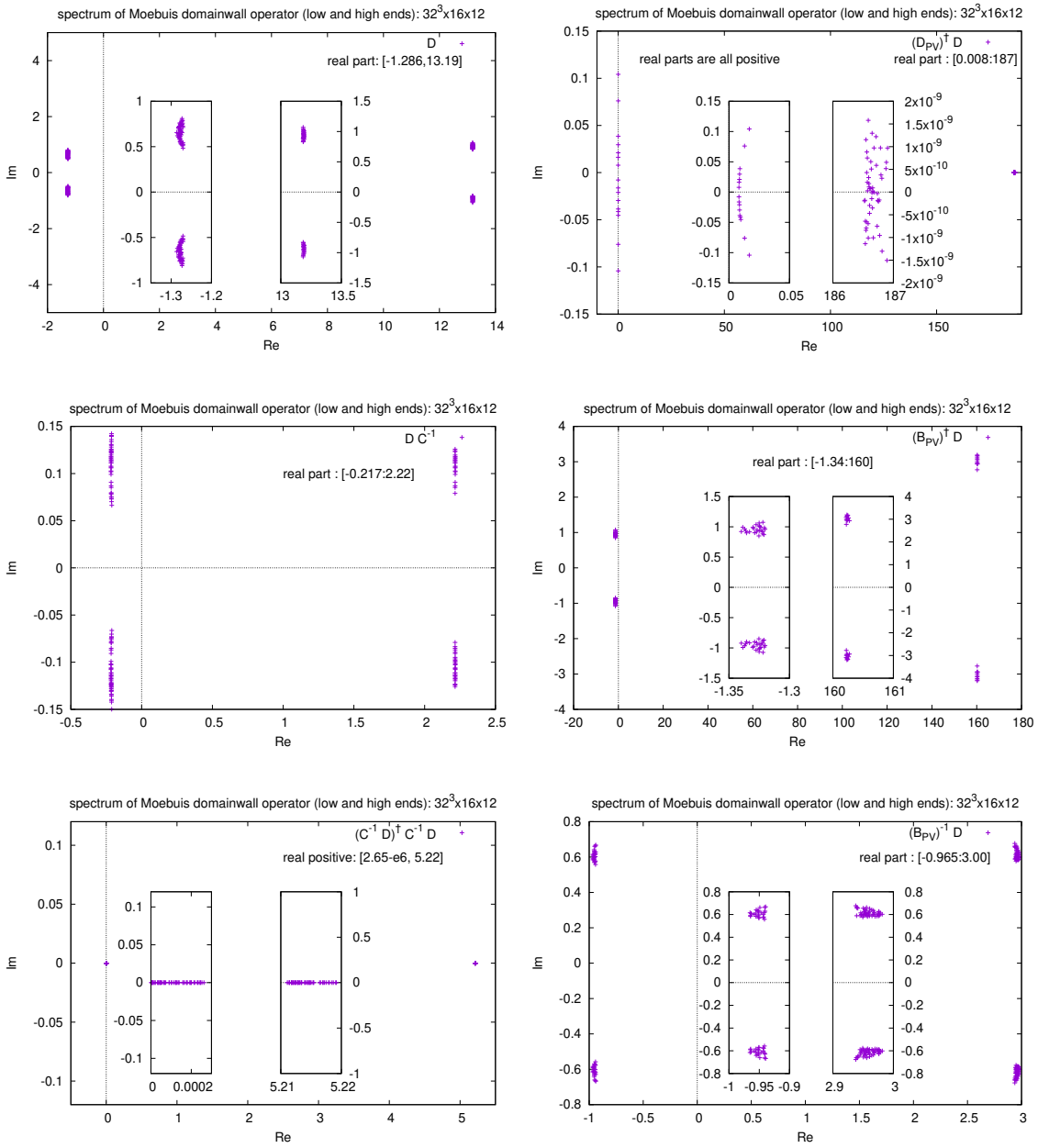

Figure 3: Spectrum of the domain-wall operators: the left panels displays the original operator and preconditioned ones with its diagonal preconditioner, C. The right panels are those preconditioned by the Pauli-Villars operator $D_{\rm PV}$ or its approximation $B_{\rm PV}$. Explicitly, D (top-left), DC^{-1} (middle-left), $(C^{-1}D)^\dagger C^{-1}D$ (bottom-left), $D_{\rm PV}^\dagger D$ (top-right), $B_{\rm PV}^\dagger D$ (middle-right), and $B_{\rm PV}^{-1}D$ (bottom-right).

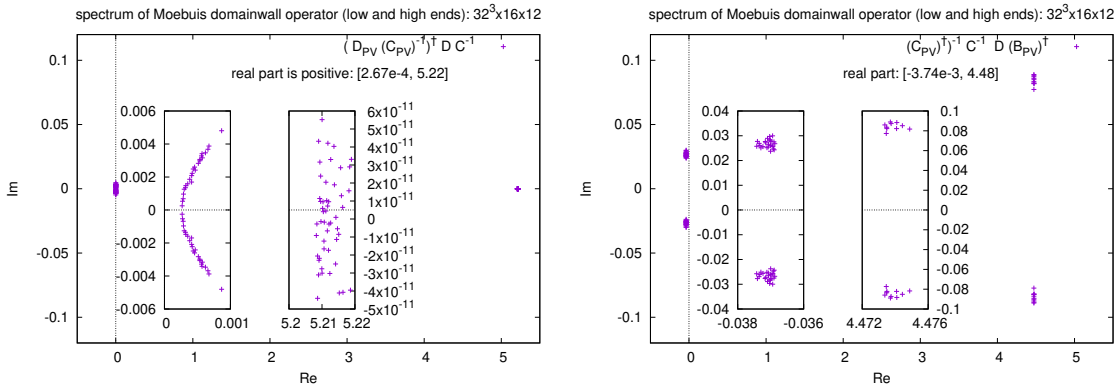

Figure 4: Spectrum of the domain-wall operators: preconditioned with the site-diagonal operator C^{-1} and the Pauli-Villars operator $D_{\rm PV}$ or its approximation $B_{\rm PV}$.

each block. The residual norms squared are typically of the order of 10^{-3}. The real part of the eigenvalues again spread to the negative values, while the largest eigenvalues are much reduced.

We finally combine the Pauli-Villars operator and the site diagonal operator to precondition D. In Fig. 4, the left panel is the spectrum of $\left(D_{\rm PV}C_{\rm PV}^{-1}\right)^\dagger DC^{-1}$. Here $C_{\rm PV}$ is the site diagonal part of the Pauli-Villas operator, $\mathrm{diag}((D_{\rm PV})_{\rm ee}, (D_{\rm PV})_{\rm oo})$. Similar to $D_{\rm PV}^\dagger D$ in Fig. 3, the real part of the spectrum is positive. In addition, the largest eigenvalue is smaller than that with $D_{\rm PV}$, which reduces the condition number from 2.34×10^4 for $D_{\rm PV}^\dagger D$ to 1.96×10^4 for this operator. Replacing $D_{\rm PV}$ with a block diagonal operator $B_{\rm PV}$ gives eigenvalues again with the negative real part as in the right panel. This situation is similarly to $B_{\rm PV}^\dagger D$ in Fig.3.

4. Summary and Outlooks

We investigated the spectrum of several preconditioned Möbius domain-wall operators. By using $D_{\rm PV}^\dagger$, the Hermitian conjugate of the Pauli-Villars operator, we obtain spectra with the positive real part. However, an approximate operator $B_{\rm PV}^\dagger$, which is obtained from $D_{\rm PV}^\dagger$ by truncating connections between neighboring blocks, develops the negative real part of the eigenvalues.

Among our trails, a combination of the site diagonal preconditioning and the Pauli-Villars operator gave the smallest condition number. Using this preconditioner may help to develop a faster solver for the domain-wall fermion.

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