

Eigenspectrum Calculation of the $O(a)$ -Improved Wilson-Dirac Operator in Lattice QCD Using the Sakurai-Sugiura Method

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Abstract We have developed a computer code to find eigenvalues and eigenvectors of non-Hermitian sparse matrices arising in lattice quantum chromodynamics (lattice QCD). The Sakurai-Sugiura (SS) method (Sakurai and Sugiura, J Comput Appl Math 159:119, 2003) is employed here, which is based on a contour integral, allowing us to obtain desired eigenvalues located inside a given contour of the complex plane. We apply the method here to calculating several low-lying eigenvalues of the non-Hermitian $O(a)$ -improved Wilson-Dirac operator D (Sakurai et al., Comput Phys Commun 181:113, 2010). Evaluation of the low-lying eigenvalues is crucial since they determine the sign of its determinant $\det D$, important quantity in lattice QCD. We are particularly interested in such cases as finding the lowest eigenvalues to be equal or close to zero in the complex plane. Our implementation is tested for the Wilson-Dirac operator in free case, for which the eigenvalues are analytically

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known. We also carry out several numerical experiments using different sets of gauge field configurations obtained in quenched approximation as well as in full QCD simulation almost at the physical point. Various lattice sizes $L_x L_y L_z L_t$ are considered from $8^3 \times 16$ to 96^4 , amounting to the matrix order $12L_x L_y L_z L_t$ from 98,304 to 1,019,215,872.

1 Introduction

The determinant of the Wilson-Dirac operator, $\det D$, plays an important role in lattice QCD. In general, the determinant of an $\mathcal{L} \times \mathcal{L}$ matrix D can be written, in terms of its eigenvalues λ_l , as

$$\det D = \prod_{l=1}^{\mathcal{L}} \lambda_l, \quad (1)$$

so that all the information about the Wilson fermion determinant, or the fermion measure, is concentrated in the eigenspectrum. This makes the eigenspectrum calculation of the Wilson-Dirac operator an interesting subject. Because the eigenspectrum possesses the vertical and horizontal symmetries and that the complex eigenvalues are therefore always paired, the determinant can be further expressed in the form:

$$\det D = \prod_{\lambda_l \in \mathbb{R}} \lambda_l \prod_{\lambda_{l'} \in \mathbb{C}} |\lambda_{l'}|^2. \quad (2)$$

We are thus particularly interested in calculating several low-lying real eigenvalues of the Wilson-Dirac operator, since the sign problem may occur due to the real, negative eigenvalues.

In this work, we develop exploratorily a computer code for calculating the low-lying eigenspectrum of the Wilson-Dirac operator. For such sparse eigenproblems as the Wilson-Dirac equation, the Implicitly Restarted Arnoldi Method (IRAM) [1] is one of the conventional choices. It is noteworthy mentioning earlier attempts to improve eigenvalue computations of the non-Hermitian Dirac operator, such as in [2]. We adopt here the Sakurai-Sugiura (SS) method since this makes it possible to set more flexibly the region for searching eigenvalues. The SS method is based on contour integrals, allowing us to calculate eigenvalues located in a given domain of the complex plane as well as the associated eigenvectors. Our computer code will be applied to calculating low-lying eigenvalues of the non-Hermitian $O(a)$ -improved Wilson-Dirac operator. We consider the spatiotemporal lattice sizes $8^3 \times 16$ and 96^4 , amounting to the matrix order of 98,304 and 1,019,215,872, respectively. Eigenvalue calculations will be performed using gauge field configurations for the free case, those generated in quenched approximation as well as those generated by a full QCD simulation, focusing on such cases as finding the low-lying eigenvalues to be localized very close to zero in the complex plane.

2 Sakurai-Sugiura Method for the Wilson-Dirac Operator

The lattice QCD is defined on a hypercubic four-dimensional lattice of finite extent expressed as $L_x \times L_y \times L_z \times L_t$ with $L_{x,y,z}$ being the three-dimensional spatial extent and L_t the temporal one. The lattice spacing is set to unity for notational convenience. The fields are defined on the sites n with periodic boundary conditions. We define two types of fields on the lattice. One is the gauge field represented by $U_\mu(n)^{a,b}$ with $\mu = 1, 2, 3, 4$ (corresponding respectively to x, y, z, t) and $a, b = 1, 2, 3$, which is a 3×3 SU(3) matrix assigned on each link. The other is the quark field $q(n)_\alpha^a$ which resides on each site carrying the Dirac index $\alpha = 1, 2, 3, 4$ and the color index $a = 1, 2, 3$. The $O(a)$ -improved Wilson-Dirac operator is written as

$$\begin{aligned}
 D_{\alpha,\beta}^{a,b}(n, m) = & \delta_{\alpha,\beta} \delta^{a,b} \delta(n, m) - \kappa \sum_{\mu=1}^4 [(1 - \gamma_\mu)_{\alpha,\beta} (U_\mu(n))^{a,b} \delta(n + \hat{\mu}, m) \\
 & + (1 + \gamma_\mu)_{\alpha,\beta} ((U_\mu(m))^{b,a})^* \delta(n - \hat{\mu}, m)] \\
 & + \kappa c_{\text{SW}} \sum_{\mu,\nu=1}^4 \frac{i}{2} (\sigma_{\nu\mu})_{\alpha,\beta} (F_{\nu\mu}(n))^{a,b} \delta(n, m), \tag{3}
 \end{aligned}$$

where $\hat{\mu}$ denotes the unit vector in the μ direction. κ is the hopping parameter, and the coefficient c_{SW} is a parameter to be adjusted for the $O(a)$ -improvement. The Euclidean gamma matrices are defined in terms of the Minkowski ones in the Bjorken-Drell convention: $\gamma_j = -i\gamma_{BD}^j$ ($j = 1, 2, 3$), $\gamma_4 = \gamma_{BD}^0$, $\gamma_5 = \gamma_{BD}^5$, and $\sigma_{\mu\nu} = \frac{1}{2}[\gamma_\mu, \gamma_\nu]$. The explicit representation for $\gamma_{1,2,3,4,5}$ are given in [3], together with the expression for the field strength $F_{\mu\nu}(n)$ in terms of the gauge field $U_\mu(n)$. The $O(a)$ -improved Wilson-Dirac operator defined in Eq. (3) is a sparse, complex non-Hermitian square matrix $D \in \mathbb{C}^{\mathcal{L} \times \mathcal{L}}$, where only 51 out of $\mathcal{L} = L_x \times L_y \times L_z \times L_t \times 3 \times 4$ entries in each row have nonzero values.

In this work, we consider an eigenproblem

$$Dx_l = \lambda_l x_l, \quad (l = 1, 2, \dots, \mathcal{L}), \tag{4}$$

where λ_l and x_l are eigenvalues and eigenvectors, respectively. In order to extract eigenpairs (λ_l, x_l) from the matrix D in Eq. (4), we adopt the Sakurai-Sugiura method, proposed in [4–6]. This method is based on contour integrals, allowing us to calculate eigenvalues located in a given domain of the complex plane, together with the associated eigenvectors. In this method, we first define matrices $S_k \in \mathbb{C}^{\mathcal{L} \times \mathcal{L}}$ as

$$S_k \equiv \frac{1}{2\pi i} \oint_{\Gamma} z^k (zI - D)^{-1} V dz, \quad k = 0, 1, \dots, M-1. \tag{5}$$

Here, Γ is a positively oriented closed curve in the complex plane inside which we seek for eigenvalues, and M denotes the maximum moment degree. The matrix

$V \in \mathbb{C}^{\mathcal{L} \times L}$, called source matrix, contains L column vectors $V = [v_1, v_2, \dots, v_L]$, and we take a random vector for each of these source vectors. We assume that Γ is given by a circle and the integration is evaluated via a trapezoidal rule on Γ . By designating the center and the radius of the circle as γ and ρ , respectively, and by defining the quadrature points as $z_j = \gamma + \rho e^{2\pi i(j-1/2)/N}$, $j = 1, 2, \dots, N$, we approximate the integral in Eq. (5) via an N -point trapezoidal rule:

$$S_k \approx \hat{S}_k \equiv \frac{1}{N} \sum_{j=1}^N z_j^k (z_j I - D)^{-1} V. \quad (6)$$

We then carry out the singular value decomposition for the matrix $\hat{S} = [\hat{S}_0, \hat{S}_1, \dots, \hat{S}_{M-1}] \in \mathbb{C}^{\mathcal{L} \times LM}$ as follows

$$\hat{S} = \tilde{Q} \Sigma W, \quad (7)$$

$$\tilde{Q} = [q_1, q_2, \dots, q_{LM}] \in \mathbb{C}^{\mathcal{L} \times LM}, \quad (8)$$

$$\Sigma = \text{diag}(\sigma_1, \sigma_2, \dots, \sigma_{LM}). \quad (9)$$

We next determine the numerical rank m of the matrix \hat{S} . The value of m is fixed as the number of singular values satisfying $\sigma_i > \delta$, with δ being the threshold for determining the numerical rank and usually set to $\delta = 10^{-12}$. The original eigenproblem is transformed to a smaller eigenproblem via the transformation matrix $Q = [q_1, q_2, \dots, q_m]$, with only the first m column vectors from \tilde{Q} are incorporated. We finally solve the smaller eigenequation $Q^H D Q u_l = \mu_l u_l$ and obtain an approximation to the eigenpairs $\lambda_l \approx \mu_l$ and $x_l \approx Q u_l$. Although our purpose is to know the eigenvalue distribution and that the eigenvectors are not necessary, we choose to calculate them since we need to check the accuracy via the relative residual norms.

As can be seen from Eq. (6), the Sakurai-Sugiura method produces a subspace with the matrix basis involving the inverses of the matrices $(z_j I - D)$. The matrix inversion can be performed solving the shifted linear equations

$$(z_j I - D)y_{jl} = v_l. \quad (10)$$

There exist several implementations based on direct methods such as LAPACK and MUMPS libraries. These implementations, however, are hardly applicable to such linear problems as arising in lattice QCD due to their large matrix sizes, and some iterative methods are desirable to solve such large sparse linear equations. In this work, we implement exploratorily the BiCGStab algorithm as is presented in Algorithm 1. The BiCGStab algorithm will be found to converge very slowly, suffering from the ill-condition problem of the shifted linear equations. We choose, however, to employ the solution vectors as are obtained from a sufficiently large number of BiCGStab iterations. The shift-invariance property of the Krylov subspace of D under any translation indicates that substantial time saving can

Algorithm 1 BiCGStab algorithm for solving $Ay \equiv (zI - D)y = v$

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1: initial guess  $y \in \mathbb{C}^{\mathcal{L}}$ ,
2: compute  $r = v - Ay$ ,
3: set  $p = r' = r$ ,
4: choose  $\tilde{r}$  such that  $(\tilde{r}, r) \neq 0$ ,
5: while  $\|r\|_2 / \|v\|_2 > \epsilon$  do:
6:    $\alpha = (\tilde{r}, r) / (\tilde{r}, Ap)$ ,
7:    $y \leftarrow y + \alpha p$ ,
8:    $r \leftarrow r - \alpha Ap$ ,
9:    $\zeta = (Ar, r) / (Ar, Ar)$ ,
10:   $y \leftarrow y + \zeta r$ ,
11:   $r \leftarrow r - \zeta Ar$ ,
12:   $\beta = (\alpha / \zeta) \cdot (\tilde{r}, r) / (\tilde{r}, r')$ ,
13:   $p \leftarrow r + \beta(p - \zeta Ap)$ ,
14:   $r' = r$ ,
15: end while.

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be achieved by solving all shifted equations with only one sequence of Krylov subspaces, which can be a subject of the future development. In practice, the center γ and the radius ρ of the contour can be determined by running the code beforehand with small values of N , L and M , which also allows us to estimate approximatively the multiplicity of eigenvalues inside Γ . Then, the default values of $N = 32$ and $M = 16$ can be mostly used, but the value of L is crucial, and need to be large in case of large multiplicity or in order to obtain higher accuracy.

Code development is carried out based on the lattice QCD simulation program LDDHMC/ ver1.3K0.52ovlpcomm1.2 developed for the K computer [7, 8]. The K computer, at the RIKEN Advanced Institute for Computational Science, consists of 82,944 computational nodes and 5184 I/O nodes connected by the so-called ‘‘Tofu’’ network, providing 11.28 Pflops of computing capability. The Tofu network topology is six-dimensional one with 3D-mesh times 3D-torus shape. Each node has a single 2.0 GHz SPARC64 VIIIfx processor equipping 8 cores with SIMD enabled 256 registers, 6 MB shared L2 cache and 16 GB of memory. The L1 cache sizes per each core are 32 KB/2WAY (instruction) and 32 KB/2WAY (data).

3 Simulation Results

Our implementation is tested here for the free-case Wilson-Dirac operator, of which the eigenspectrum can be analytically obtained. For the free case, $(U_\mu(n))^{a,b} = \delta_{ab}$, the Wilson-Dirac action, in the momentum space ($\psi(x) = \int dk \exp(ikx) \tilde{\psi}(k)$), turns out to be

$$\tilde{D}(k) = 1 - \kappa \sum_{\mu=1}^4 [2 \cos(k_\mu) - 2i\gamma_\mu \sin(k_\mu)]. \quad (11)$$

Since the allowed momentum components must be the discrete elements of the Brillouin zone ($k_\mu = \frac{2\pi}{L_\mu}l_\mu$), we then obtain the expression for the free Wilson-Dirac eigenvalues as

$$\lambda_{\{l_\mu\}}^{\text{free}} = 1 - 2\kappa \left[\sum_{\mu=1}^4 \cos\left(\frac{2\pi}{L_\mu}l_\mu\right) \pm i \sqrt{\sum_{\mu=1}^4 \sin^2\left(\frac{2\pi}{L_\mu}l_\mu\right)} \right], \quad l_\mu = 0, 1, \dots, L_\mu - 1. \quad (12)$$

Each set of the numbers $\{l_\mu\}$ correspond to 12 eigenvalues, 2 sets of 6 multiple eigenvalues with the plus and minus signs in Eq. (12). Note also that for the hopping parameter $\kappa = 1/8$, the minimum eigenvalue coincide with the origin, $z = 0$.

Figure 1 shows the eigenvalues of the free-case Wilson-Dirac operator calculated by the SS method for the lattice size $8^3 \times 16$ and the hopping parameter $\kappa = 1/8$. We have used the number of quadrature $N = 32$, the number of source vector $L = 64$ and the maximum moment degree $M = 16$. We notice three sets of eigenvalues inside the integration contour of which the quadrature points z_j are indicated by asterisks. Each of these three sets contains 12 multiple eigenvalues, so that in total 36 eigenvalues are found inside the integration contour. The BiCGStab algorithm used for solving the shifted linear equation (10) is found to converge very slowly for some quadrature points z_j , due to the ill-condition problem: for the quadrature point the most on the right-hand side z_1 , the residual $\|r\|_2/\|v\|_2$ decreases only to about $10^{-8} \sim 10^{-10}$ with 1000 BiCGStab iterations, while it decreases less than 10^{-14} with about 200 BiCGStab iterations for the quadrature point the most on the left-hand side z_{17} . However, using the solution vectors obtained

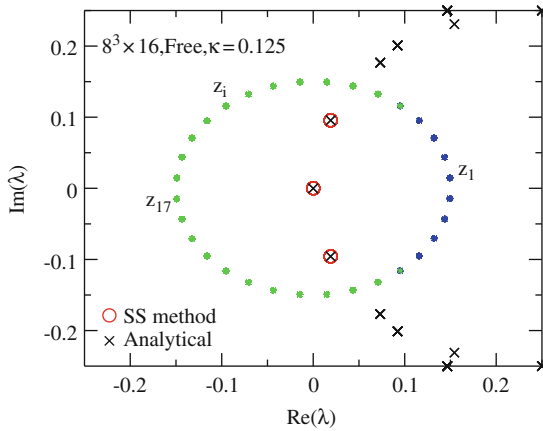


Fig. 1 Eigenvalues of the free-case Wilson-Dirac operator in a $8^3 \times 16$ lattice for the hopping parameter $\kappa = 1/8$. The eigenvalues obtained from the SS method are indicated as *red circles*, those obtained from the analytical expression are indicated as *black crosses*. *Green (blue) asterisks* indicate the quadrature points z_j for which the BiCGStab algorithm converges (does not converge) to less than 10^{-14} of the relative residuals norms with 1000 iterations

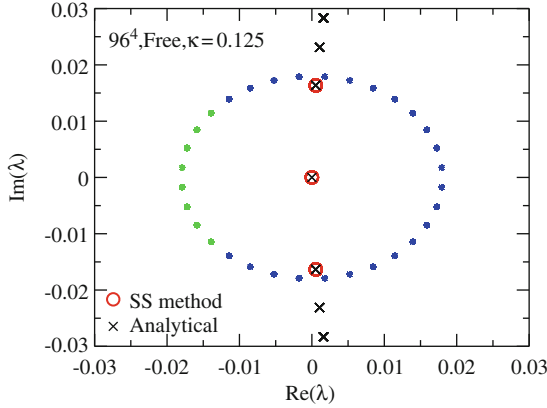


Fig. 2 The same as in Fig. 1, but for the lattice size 96^4

with about 1000 iterations, we have been able to obtain the above eigenvalues accurately with the relative residual norms about 10^{-7} . This may indicate that even if the shifted equations (10) are not solved with high precision, we can obtain a certain precision about the eigenvalues. If we decrease the number of BiCGStab iterations, we could still obtain acceptable values for the eigenvalues but with more or less lower accuracy. Our eigenvalues obtained by the SS method are visually indistinguishable from those obtained from the analytical expression in Eq. (12). Figure 2 shows the same results but for the larger lattice size, 96^4 . We have used the parameters for the SS method $(N, L, M) = (32, 128, 16)$. Here, inside the integration contour, we have found one set of 12 multiple eigenvalues at the origin and 2 sets of 36 multiple eigenvalues above and below the origin, 84 eigenvalues in total. The relative residual norms have been found to be around 5×10^{-4} . These eigenvalues calculated by the SS method are also shown to be indistinguishable from those from the analytical expression in Eq. (12). Note that, we set $L = 128$ since it must be greater than or equal to the maximum multiplicity of the eigenvalues in Γ . If there is no multiplicity, we usually set a small value to L e.g. $L = 8$.

We have also carried out eigenvalue calculations with a sample of gauge field configurations generated in quenched approximation. We generate these configurations on a $8^3 \times 16$ lattice with the Iwasaki gauge action $\beta = 1.9$ using the lattice QCD program LDDHMC/ver1.3K0.52ovlpcomm 1.2 [7, 8]. Figure 3 shows the eigenvalues of the $O(a)$ -improved Wilson-Dirac operator with these gauge configurations in quenched approximation for the parameters $\kappa = 0.1493$ and $c_{SW} = 1.6$. These values of κ and c_{SW} have been chosen so that the minimum real eigenvalue is close to the origin in the complex plane. We have used the parameters for the SS method $(N, L, M) = (32, 96, 16)$. The relative residual norms of the eigenvalues have been found to be around 10^{-5} .

Finally, we have performed eigenvalue calculations using a set gauge field configurations generated in a full QCD calculation. These gauge field configurations

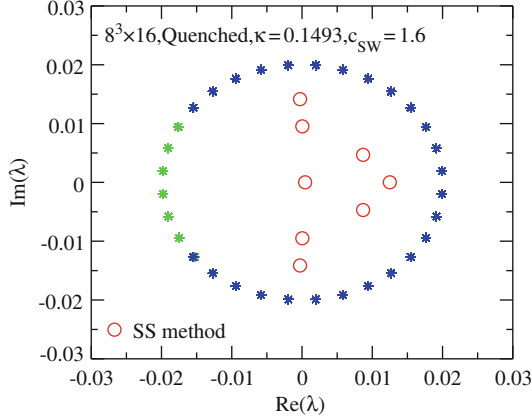


Fig. 3 Eigenvalues of the $O(a)$ -improved Wilson-Dirac operator in a $8^3 \times 16$ lattice for the hopping parameter $\kappa = 0.1493$ and the improvement parameter $c_{\text{SW}} = 1.6$, with gauge field configurations generated in quenched approximation. The eigenvalues obtained from the SS method are indicated as *red circles*. *Green (blue) asterisks* indicate the quadrature points z_j for which the BiCGStab algorithm converges (does not converge) to less than 10^{-14} of the relative residuals norms with 1000 iterations

are generated by a $2 + 1$ flavor QCD simulation near the physical point on a 96^4 lattice [9] with the hopping parameters $(\kappa_{\text{ud}}, \kappa_s) = (0.126117, 0.124700)$ and $c_{\text{SW}} = 1.110$. The other details are given in [9]. Figure 4 shows the eigenvalues calculated by the SS method for the hopping and improvement parameters $\kappa = 0.126117$ and $c_{\text{SW}} = 1.110$. We have used the parameters for the SS method $(N, L, M) = (32, 16, 16)$, and the maximum number of BiCGStab iterations 30,000 for solving the shifted linear equations. The relative residual norms of the eigenvalues have been found to be around 5×10^{-4} .

The above eigenvalue calculations have been performed on the K computer, using 16 nodes for the lattice size $8^3 \times 16$ and 16,384 nodes for the lattice size 96^4 . Almost the whole computer time is consumed in the multiplication of the quark field by the Wilson-Dirac operator. The time spent by each matrix-vector multiplication is found to be 1.29×10^{-3} s for the lattice size $8^3 \times 16$, and 5.5×10^{-3} s for the lattice size 96^4 . For the $8^3 \times 16$ free case, the elapsed time amounts to 2160 s with about 1.67×10^6 matrix-vector multiplications being performed. For the 96^4 free case, the elapsed time is 21,500 s with about 3.93×10^6 matrix-vector multiplications. For the $8^3 \times 16$ quenched-approximation case, the elapsed time is found to be 3480 s with about 3.01×10^6 matrix-vector multiplications, while for the 96^4 Full QCD case, we have found the elapsed time to be 65,300 s with 1.27×10^7 matrix-vector multiplications. In Fig. 5, we show the performance per node of the matrix-vector multiplication as a function of the lattice size.

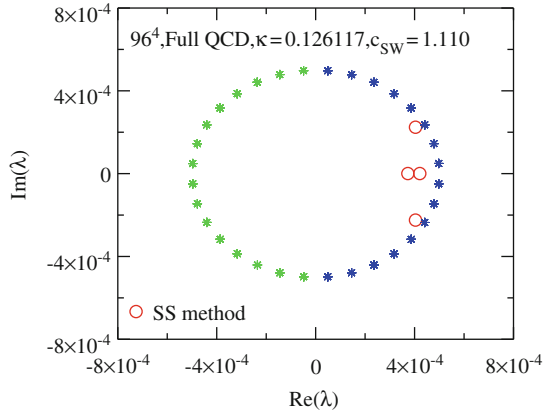


Fig. 4 Eigenvalues of the $O(a)$ -improved Wilson-Dirac operator in a 96^4 lattice for the hopping parameter $\kappa = 0.126117$ and the improvement parameter $c_{\text{SW}} = 1.110$, with gauge field configurations generated in a full QCD simulation. The eigenvalues obtained from the SS method are indicated as *red circles*. *Green (blue) asterisks* indicate the quadrature points z_j for which the BiCGStab algorithm converges (does not converge) to less than 10^{-14} of the relative residuals norms with 30,000 iterations

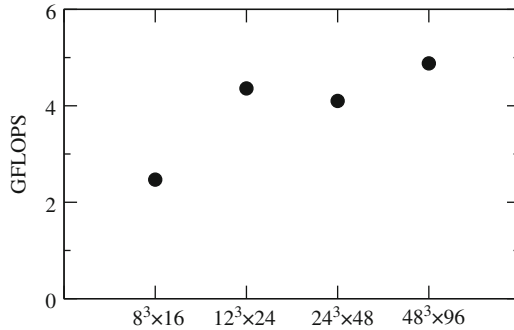


Fig. 5 Performance (in GFLOPS) per node of the matrix-vector multiplication as a function of the lattice size. Note that for the lattice sizes $8^3 \times 16$, $12^3 \times 24$, $24^3 \times 48$, and $48^3 \times 96$, we use respectively 16, 16, 256, and 2048 nodes of the K computer

4 Summary

In this work, we have exploratorily developed a computer code for calculating eigenvalues and eigenvectors of non-Hermitian matrices arising in lattice QCD, using the Sakurai-Sugiura method. We have applied our implementation to calculating low-lying eigenvalues of the $O(a)$ -improved Wilson-Dirac operator with gauge field configurations for the free case and those generated in quenched approximation and in full QCD. Eigenvalues have been obtained with relative residual norms from about 10^{-7} to 5×10^{-4} , with the accuracy being limited by the slow convergence

of the BiCGStab algorithm for solving the shifted linear equations. We think that the Sakurai-Sugiura method is a promising way to solve eigenvalue problems in lattice QCD under the condition that it is combined with a more efficient shifted linear equation solver, which is desirable in order to improve the accuracy of these eigenvalues. For the future work, some preconditioner might be necessary for the iterative linear solver. We are actually carrying out implementation of a Krylov subspace iterative method specifically for solving shifted linear systems [10].

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