Eigenspectrum calculation of the non-Hermitian O(a)-improved Wilson-Dirac operator using the Sakurai-Sugiura method

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Motivation

- The determinant of the Wilson-Dirac operator

$$\det D$$

  plays an important role in lattice QCD.
- This can be written as

$$\det D = \lambda_1 \lambda_2 \cdots \lambda_{\mathcal{N}}$$

  where λ_i's satisfy the eigenequation:

$$D x_i = \lambda_n x_i,\ i = 1, 2, \cdots, \mathcal{N}$$

- Low-lying eigenvalues (small $\mathrm{Re}(\lambda_i)$) are particularly important, since they determine
  - the sign of $\det D$
  - the condition number of the matrix D
- Our goal: develop a way to calculate eigenvalues of D in a given domain of the complex plane.

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O(a)-improved Wilson-Dirac operator

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

$n,m=1,2,\ldots,L_xL_yL_zL_t$ (lattice volume)

$\alpha,\beta=1,2,3,4$ (spin indices)

$a,b=1,2,3$ (color indices)

$(U_\mu(n))^{a,b}$: gauge field at site n w/ 4D indices $\mu=1,2,3,4$

Gamma matrices:

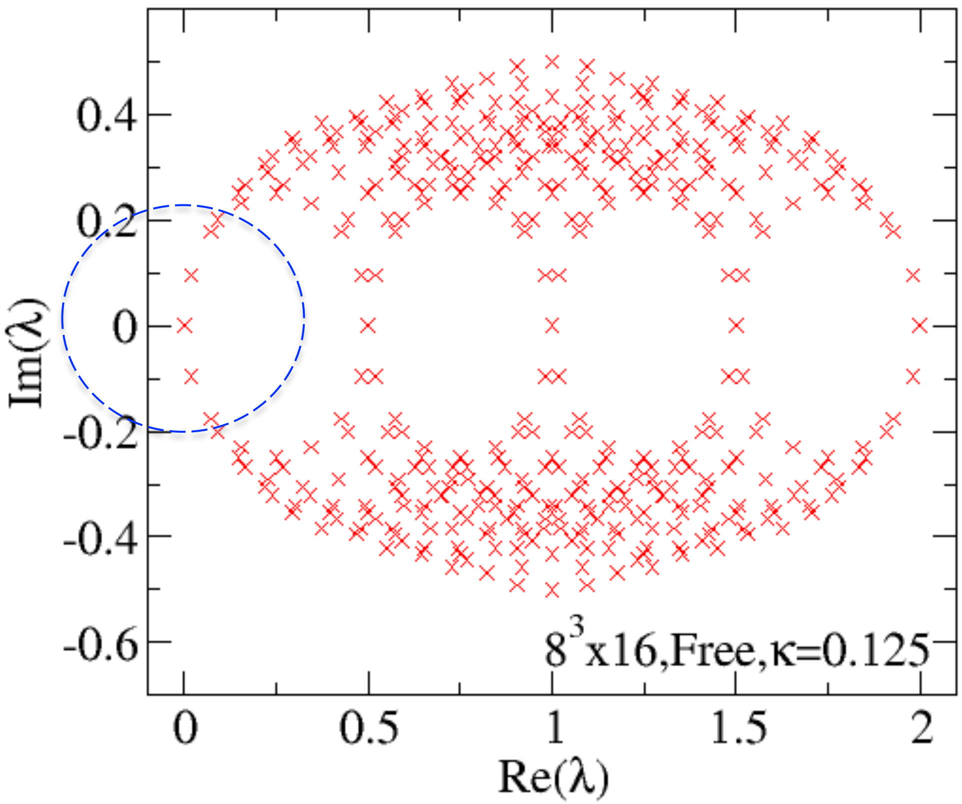
$$
\gamma_1 = \begin{pmatrix} 0 & 0 & 0 & -i \\ 0 & 0 & -i & 0 \\ 0 & i & 0 & 0 \\ i & 0 & 0 & 0 \end{pmatrix}, \gamma_2 = \begin{pmatrix} 0 & 0 & 0 & -1 \\ 0 & 0 & 1 & 0 \\ 0 & 1 & 0 & 0 \\ -1 & 0 & 0 & 0 \end{pmatrix}, \gamma_3 = \begin{pmatrix} 0 & 0 & -i & 0 \\ 0 & 0 & 0 & i \\ i & 0 & 0 & 0 \\ 0 & -i & 0 & 0 \end{pmatrix}, \gamma_4 = \begin{pmatrix} 1 & 0 & 0 & 0 \\ 0 & 1 & 0 & 0 \\ 0 & 0 & -1 & 0 \\ 0 & 0 & 0 & -1 \end{pmatrix}.
$$

- Sparse matrix: only 51 elements out of $12L_xL_yL_zL_t$ are nonzero

Eigenspectrum for the free case

- For the free case $U_\mu(n)=1$, the eigenspectrum can be analytically calculated.

$$\lambda_{\mathrm{W}} = 1 - 2\kappa\left[\sum_{\mu}^{4}\cos(k_\mu) \pm 2i\sqrt{\sum_{\mu}^{4}\sin^2(k_\mu)}\right]$$



Sakurai-Sugiura (SS) method

- The SS method allows us to calculate eigenvalues and eigenvectors of sparse matrices in a given domain of the complex plane.
- Produce a subspace with contour integrals

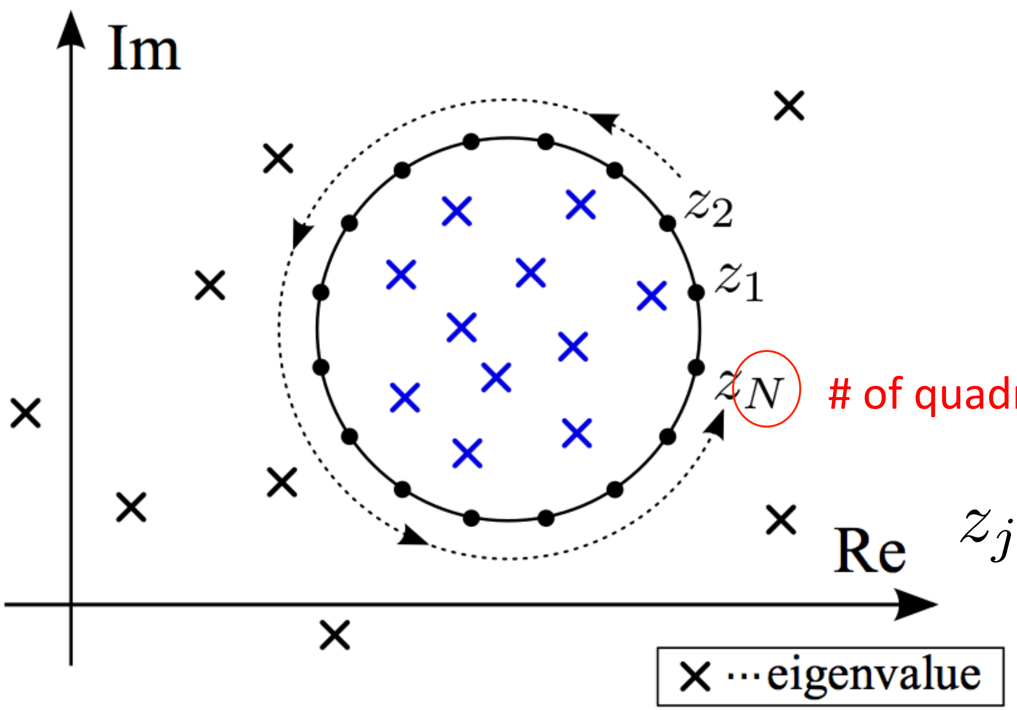
Max. momentum degree

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

$$V = [v_1, v_2, \ldots, v_L]$$

\# of source vec.

$$S_k, V \in \mathbb{C}^{\mathcal{N} \times L}$$



\# of quadrature pts.

$$z_j = \gamma + \rho e^{2\pi i (j-1/2)/N}$$

Sakurai-Sugiura (SS) method

1. $S \equiv [S_0, S_1, \ldots, S_{M-1}] \in \mathbb{C}^{\mathcal{N} \times LM}$
2. $\tilde{Q}\Sigma W = \mathrm{SVD}(S)$
3. From Σ, we obtain the rank m of S.
4. $Q = \tilde{Q}(:, 1:m)$
5. Solve a smaller eigenproblem: $Q^{\mathrm{H}} D Q \vec{u} = \mu \vec{u}$
6. Obtain approximatively eigenpairs: $\lambda \approx \mu, \vec{x} \approx Q\vec{u}$

Accuracy evaluated by relative residual norms:

$$\mathrm{res(i)} = \frac{||D\vec{x}_i - \lambda_i \vec{x}_i||_2}{||D\vec{x}_i||_2 + |\lambda_i|||\vec{x}_i||_2}$$

- T. Sakurai and H. Sugiura, J. Comput. Appl. Math. 159 (2003) 119.
- Software named "z-Pares" available at the web site http://zpares.cs.tsukuba.ac.jp/.

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Calculating $(zI\text{-}D)^{-1}$

Matrix inversion is carried out at each quadrature points z_i by solving the shifted linear equations

$$Ay_{jl} = (z_j I - D)y_{jl} = v_l$$

using the BiCGStab algorithm.

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initial guess $y \in \mathbb{C}^{\mathcal{N}}$,
compute $r = v - Ay$,
set $p = r$,
choose $\tilde{r}$ such that $(\tilde{r}, r) \neq 0$,
while $|r|/|b| > \epsilon$ **do**
    $\alpha = (\tilde{r}, r)/(\tilde{r}, Ap)$,
    $y \leftarrow y + \alpha p$,
    $r \leftarrow r - \alpha Ap$,
    $\zeta = (Ar, r)/(Ar, Ar)$,
    $y \leftarrow y + \zeta r$,
    $r \leftarrow r - \zeta Ar$,
    $\beta = (\alpha/\zeta) \cdot (\tilde{r}, r)/(\tilde{r}, r')$,
    $p \leftarrow r + \beta(p - \zeta Ar)$,
    $r' = r$
end while

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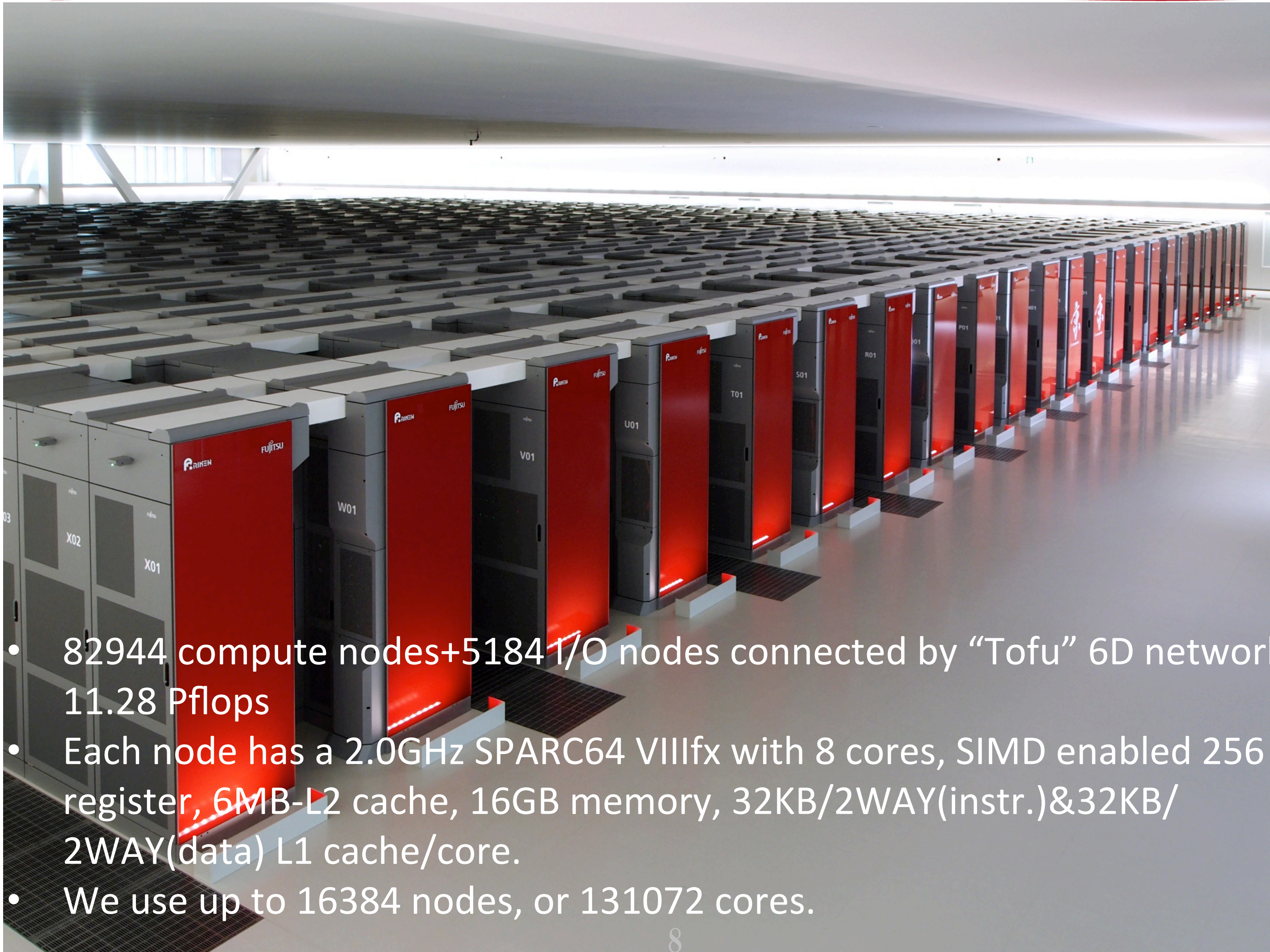

- 82944 compute nodes+5184 I/O nodes connected by “Tofu” 6D network
  11.28 Pflops
- Each node has a 2.0GHz SPARC64 VIIIfx with 8 cores, SIMD enabled 256 register, 6MB-L2 cache, 16GB memory, 32KB/2WAY(instr.)&32KB/ 2WAY(data) L1 cache/core.
- We use up to 16384 nodes, or 131072 cores.

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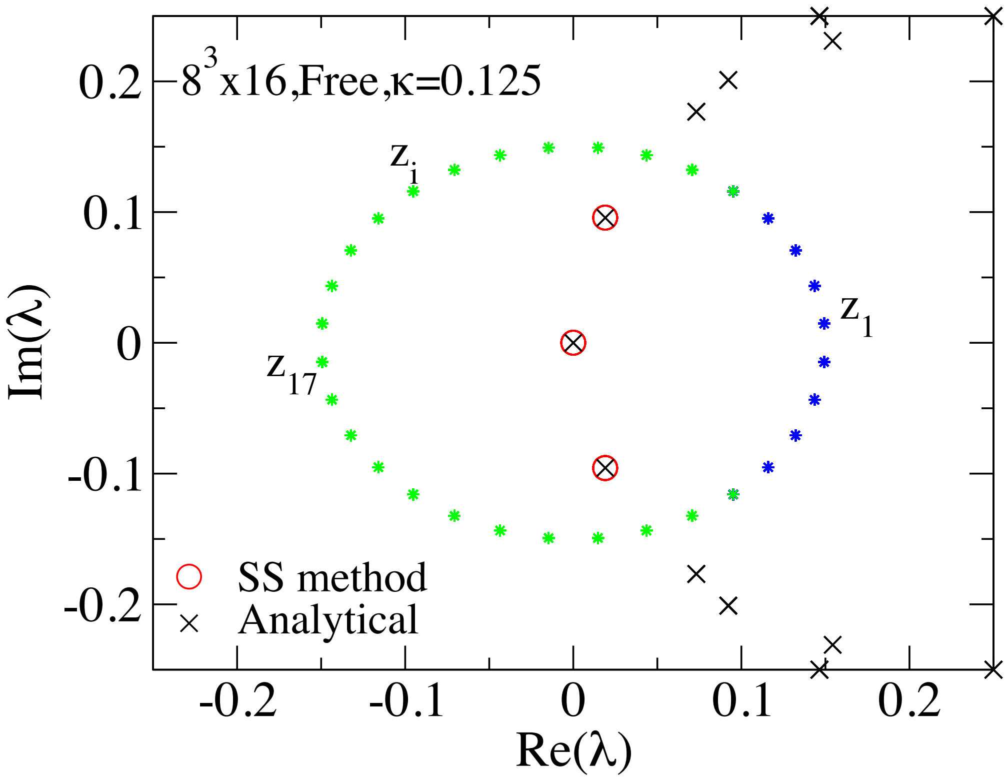
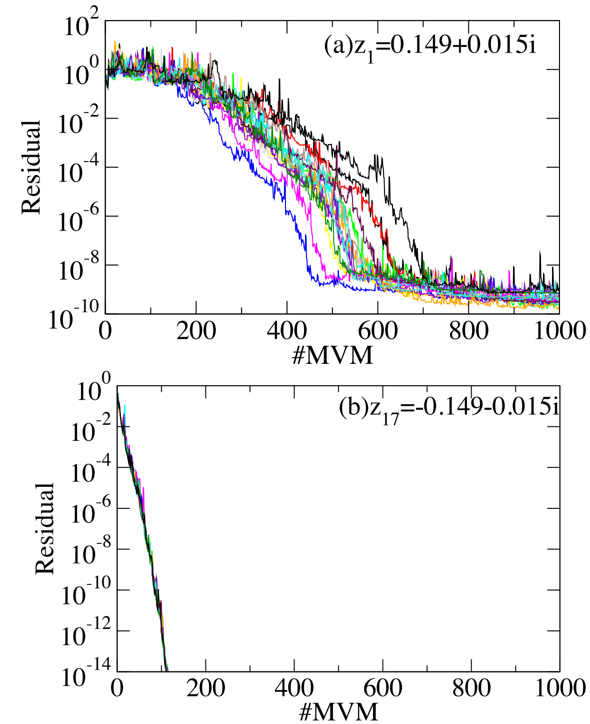
Results for the free case

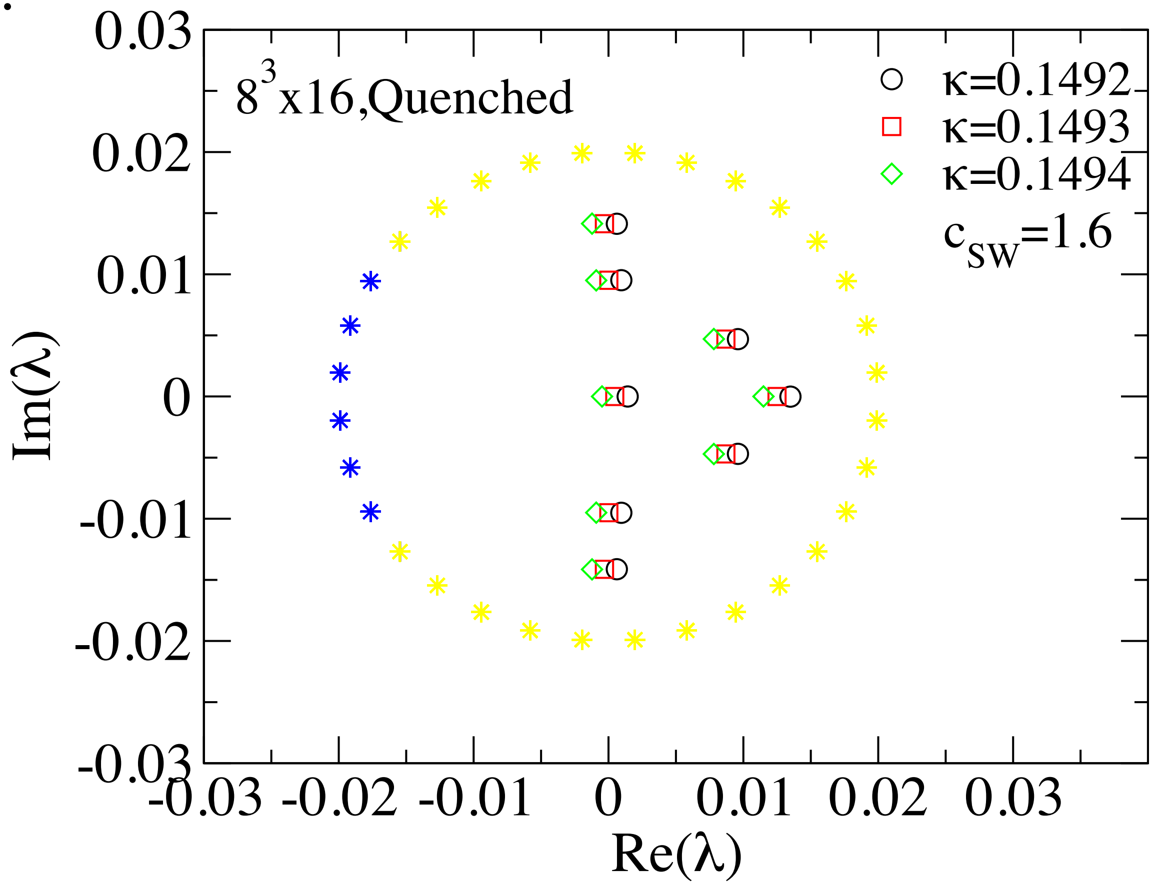




- BiCGStab converges very slowly at some z_i points, but we use the solutions obtained after 1000 BiCGStab iterations.
  ❖ converged, ❖ not converged to 10^{-14}.
- Convergence slow when # of eigenvalues is large close to z_i.
- N=32,L=64,M=16, Relative residual norms ≈ 10^{-7}

Results

- We use $U_\mu(n)$ generated in quenched approximation with β=1.9.



- N=32,L=96,M=16,Relative residual norms ≈ 10^{-5}

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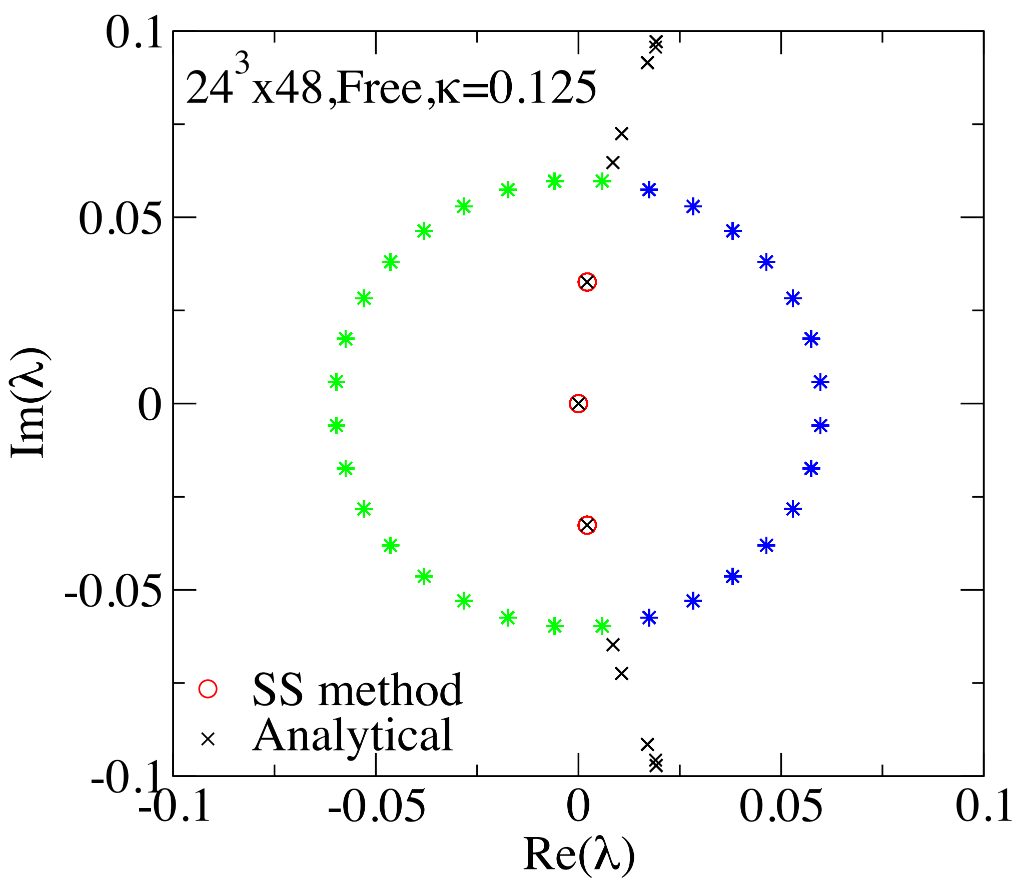
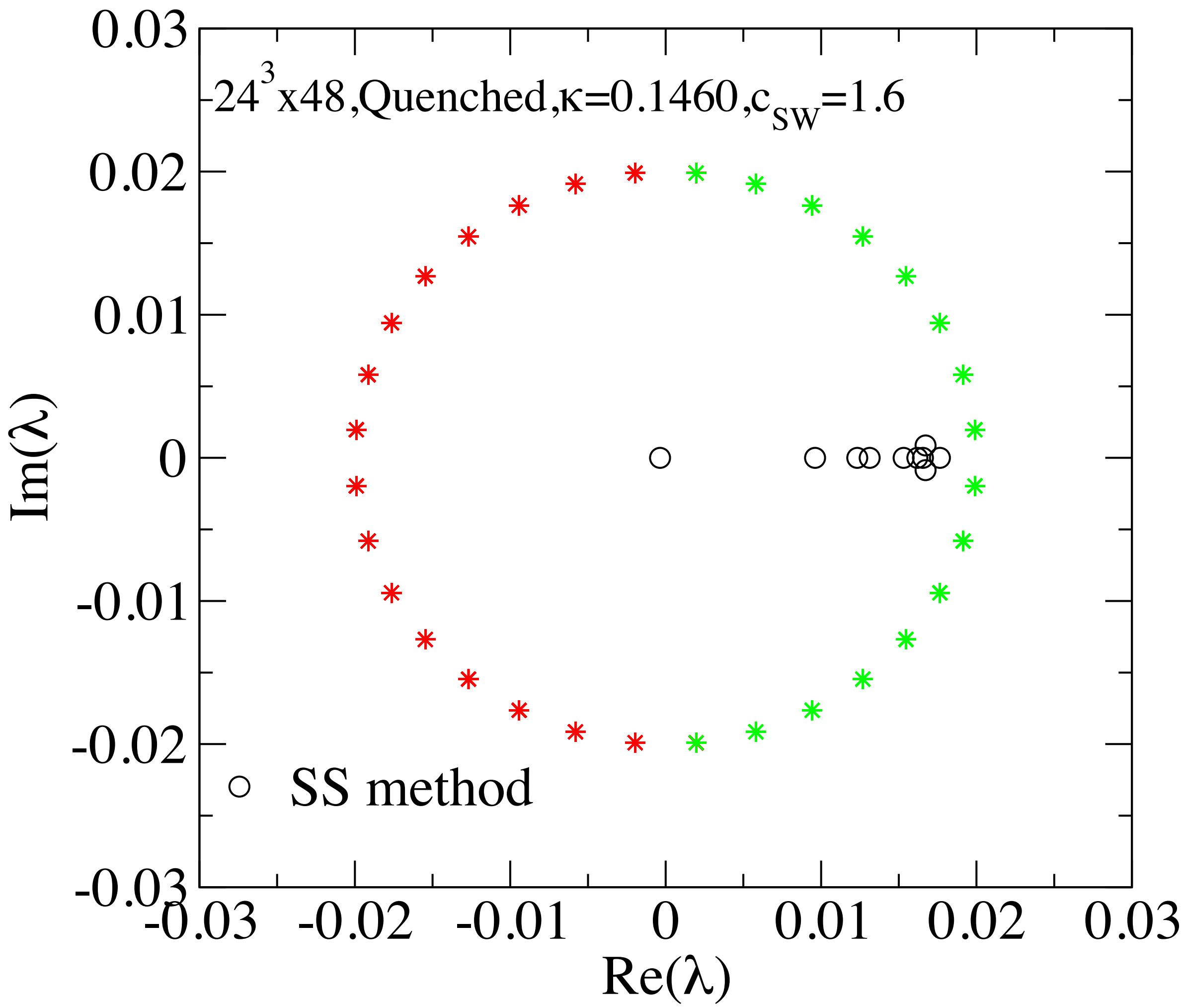
Results

- We also try a larger size of lattice.



- N=32,L=64,M=16, Relative residual norms ≈ 10^{-4}

Results



- N=32,L=196,M=16,Relative residual norms ≈ 10^{-4}

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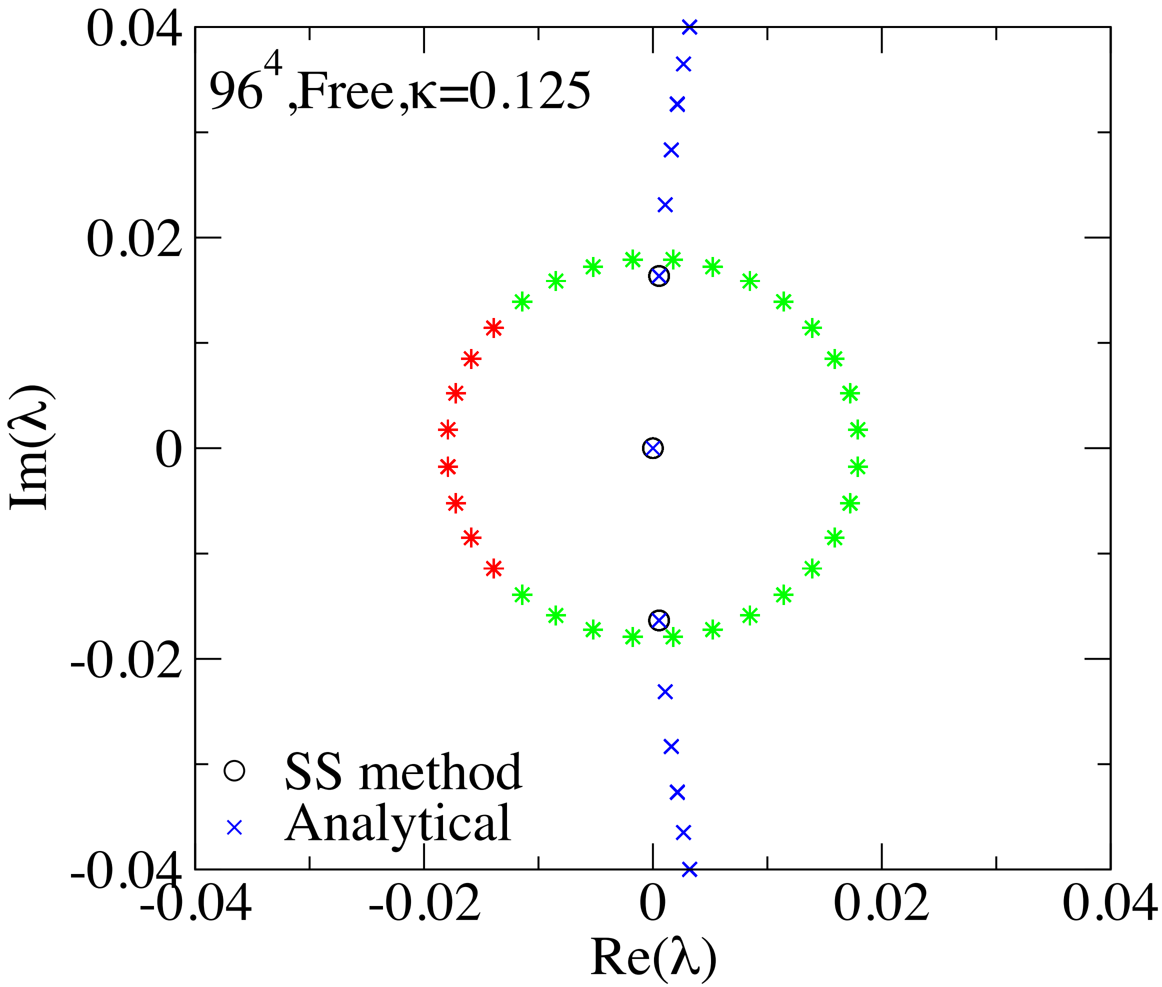
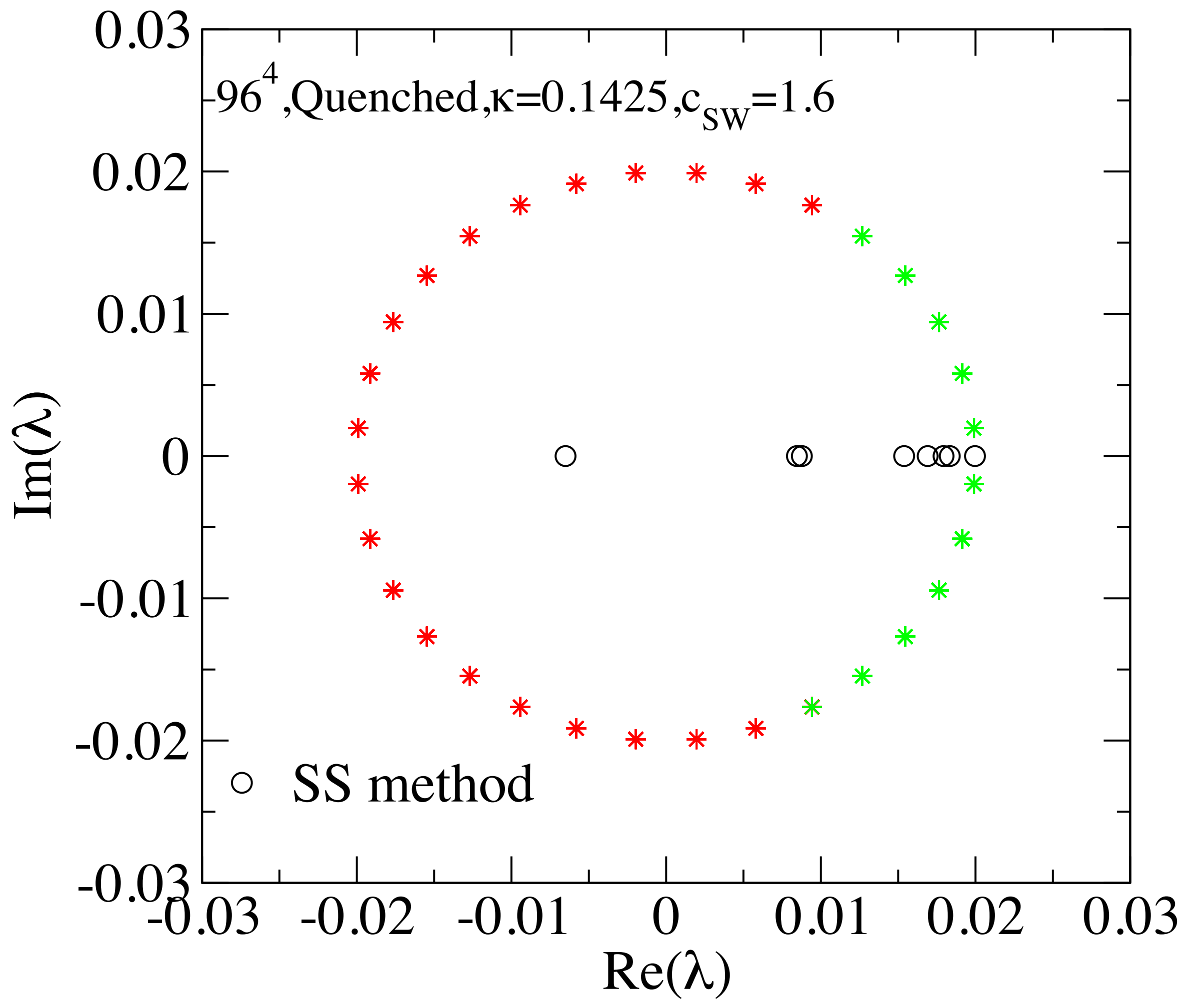
Results



- N=32,L=128,M=16,Relative residual norms ≈ 5×10^{-4}

Results



- N=32,L=32,M=16,Relative residual norms ≈ 10^{-6}

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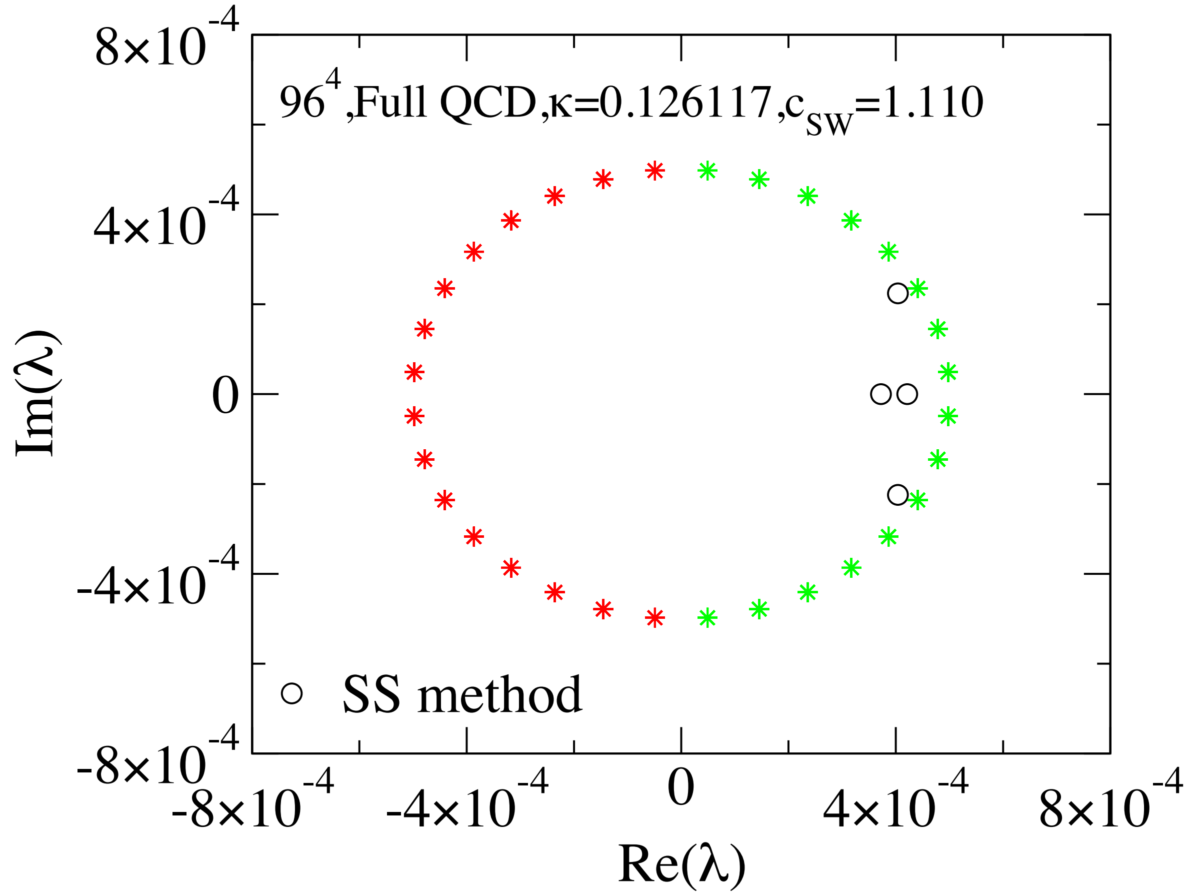
Results



- Full QCD (near the physical point) $U_{\mu}(n)$ data courtesy of Dr. Ukita (Tsukuba Univ.)
- N=32,L=16,M=16, Relative residual norms ≈ $5\text{x}10^{-4}$

Summary

- We have tried to calculate low energy eigenspectrum of the O(a)-improved Wilson-Dirac operator.
- We have implemented the Sakurai-Sugiura method.
- We have dealt with the lattice size up to 96^4.
- We have considered gauge field configurations for free case, quenched approximation, and full QCD.
- Relative residual norms vary from 10^{-7} to 5×10^{-4}.
- Accuracy limited due to slow convergence of the BiCGStab used to solve the shifted linear equations, but we can think that the eigenvalues can be estimated with 3 or more digits of accuracy.
- We need a more efficient iterative solver to the shifted linear equations in order to improve the accuracy.

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