A filtering technique for the temporally reduced matrix of the Wilson fermion determinant

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Motivation

- \( \det \Delta(\mu) \) is a key quantity in finite density lattice QCD.

- **Reduction formula**
  - calculate t-part of \( \det \Delta \) analytically
  \[
  \det \Delta = \xi^{-N_{\text{red}}/2} C_0 \det(\xi + Q)
  \]
  \[
  \xi = e^{-\mu/T}
  \]
  \[
  N_{\text{red}} = 4N_cN_s^3
  \]
  - reduction of the rank of determinant
  - analytic function of \( \mu \)

- The formula requires the eigenvalue calculation of \( Q \).
  - this prohibits the application of the formula to large volume.

- **Purpose**: We would like to develop a way to calculate eigenvalues of the reduced matrix with milder volume dependence.
**Reduced matrix**

\[ Q = (\alpha_1^{-1}\beta_1) \cdots (\alpha_{Nt}^{-1}\beta_{Nt}) \]

Reduced matrix = temporal quark line 
\sim generalization of Polyakov loop

**Block matrices**

\[ \alpha_i = B_ir_- - 2\kappa r_+ \]
\[ \beta_i = (B_ir_+ - 2\kappa r_-)U_A \]

- Spatial hop at t=i
- Temporal link variables
Spectrum of reduced matrix

- Example of eigenvalue distribution

Are there some important eigenvalues, which dominate observables?
Which are physical eigenvalues?

- **Evs near the unit circle** are related to the pion mass at large Nt [Gibbs(’86), Fodor, Szabo, Toth(’07)]
  - reduced matrix \( \sim \) temporal quark line

- **Evs** are related to quasi energy state of quarks
  - reduced matrix \( \sim \) Polyakov loop
  - Nt scaling property [Nagata, et.al. PTEP’13]
    \[
    \lambda_n = e^{-\epsilon_n/T + i\theta_n}
    \]
  - low energy modes are located close to \(|\lambda| \sim 1\) (unit circle)

- **Quark number operator and reduced matrix** [Nagata, 2012]
  - similar to Fermi distribution
  - low energy modes have large contributions

\[
\hat{n} \propto \sum_n \left( \frac{1}{1 + e^{(\epsilon_n - \mu)/T - i\theta_n}} + \frac{1}{1 + e^{(\epsilon_n + \mu)/T + i\theta_n}} \right)
\]
Which are physical eigenvalues?

- Eigenvalues near the unit circle are physically important.

How do we obtain middle eigenvalues efficiently?
Methods

- Physical eigenvalues of the reduced matrix are in the middle of its eigenspectrum

- Sakurai-Sugiura (SS) method
  - An algorithm to obtain eigenvalues that lie in a given domain on the complex plane using contour integrals
  - single version [Sakurai, Sugiura 2003]
  - blocked version [Sakurai, Futamura, Tadano 2013]
Algorithm of SS method

- A generalized eigenvalue problem for matrices A and B
  \[ Ax = \lambda Bx, \quad (A, B \in \mathbb{C}^{n \times n}) \]

- Define a function of \( z \)
  \[ f(z) = u^\dagger (zB - A)^{-1}v, \quad (z \in \mathbb{C}, u, v \in \mathbb{C}^n) \]

  - using a Weirstrass’s canonical form
    \[ P(zB - A)Q = \begin{pmatrix} zI_d - J_d & O \\ O & zN_{n-d} - I_{n-d} \end{pmatrix} \]

- single version: one vector \( v \)
- blocked version: multiple vector for \( v \)
  - Numerical stability is improved with multiple vectors.
Algorithm of SS method (blocked ver.)

- Numerical stability is improved with multiple vectors.
  - useful for the case where the target domain contains many eigenvalues.

\[ S_k = \frac{1}{2\pi i} \int_{\Gamma} z^k (zB - A)^{-1} BV \, dz, \quad k = 1, 2, \ldots, m \]

\[ V = \{ v_1, v_2, \ldots v_L \} \in \mathbb{R}^{n \times L} \]

- Sk gives a rectangular matrix.
- Perform a singular value decomposition for \( S = (S_1, S_2, \ldots S_m) \)

\[ S = U\Sigma W^\dagger \quad S \in \mathbb{C}^{n \times mL} \]

- \( m \) and \( L \) have to be chosen appropriately
Algorithm of SS method (blocked ver.)

- Determine $l$ large singular values

\[ S = U\Sigma W^\dagger \]

\[ \Sigma = (\sigma_1, \sigma_2, \cdots, \sigma_l, \cdots) \]

\[ U = (u_1, u_2, \cdots, u_l, \cdots) \]

- Projection to a small eigen problem

\[ A_l = U_l^\dagger AU_l, \quad B_l = U_l^\dagger BU_l \]

\[ A_l r_j = \omega_j B_l r_j, \]

\[ \lambda_j = \omega_j, \quad \text{Eigen pairs of the original problem} \]

\[ x_j = U_m r_j \]
Note 1: Ring region

- bSS method is extended to a domain surrounded by two boundaries by taking a subtraction:

\[ S_k = \frac{1}{2\pi i} \left( \int_{\Gamma_1} - \int_{\Gamma_2} \right) z^k (z - Q)^{-1} V \, dz \]
Note2 : Cost

• Numerical cost is mostly for $S_k$

$$S_k = \frac{1}{2\pi i} \int_\Gamma z^k (zB - A)^{-1} BV dz,$$

$$V = \{v_1, v_2, \cdots v_L\} \in \mathbb{R}^{n \times L}$$

# of inversion = (Integral points) x (L-vectors)

• If shifted CG algorithm works, it would be one of efficient way to obtain $S_k$.

• But, it turned out that CG converges quite slowly for the reduced matrix.

• We employ the direct method for the inversion.
Result

– Size : $4^4$, Nr=768 (ZGEES : LAPACK, Shur dec.)

$(4^4, L=10, m=24, \varepsilon_{SVD}=1.d-25)$

green points are integral points : 100 for each circle (Probably, it can be reduced to 50 pt.)

• bSS method works well, and are stable for sparse regions.
Result: dense region

- Size: $4^4$, $N_r=768$ (ZGEES: LAPACK, Shur dec.)

- ZGEES and bSS fails for some eigenvalues in dense regions.
Division of rings further

\[(4^4, L=10, m=24, \varepsilon_{\text{SVD}}=1.d-25)\]
other prescriptions for dense region

- Include more vectors in $U$, by decreasing $\varepsilon_{\text{SVD}}$

$$U = (u_1, u_2, \cdots, u_I, \cdots)$$

- increase $m = \max(k)$
- increase the number of vectors $L$
- increase integral points

$$S_k = \frac{1}{2\pi i} \left( \int_{\Gamma_1} - \int_{\Gamma_2} \right) z^k (z - Q)^{-1} V \, dz$$
Dependence on # of vectors in U ($m$)

- $(4^4, L=10, m=24, \varepsilon_{\text{SVD}}=1.d-25)$
- Case 1: $(77, 10, 24, -25)$
- Case 2: $(95, 10, 24, -35)$
- decrease more singular values

- $(\text{# of obtained ev, } L, \text{ max}(k), \text{eps (SVD)})$ (97 eigenvalues inside)
Dependence on # of vectors $L$

(4, $L=10$, $m=24$, $\epsilon_{SVD}=1.d-25$)

• ( # of obtained ev, $L$, max(k), eps (SVD)) (97 eigenvalues inside)
• case 1 : (77, 10, 24, -25)
• case 3 : (99, 20, 24, -25)
• include more vectors
Summary and future work

- blocked SS method successfully reproduces eigenvalues near the unit circle.
- It also works for dense region with some prescriptions.
- The inversion was done using the direct method due to ill-conditioned problem of the reduced matrix.
- We need to find an iterative method to calculate the inversion for the reduced matrix.
Algorithm of SS method (single ver.)

• Calculate moments for a given contour

\[
\mu_k = \frac{1}{2\pi i} \int_{\Gamma} (z - \gamma)^k f(z) \, dz
\]

\[
= \sum_{i=1}^{m} a_i (\lambda_i - \gamma)^k
\]

• An eigen problem for the following matrices reproduces the eigenvalues of the original eigen problem

\[
H_1 = \begin{pmatrix}
\mu_0 & \mu_1 & \cdots & \mu_{m-1} \\
\mu_1 & \mu_2 & \cdots & \mu_m \\
\vdots & \vdots & \ddots & \vdots \\
\mu_{m-1} & \mu_m & \cdots & \mu_{2m-2}
\end{pmatrix}
\]

\[
H_2 = \begin{pmatrix}
\mu_1 & \mu_2 & \cdots & \mu_m \\
\mu_2 & \mu_3 & \cdots & \mu_{m+1} \\
\vdots & \vdots & \ddots & \vdots \\
\mu_m & \mu_{m+1} & \cdots & \mu_{2m-1}
\end{pmatrix}
\]

\[
H_2 = \eta H_1 \quad \eta = \lambda - \gamma
\]
Dependence on integral points

- $N_{\text{int}} = 50$ and $100$
• singular values
Result (singular values dependence)

(4x4x4x4, L=10, m=40)

<table>
<thead>
<tr>
<th>$[r_1, r_2]$</th>
<th>$N_{ev}$</th>
<th>$N_{ev}(\epsilon = 10^{-25})$</th>
<th>$N_{ev}(\epsilon = 10^{-35})$</th>
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<tbody>
<tr>
<td>[0.03, 0.02]</td>
<td>4</td>
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<td>[0.02, 0.01]</td>
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<td>[0.01, 0.008]</td>
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<td>31</td>
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<tr>
<td>[0.008, 0.006]</td>
<td>55</td>
<td>50</td>
<td>51</td>
</tr>
<tr>
<td>[0.006, 0.008]</td>
<td>97</td>
<td>77</td>
<td>95</td>
</tr>
</tbody>
</table>
Result (L-dependence)

- Results

(4x4x4x4, L=10, m=40)

![Graph showing the dependence of L on the results]
Result-Nt-dependence

- Nt

bSS(L=10, m=24)

Re[λ]

Im[λ]

LAPACK

bSS

25
Algorithm (chart)

1. preparation
   1. set the integral domain (annulus with r1, r2)
   2. prepare L vectors, which has 1 or -1 for each element at random
   3. determine moments m

2. integral and obtain moments
   1. the inversion $(A-zB)^{-1}$ for each point on the contours
   2. (this work, we employ direct method)

3. filtering for a subspace
   1. m is determined according to a criterion, which determines the number of relevant singular value.

4. solve the small eigen problem
**Reduction formula for fermion determinant**

- Fermion determinant: $\det \Delta$
  - It includes chemical potential, and causes the sign problem.
  - It appears in a reweighting factor in avoiding the sign problem.

- Reduction formula/propagator matrix method
  - Perform the temporal part of $\det \Delta$ **analytically**

\[
\Delta = B - e^{\mu a} V - e^{-\mu a} V^\dagger
\]

\[
\Delta = \begin{pmatrix}
\square & \triangle & \triangle \\
\triangle & \square & \triangle \\
\triangle & \cdot & \cdot \\
\cdot & \cdot & \triangle \\
\triangle & \triangle & \square 
\end{pmatrix}
\]
Which are physical eigenvalues?

- Eigenvalues near the unit circle are physical modes.