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 Δ analytically

$$\det \Delta = \xi^{-N_{\rm red}/2} C_0 \det(\xi + Q)$$

$$\xi = e^{-\mu/T}$$

$$N_{\rm red} = 4 N_c N_s^3$$

  - reduction of the rank of determinant
  - analytic function of μ

[Gibbs ('86). Hasenfratz, Toussaint('92). Adams('03, '04), Borici('04). KN&AN('10), Alexandru &Wenger('10)]

- 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

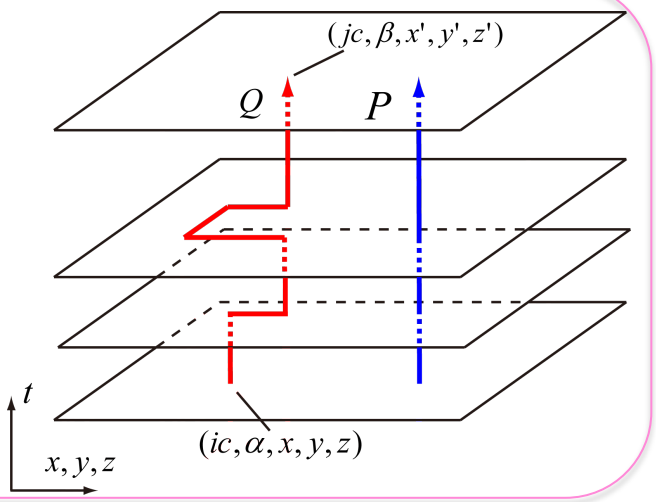
Nagata, Nakamura ('10)

- Reduced matrix

$$Q = (\alpha_1^{-1}\beta_1)\cdots(\alpha_{N_t}^{-1}\beta_{N_t})$$

reduced matrix = temporal quark line

~ generalization of Polyalov loop



- Block matrices

$$\alpha_i = B_i r_- - 2\kappa r_+,$$

spatial hop at t=i

$$\beta_i = (\underline{B_i r_+} - 2\kappa r_-)U_4$$

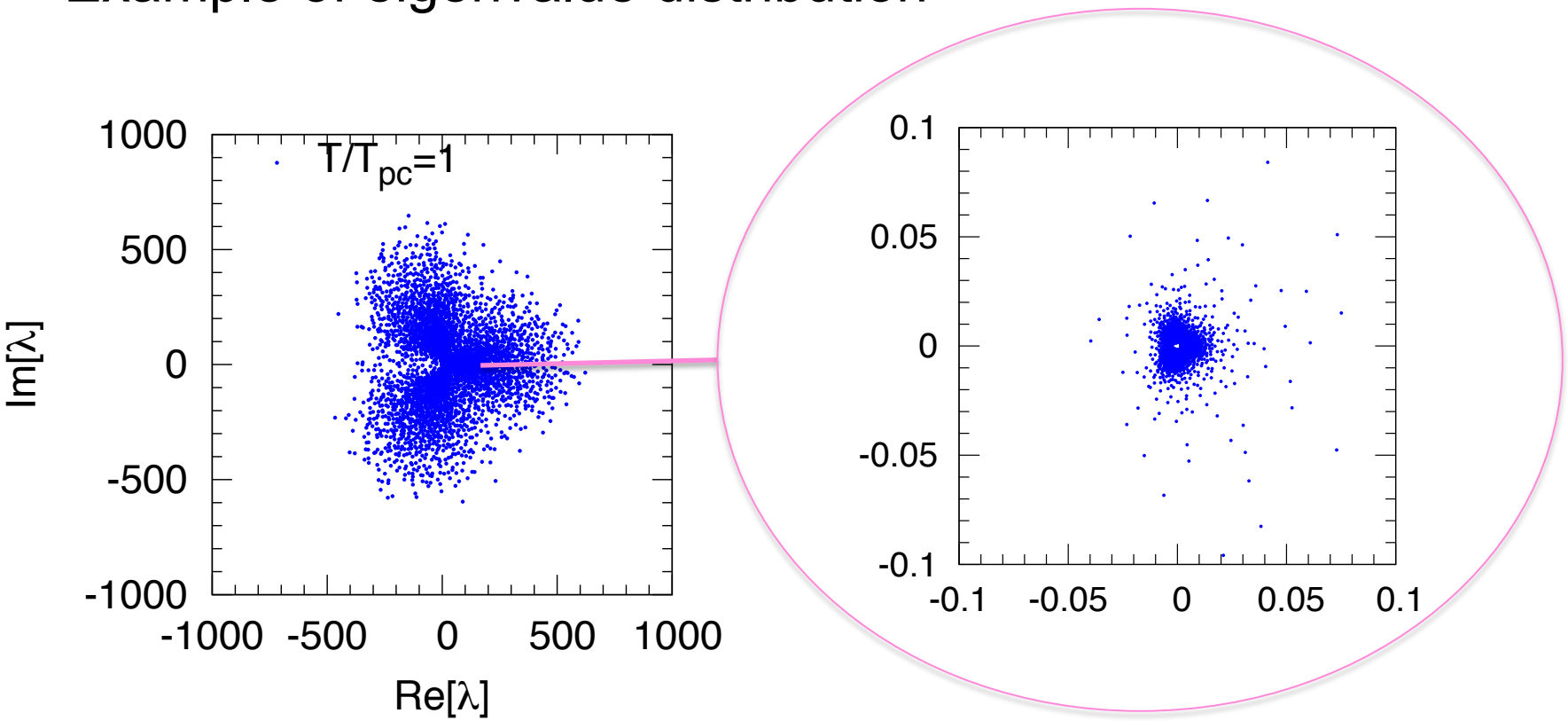
spatial hop at t=i & tempral hop to t=i+1

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 ~ temporal quark line

- Evs are related to quasi energy state of quarks
  - reduced matrix ~ Polyakov loop
  - Nt scaling property [Nagata, et.al. PTEP'13]

$$\lambda_n = e^{-\epsilon_n/T + i\theta_n}$$

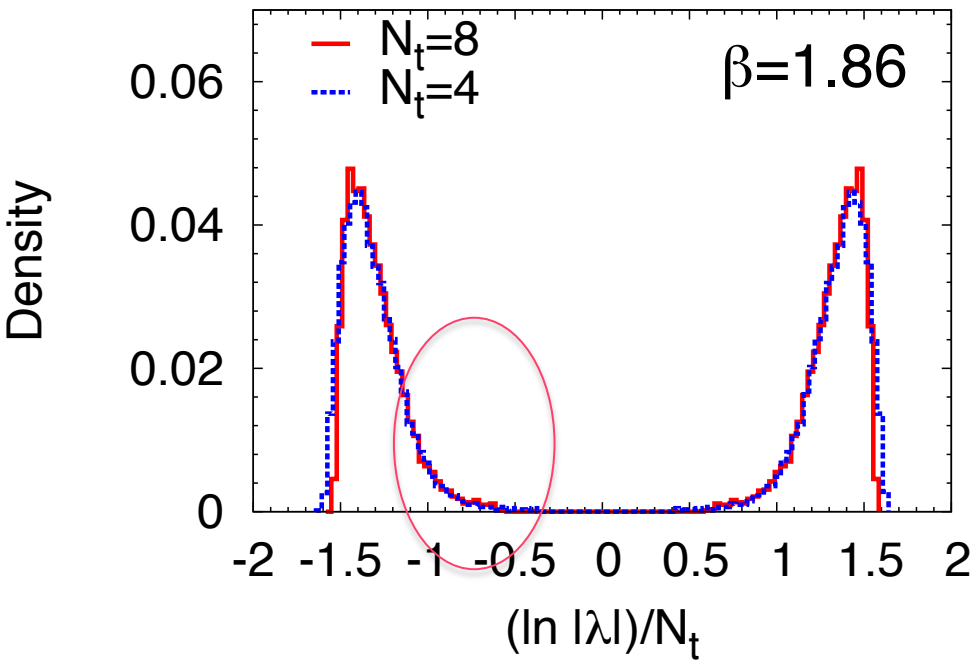
  - low energy modes are located close to $|\lambda| \sim 1$ (unit circle)

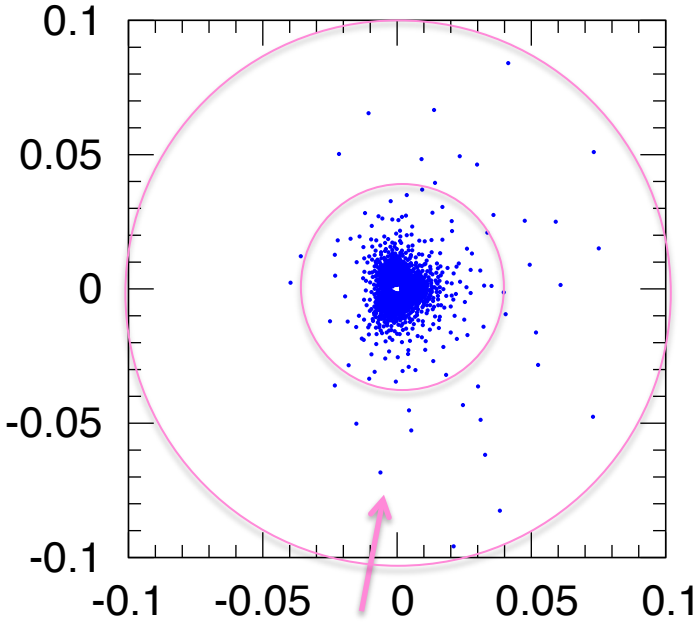
- Quark number operator and reduced matrix [Nagata, 2012]
  - similar to Fermi distribution
  - low energy modes have large contributions

$$\hat{n} \propto \sum_n \left(\frac{1}{1 + e^{(\epsilon_n - \mu)/T - i\theta_n}} + \frac{1}{1 + e^{(\epsilon_n + \mu)/T + i\theta_n}} \right)$$

Which are physical eigenvalues ?

- eigenvalues near the unit circle are physically important



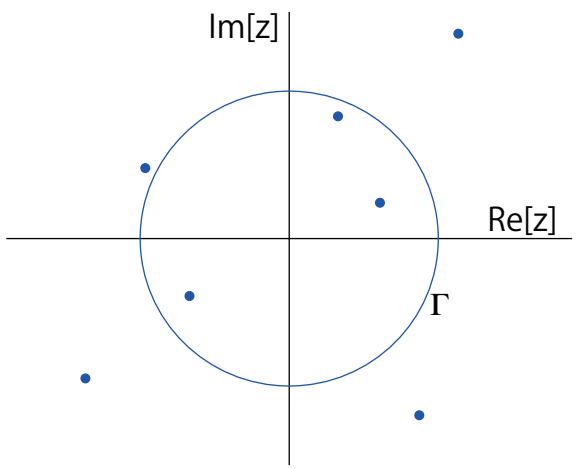


How do we obtain middle eigenvalues efficiently ?

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

$$Ax = \lambda Bx, (A, B \in \mathbb{C}^{n \times n})$$

- Define a function of z

$$f(z) = u^{\dagger}(zB - A)^{-1}v, (z \in \mathbb{C}, u, v \in \mathbb{C}^{n})$$

  – using a Weirstrass's canonical form

$$= \sum_{i=1}^{d} a_i \frac{1}{z - \lambda_i} + \underline{g(z)}$$

analytic part

$$P(zB - A)Q = \begin{pmatrix} zI_d - J_d & O \\ O & zN_{n-d} - I_{n-d} \end{pmatrix}$$

- 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.

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

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

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

$$S = U\Sigma W^\dagger \qquad S \in C^{n\times mL}$$

  - *m* and *L* have to be chosen appropriately

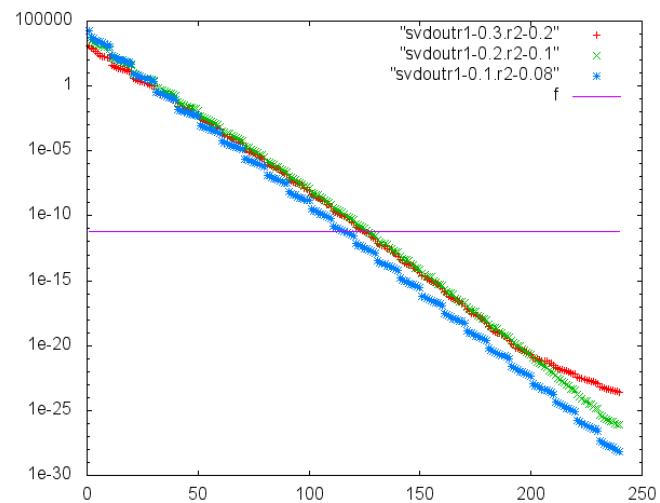
Algorithm of SS method (blocked ver.)

- Determine *l* large singular values

$$S = U\Sigma W^{\dagger}$$

$$\Sigma = \underline{(\sigma_1, \sigma_2, \cdots, \sigma_l,} \cdots)$$

$$U = \underbrace{(u_1, u_2, \cdots, u_l,}_{U_l} \cdots)$$



- Projection to a small eigen problem

$$A_l = U_l^{\dagger} A U_l, B_l = U_l^{\dagger} B U_l$$

$$A_l r_j = \omega_j B_l r_j,$$

$$\lambda_j = \omega_j,$$

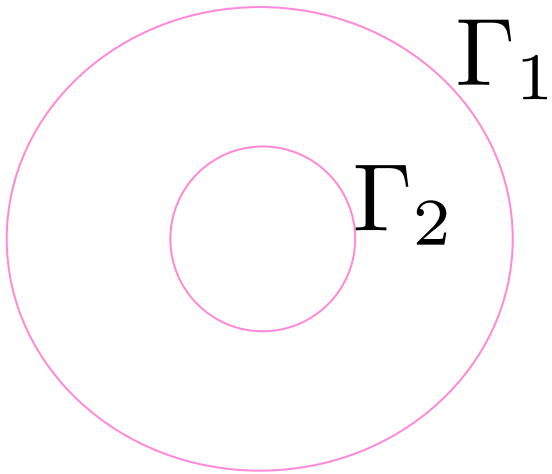
$$x_j = U_m r_j$$

Eigen pairs of the original problem

Note 1: Ring region

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

$$S_k = \frac{1}{2\pi i}\left(\int_{\Gamma_1} - \int_{\Gamma_2}\right) z^k (z-Q)^{-1} V dz$$



Note2 : Cost

- Numerical cost is mostly for Sk

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

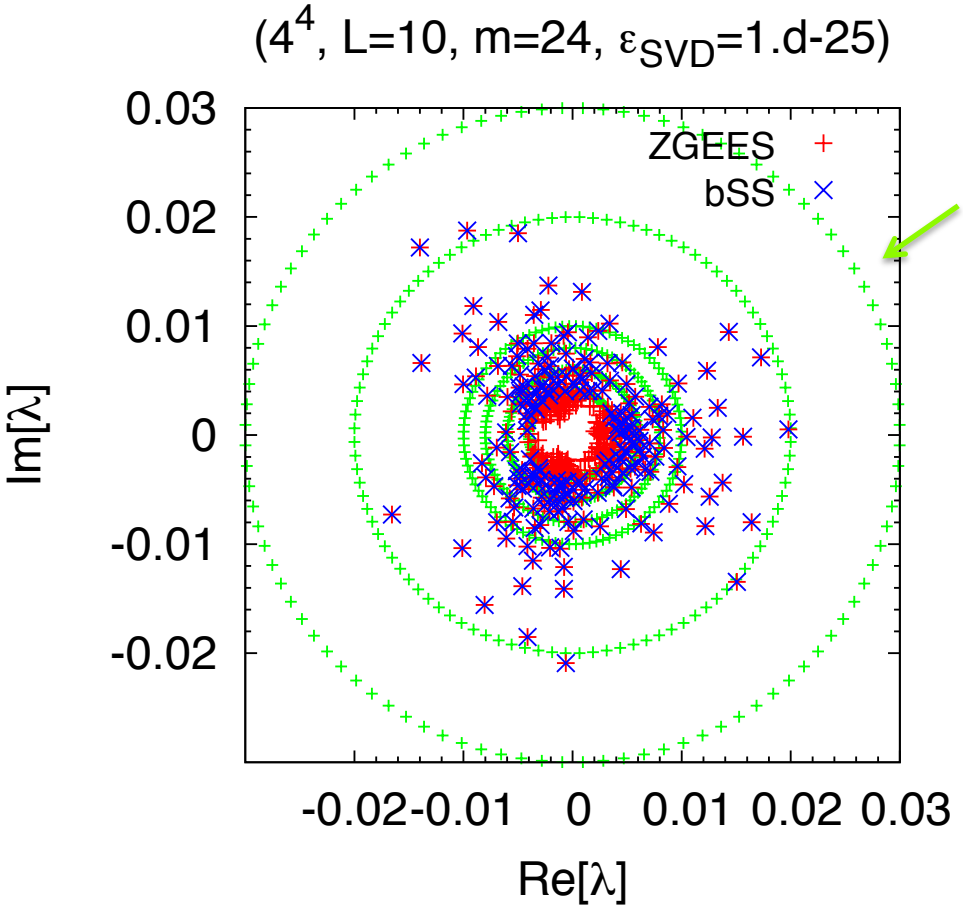
$$V = \{v_1, v_2, \cdots v_L\} \in \mathbb{R}^{n\times L}$$

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

- If shifted CG algorithm works, it would be one of efficient way to obtain Sk.
- 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.)

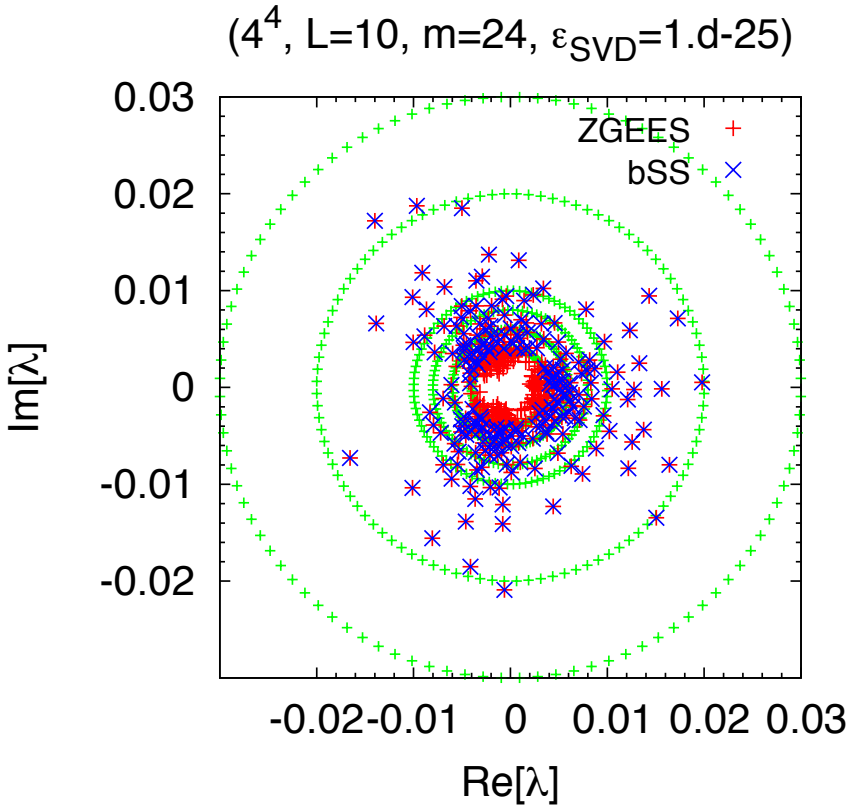


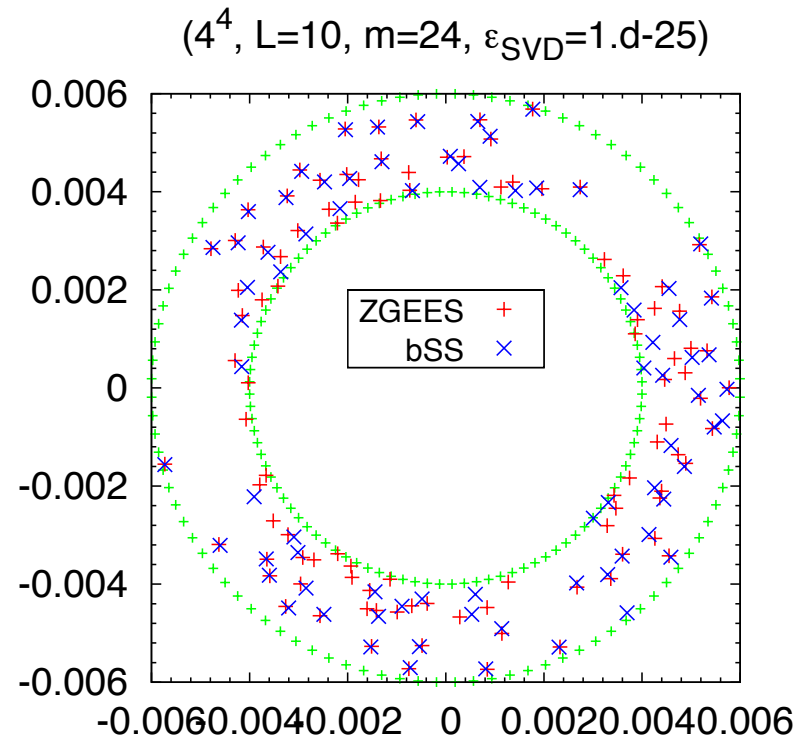
green points are integral points : 100 for each circle (Probably, it can be reduced to 50 pt.)

- bSS method works well, and are stable for sparse regions.

Result : dense region

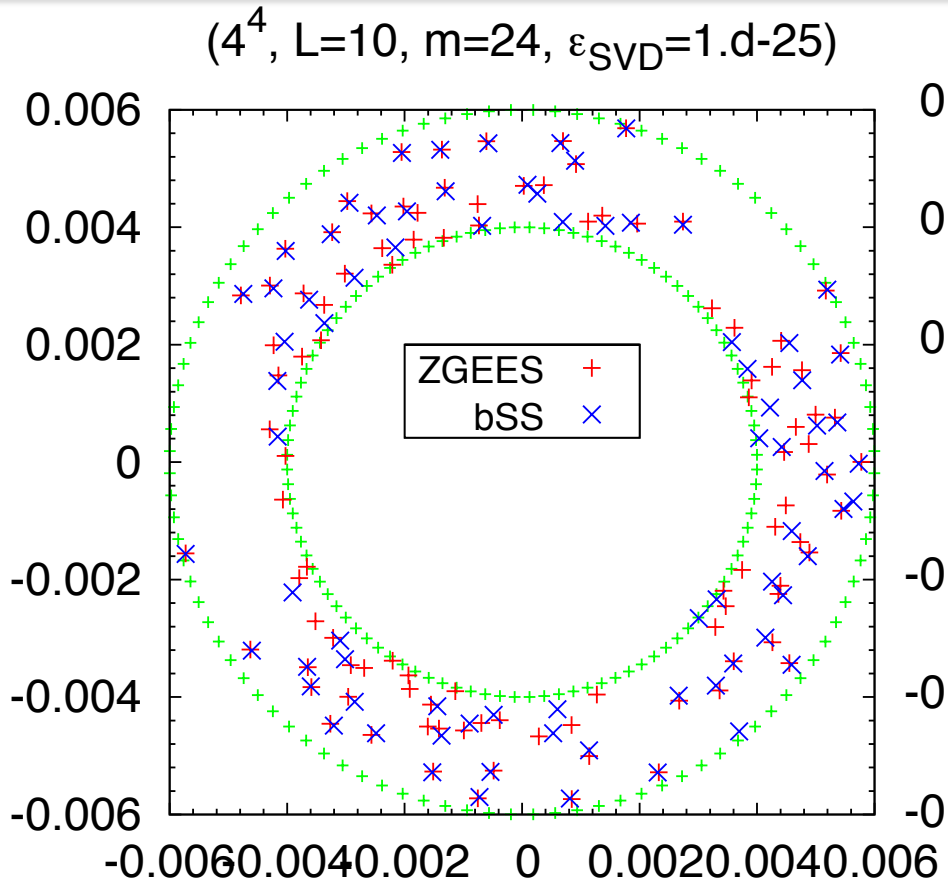
– Size : 4^4, Nr=768 (ZGEES : LAPACK, Shur dec.)

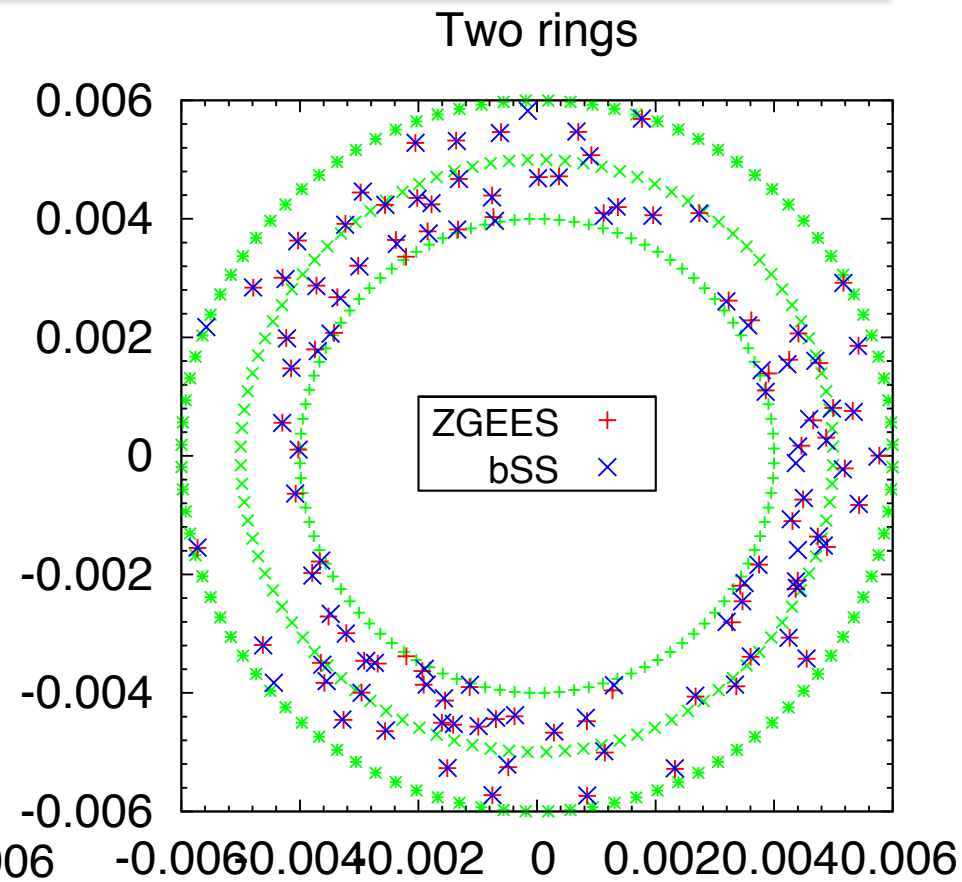




- bSS fails for some eigenvalues in dense regions.

Division of rings further

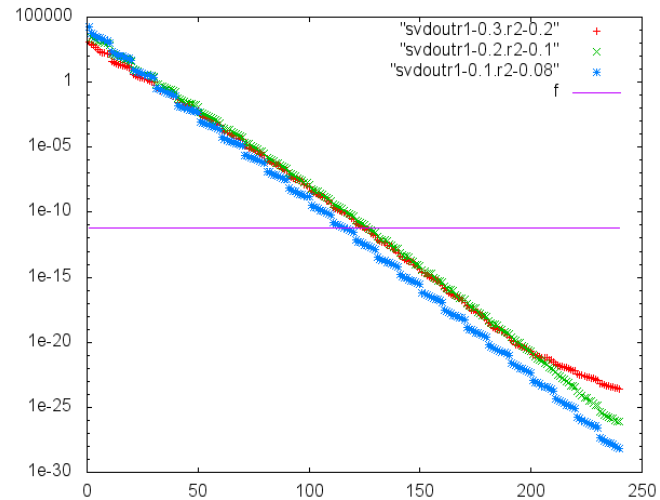




other prescriptions for dense region

- Include more vectors in U, by decreasing ε_{SVD}

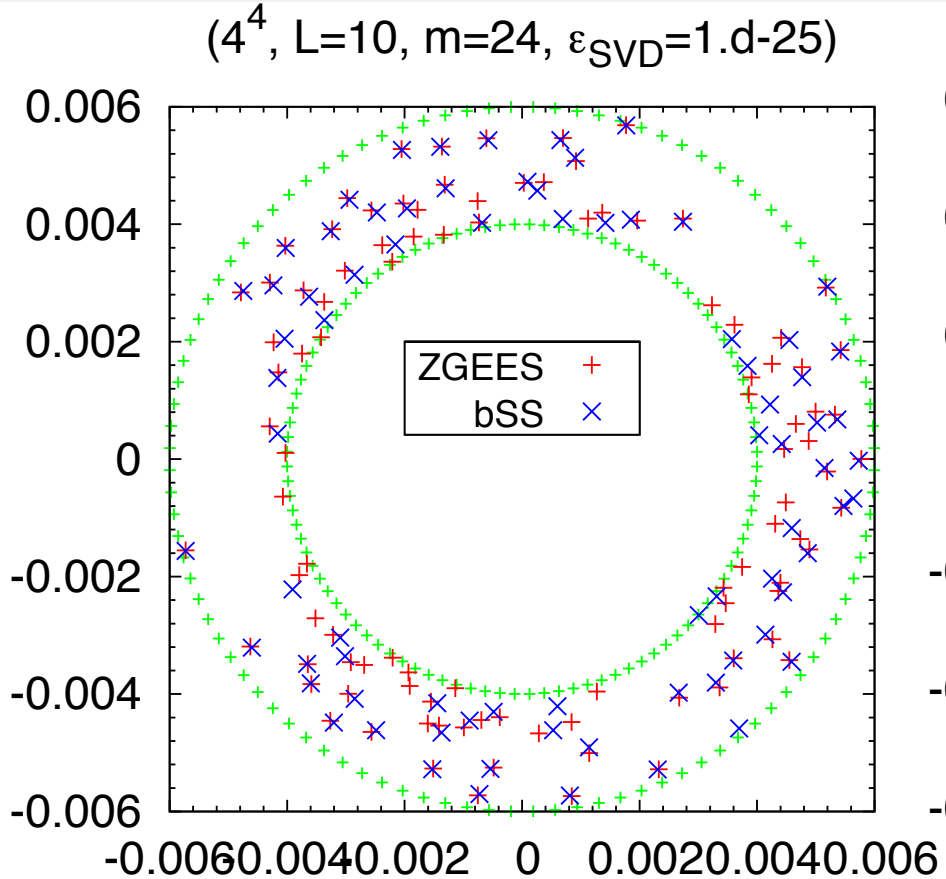
$$U = (u_1, u_2, \cdots, u_l, \cdots)$$

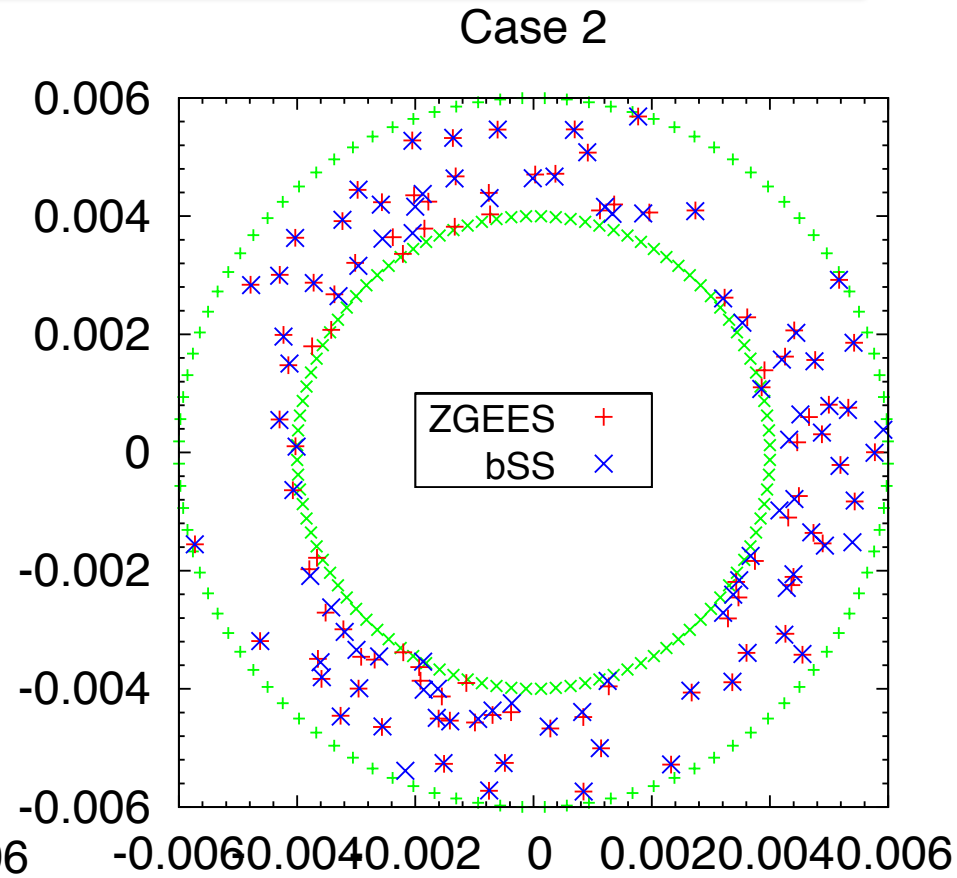


- increase m =max(k)
- increase the number of vectors L
- increase integral points

$$S_k = \frac{1}{2\pi i}\left(\int_{\Gamma_1} - \int_{\Gamma_2}\right) z^k (z-Q)^{-1} V dz$$

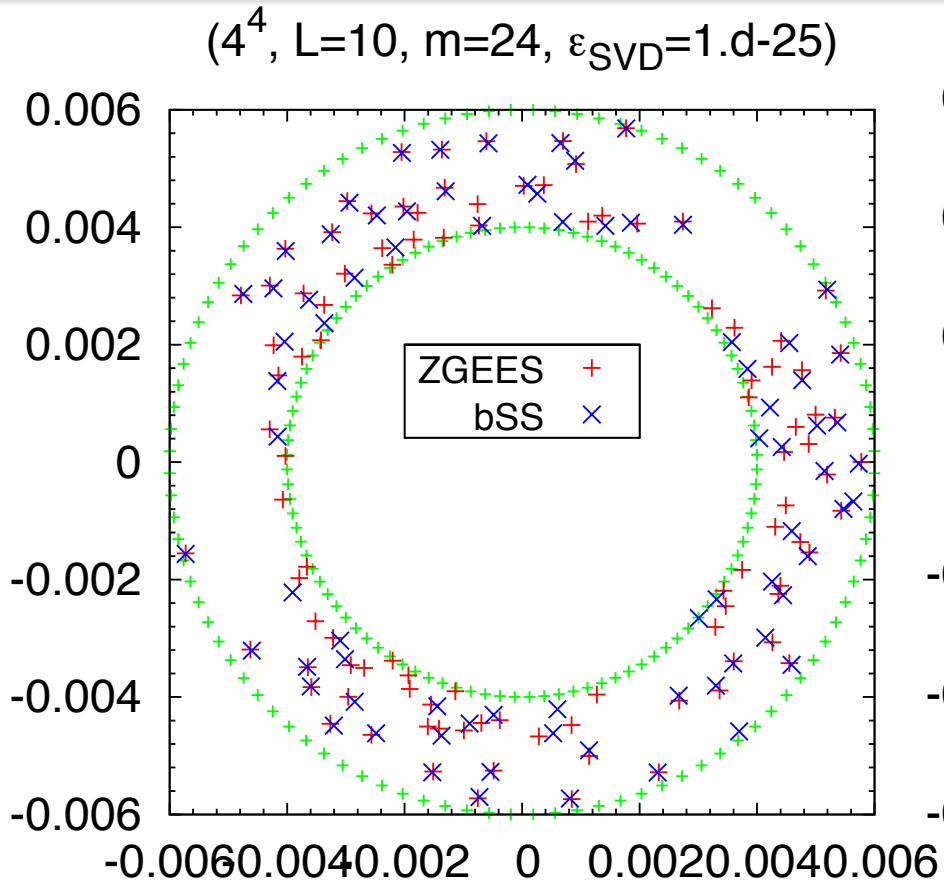
Dependence on # of vectors in U (*m*)

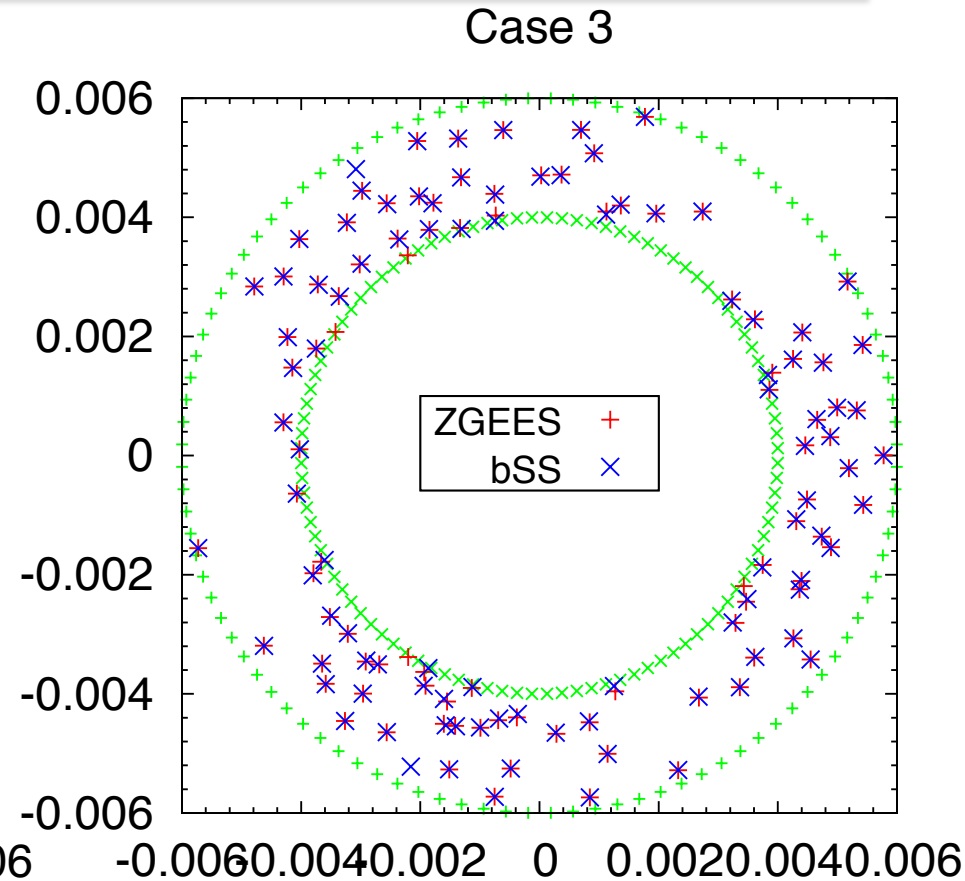




- (# of obtained ev, L, max(k), eps (SVD)) (97 eigenvalues inside)
- case 1 : (77, 10, 24, -25)
- case 2 : (95, 10, 24, -35)
- decrease more singular values

Dependence on # of vectors *L*





- (# 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.

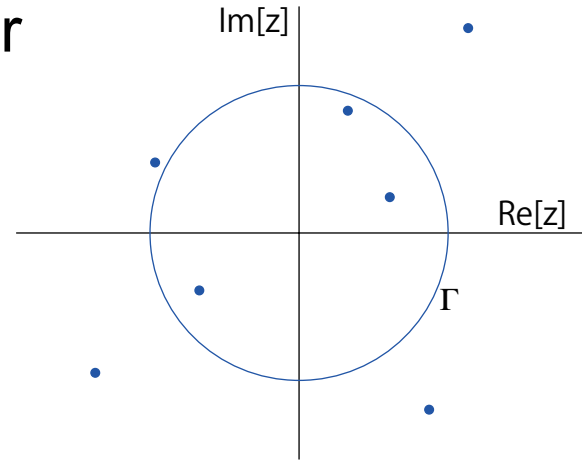
- The inversion was done using the direct method due to ill-conditioned problem of the reduced matrix.

- 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

$$\mu_k = \frac{1}{2\pi i}\int_\Gamma (z-\gamma)^k f(z)dz$$
$$= \sum_{i=1}^{m} a_i(\lambda_i - \gamma)^k$$



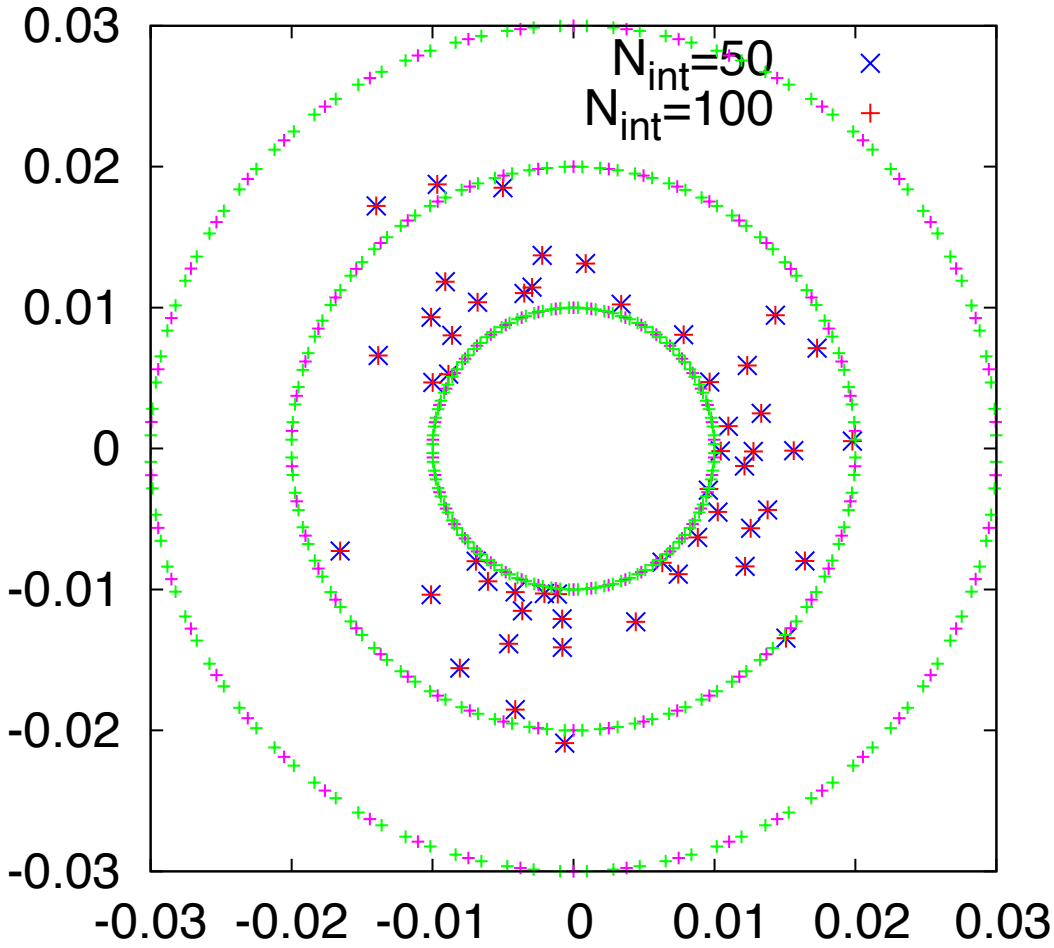
- An eigen problem for the following matrices reproduces the eigenvalues of the original eigen problem

$$H_1 = \begin{pmatrix} \mu_0 & \mu_1 & \cdots & \mu_{m-1} \\ \mu_1 & \mu_2 & \cdots & \mu_m \\ \vdots & \vdots & & \vdots \\ \mu_{m-1} & \mu_m & \cdots & \mu_{2m-2} \end{pmatrix} \qquad H_2 = \begin{pmatrix} \mu_1 & \mu_2 & \cdots & \mu_m \\ \mu_2 & \mu_3 & \cdots & \mu_{m+1} \\ \vdots & \vdots & & \vdots \\ \mu_m & \mu_{m+1} & \cdots & \mu_{2m-1} \end{pmatrix}$$

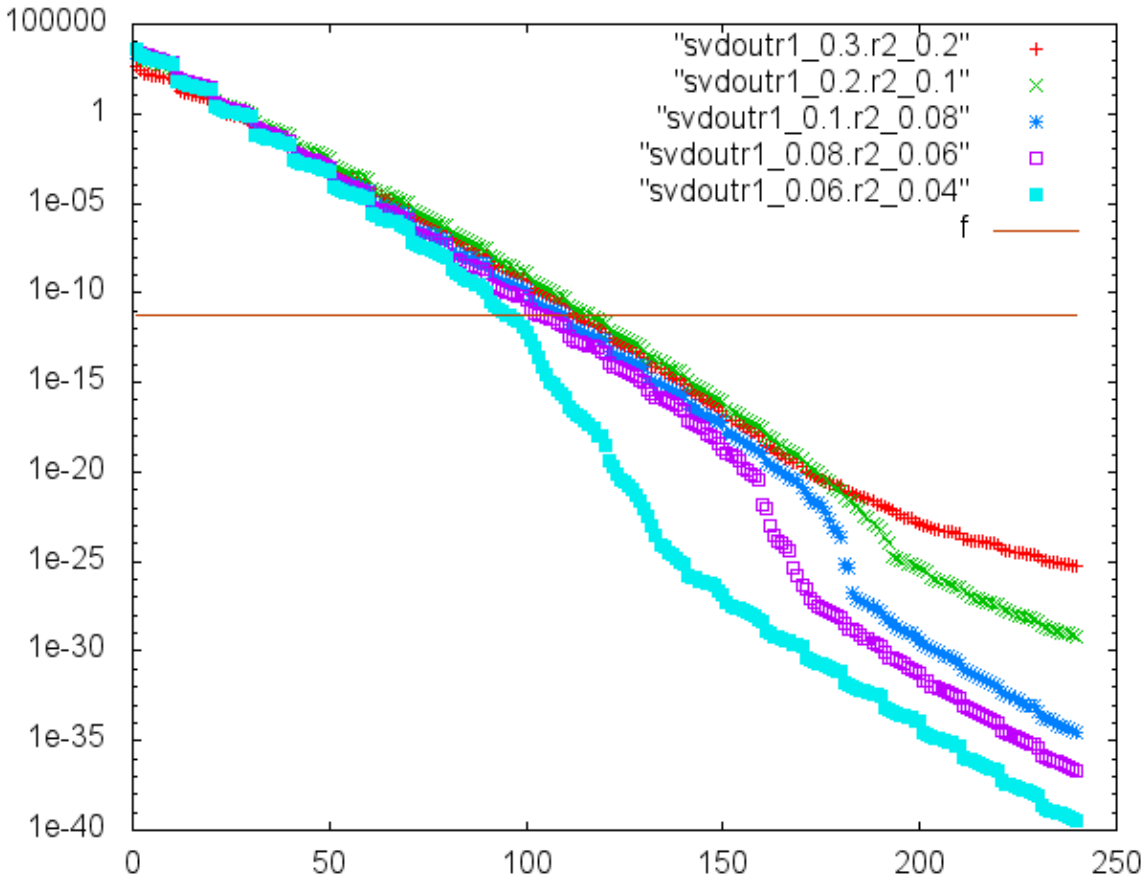
$$H_2 = \eta H_1 \qquad \eta = \lambda - \gamma$$

Dependence on integral points

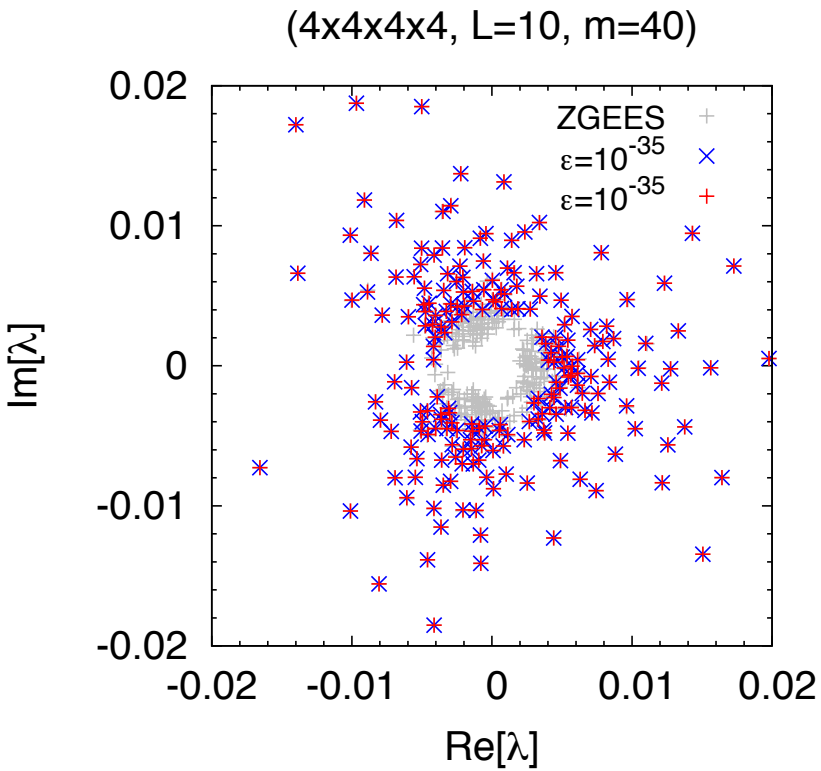
- Nint = 50 and 100



- singular values



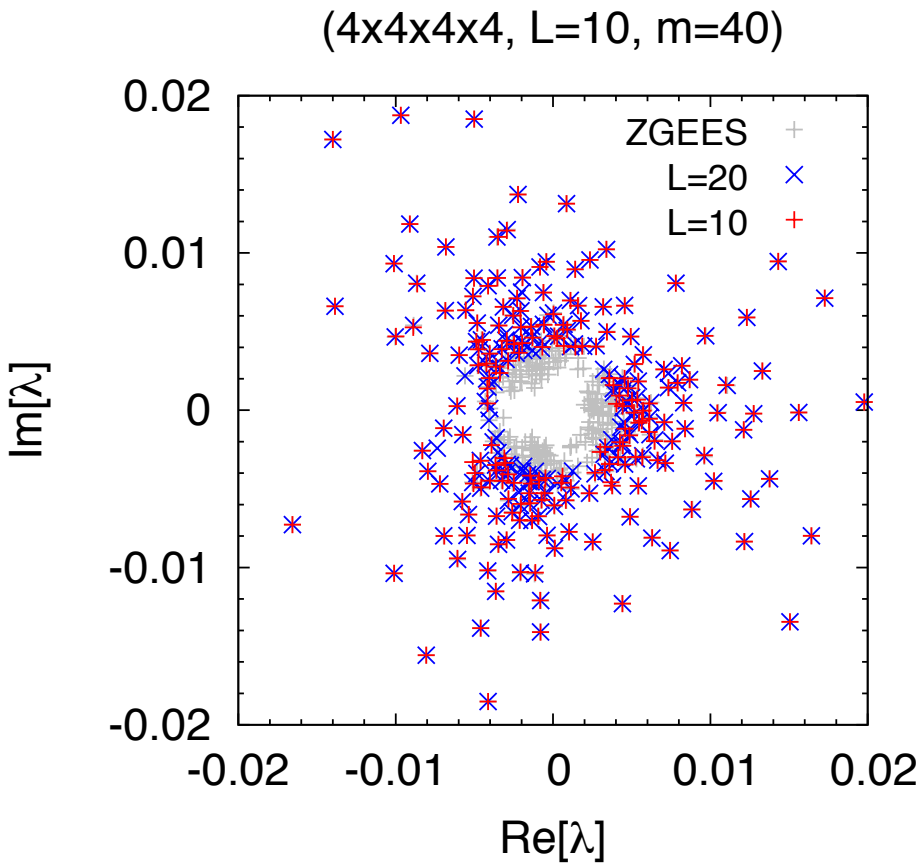
Result (singular values dependence)



$[r_1, r_2]$	$N_{\rm ev}$	$N_{\rm ev}(\epsilon = 10^{-25})$	$N_{\rm ev}(\epsilon = 10^{-35})$
$[0.03, 0.02]$	4	4	4
$[0.02, 0.01]$	48	48	48
$[0.01, 0.008]$	29	29	31
$[0.008, 0.006]$	55	50	51
$[0.006, 0.008]$	97	77	95

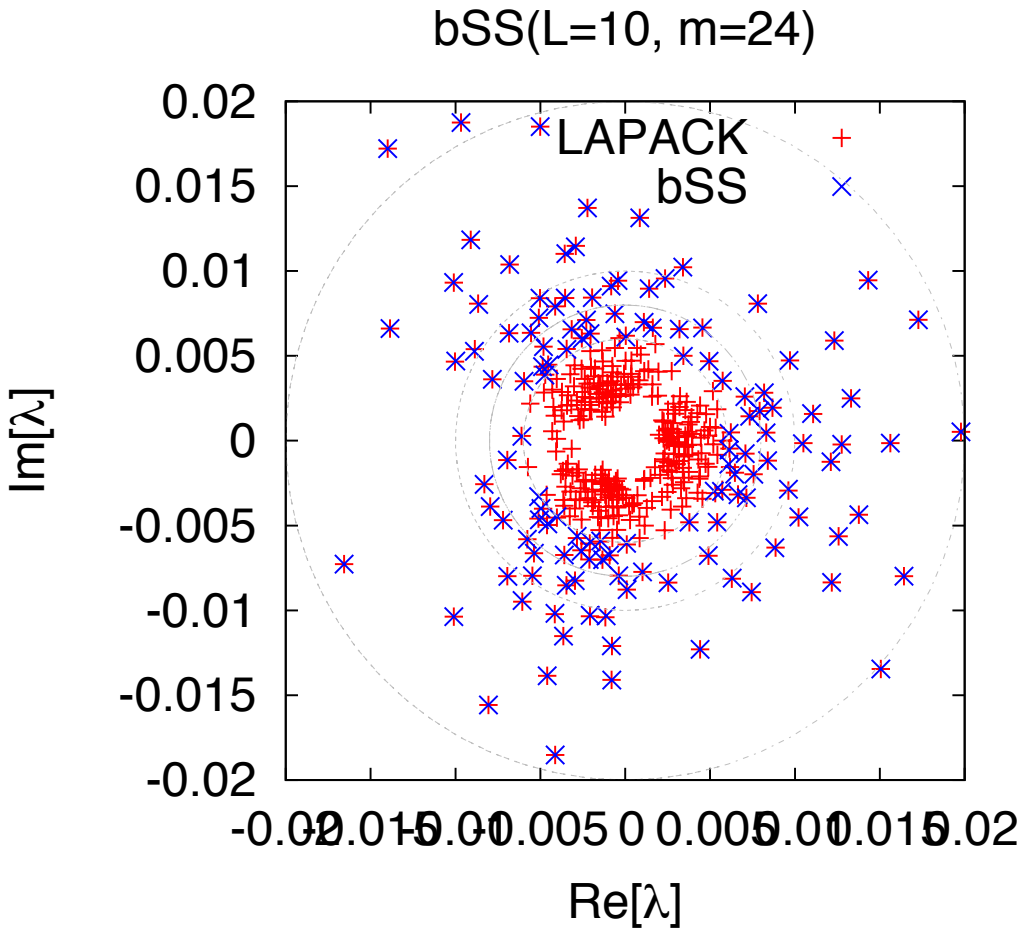
Result(L-dependence)

- Results



Result-Nt-dependence

- Nt



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 Δ
  - 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 Δ analytically

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

$$\Delta = \begin{pmatrix} \square & \triangle & & & \triangle \\ \triangle & \square & \triangle & & \\ & \triangle & \ddots & & \\ & & & \ddots & \triangle \\ \triangle & & & \triangle & \square \end{pmatrix}$$

Which are physical eigenvalues ?

- eigenvalues near the unit circle are physical modes