Comparing iterative methods to compute the overlap Dirac operator at nonzero chemical potential

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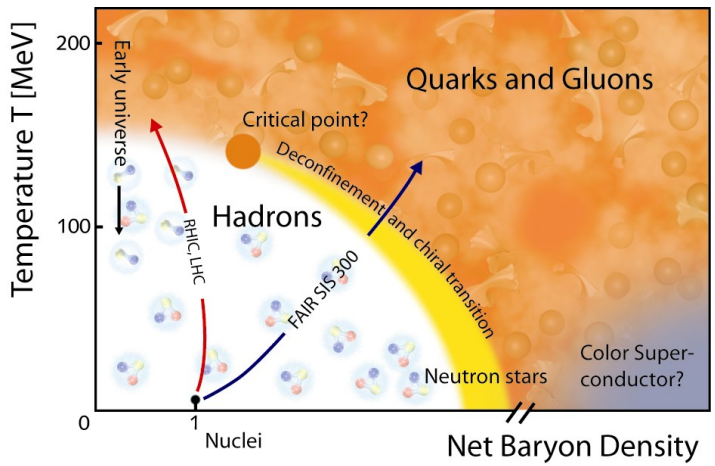
Outline

1. Lattice implementation of chiral symmetry at nonzero quark density
   - Overlap Dirac operator at nonzero quark chemical potential
   - Sign function of non-Hermitian matrix
2. Iterative methods for function of non-Hermitian matrix
   - Arnoldi approximation
   - Two-sided Lanczos approximation
   - Deflation
   - Results



Chiral symmetry on the lattice

- chiral symmetry on the lattice – Ginsparg-Wilson relation:

$$\{D, \gamma_5\} = aD\gamma_5 D$$

- massless overlap Dirac-operator (Neuberger-Narayanan)

$$D_{\text{ov}} = \mathbb{1} + \gamma_5 \,\text{sign}(\gamma_5 D_W)$$

- D_{ov} satisfies GWR because $\text{sign}^2(A) = \mathbb{1}$
- kernel $\gamma_5 D_W$ Hermitian $\rightarrow \gamma_5 D_{\text{ov}} = D_{\text{ov}}^\dagger \gamma_5$ (γ_5-Hermiticity)
- D_{ov} has exact zero modes with definite chirality $\langle \gamma_5 \rangle = \pm 1$ reflecting topological charge of gauge configuration (Atiyah-Singer index theorem)

Chiral symmetry on the lattice at nonzero quark density

Generalize overlap Dirac operator to nonzero quark chemical potential

- replace D_W by $D_W(\mu)$ in overlap definition:

Overlap operator at $\mu \neq 0$

$$D_{\text{ov}}(\mu) = \mathbb{1} + \gamma_5 \,\text{sign}(\gamma_5 D_W(\mu))$$

JB, Wettig PRL97(012003) 2006

Wilson-Dirac operator at $\mu \neq 0$

$$D_W(\mu) = 1 - \kappa \sum_{i=1}^{3} (T_i^+ + T_i^-) - \kappa (e^{\mu} T_4^+ + e^{-\mu} T_4^-)$$

with $\quad (T_\nu^\pm)_{yx} = (1 \pm \gamma_\nu) U_{x,\pm\nu} \delta_{y,x\pm\hat{\nu}}$

Hasenfratz-Karsch 1983, Kogut et al. 1983

- kernel $\gamma_5 D_W(\mu)$ no longer Hermitian:

$D_{\text{ov}}(\mu)$ requires definition of sign of a non-Hermitian matrix

Function of a matrix

- spectral definition of matrix function:
  - if A diagonalizable: $A = U\,\mathrm{diag}\{\lambda_i\}U^{-1}$

$$f(A) = U\,\mathrm{diag}\{f(\lambda_i)\}U^{-1}$$

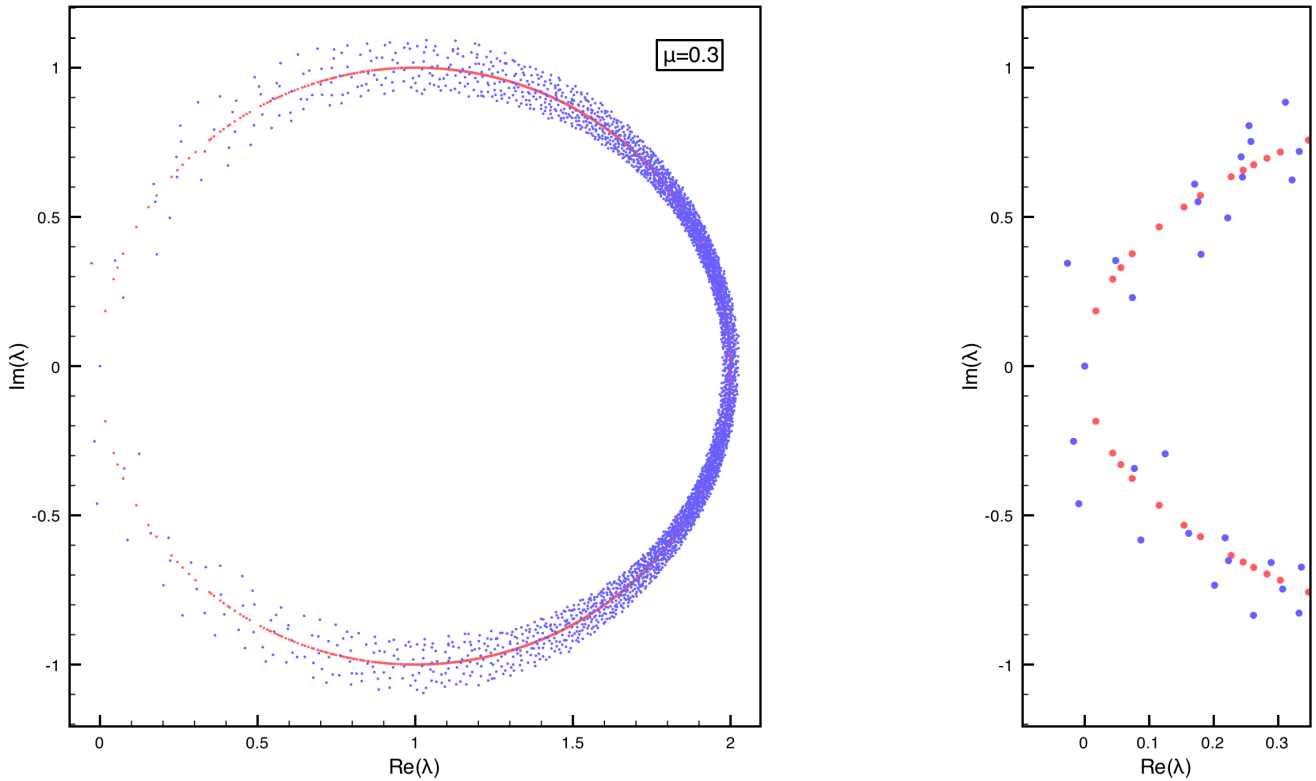
    with complex eigenvalues $\lambda_1, \ldots, \lambda_N$ and eigenvector matrix U
  - if A not diagonalizable: spectral definition using Jordan canonical form
- Sign function of non-Hermitian matrix requires sign of complex number:

$$\mathrm{sign}(z) = \frac{z}{\sqrt{z^2}} = \mathrm{sign}(\mathrm{Re}\, z)$$

  - ensures $\mathrm{sign}^2(z) = 1$
  - gives correct result for $z \in \mathbb{R}$
- definition ensures $\mathrm{sign}^2(A) = \mathbb{1}$

Typical spectrum ($V = 4^4, \beta = 5.1, m_W = -2$)

$$\mu = 0.3$$



- $D_{\text{ov}}(\mu)$ satisfies Ginsparg-Wilson relation → lattice chiral symmetry
- exact zero modes with definite chirality
- naturally violates γ_5-Hermiticity → spectrum no longer on circle

Iterative method for function of non-Hermitian matrix

- exact computation of $\mathrm{sign}(A)$ only possible for small volumes
  - memory requirements (store full matrix)
  - computation time (compute full diagonalization)
- develop iterative method to compute $f(A)b$ for non-Hermitian A
- exact statement: for the unique polynomial $P_K(z)$ which interpolates $f(z)$ at all eigenvalues of A,

$$P_K(A)b = f(A)b \quad \text{for any vector } b$$

- approximation method for $y = f(A)b$:

  construct good low degree polynomial approximation to f on $\lambda(A)$ wrt b
  - depends on spectrum of A
  - depends on decomposition of b in eigenvectors of A

Constructing an Arnoldi basis

- Krylov subspace: $K_k(A, b) = \text{span}(b, Ab, A^2 b, \ldots, A^{k-1} b)$.
  - contains all vectors resulting from action of arbitrary polynomial of degree $\leq k-1$ in A on vector b
  - one of these vectors minimizes $||P_{k-1}(A)b - f(A)b||$ over all polynomials of degree $\leq k-1 \rightarrow$ namely, the projection of $f(A)b$ on the Krylov subspace

- Arnoldi method uses the recursive scheme

  with
  $$AV_k = V_k H_k + \beta_k v_{k+1} e_k^T$$

  $$V_k^\dagger A V_k = H_k$$

  to build an orthonormal basis $V_k = (v_1, \ldots, v_k)$ in $K_k(A, b)$, where:
  - H_k is a $k \times k$ Hessenberg matrix (upper triangular + one subdiagonal)
  - eigenvalues of H_k are Ritz values of A w.r.t. $K_k(A, b)$
  - $v_1 = b/|b|$
  - β_k: normalization of v_{k+1}, e_k is the k-th basis vector in $\mathbb{C}^k$.

Arnoldi approximation for function of non-Hermitian matrix

- projection of $y = f(A)b$ on $K_k(A, b)$:

$$y \approx y_{\text{proj}} = V_k V_k^\dagger f(A) b = V_k \underbrace{V_k^\dagger f(A) V_k}_{\approx f(H_k) \rightarrow \text{Ritz approximation}} V_k^\dagger b$$

- approximation to y_{proj} using $V_k^\dagger f(A) V_k \approx f(H_k)$

$$y_{\text{proj}} \approx \tilde{y} = |b| V_k f(H_k) e_1$$

  - $\tilde{y} \in K_k(A, b)$
  - $f(x)$ interpolated at Ritz values of A wrt $K_k(A, b)$
  - problem reduced to computation of $f(H_k)$ ($\dim H_k \ll \dim A$)

- $f(H_k)$ computed with suitable method
  - exactly with spectral decomposition
  - suitable approximation method
    e.g., for sign function use Roberts' matrix-iterative method:

$$S^{n+1} = \frac{1}{2}\left[S^n + (S^n)^{-1}\right] \quad , \quad \text{with} \quad S^0 = A$$

Sign function and deflation – Hermitian case

- problem: need large Krylov space if A has small eigenvalues
- reason: in region of $\mathbb{C}$ where f changes rapidly
  $\rightarrow$ hard to approximate f by low-degree polynomial
- solution: improve efficiency by using exact value of f for critical eigenvalues of A
- Hermitian case: deflation straightforward because any # eigenvectors form subspace orthonormal to remaining eigenvectors:

$$f(A)b = Uf(\Lambda)U^\dagger b = \sum_{i=1}^{m} \underbrace{f(\lambda_i)(u_i^\dagger b)\,u_i}_{\text{exact}} + \underbrace{f(A)b_\perp}_{\text{approximation}}$$

  - u_i eigenvector corresp. to λ_i, and $b_\perp = b - \sum_{i=1}^{m}(u_i^\dagger b)u_i$
  - compute eigenvalues and eigenvectors needed for deflation once $\forall\, b$
  - approximation for $f(A)b_\perp$ in space $\perp \operatorname{span}(u_1, \ldots, u_m)$
- simple decomposition does not work in the non-Hermitian case since eigenvectors of A are not orthonormal

Non-Hermitian case: Left-Right deflation

- use left and right eigenvectors belonging to m critical eigenvectors

$$AR_m = R_m \Lambda_m$$

$$L_m^\dagger A = \Lambda_m L_m^\dagger$$

  - Λ_m is the diagonal eigenvalue matrix for the m critical eigenvalues
  - $R_m = (r_1, \ldots, r_m)$ is the matrix of right eigenvectors
  - $L_m = (\ell_1, \ldots, \ell_m)$ is the matrix containing the left eigenvectors
  - $L_m^\dagger R_m = I_m$, and $R_m L_m^\dagger$ is oblique projector on the subspace Ω_m

- decompose b as

$$b = b_\parallel + b_\ominus$$

where $b_\parallel = R_m L_m^\dagger b$ is oblique projection of b on Ω_m and $b_\ominus = b - b_\parallel$

$$f(A)b = f(A)R_m L_m^\dagger b + f(A)b_\ominus$$

Left-Right deflation – the approximation

- 1st term: exact contribution

$$f(A)R_m L_m^\dagger b = R_m f(\Lambda_m) L_m^\dagger b$$

- 2nd term: Arnoldi method in the Krylov subspace $K_k(A, b_\ominus)$

$$AV_k = V_k H_k + \beta_k v_{k+1} e_k^T$$

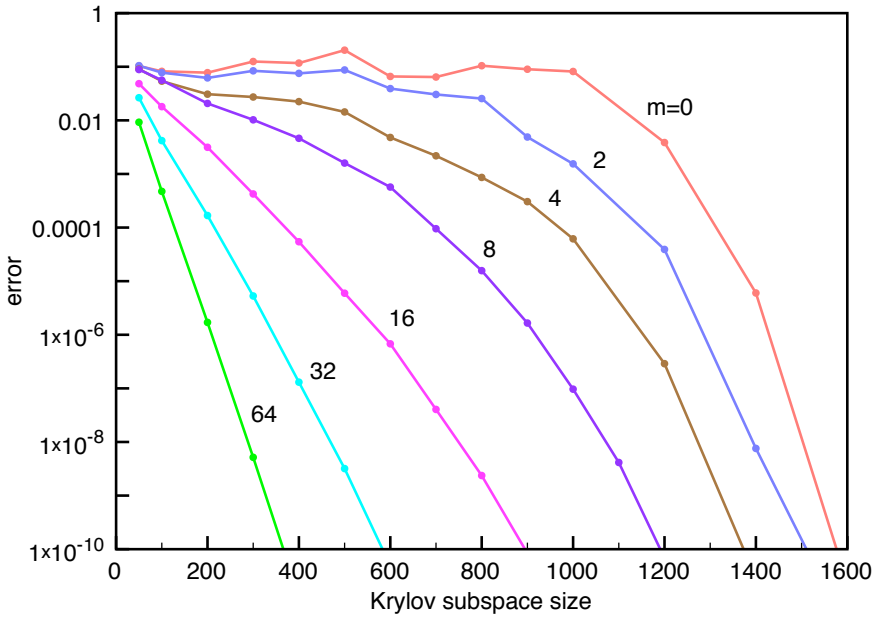
- Finally,

$$f(A)b \approx R_m f(\Lambda_m) L_m^\dagger b + |b_\ominus| V_k f(H_k) e_1$$

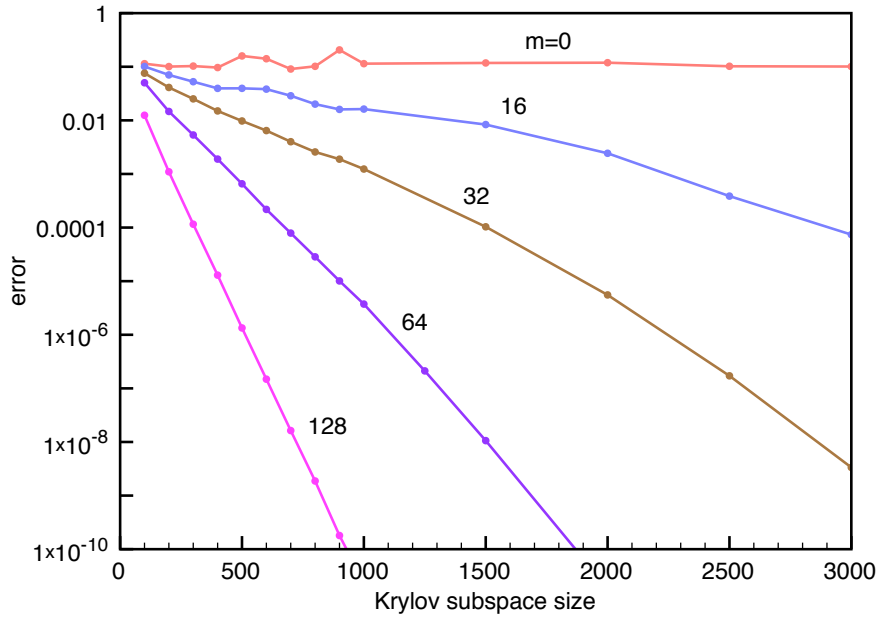
  - compute $f(H_k)$ with suitable method
  - only needs first column of $f(H_k)$
  - requires left and right critical eigenvectors

Deflation and convergence for $D_{\mathrm{ov}}(\mu)b$

4^4 lattice (dim=3072)



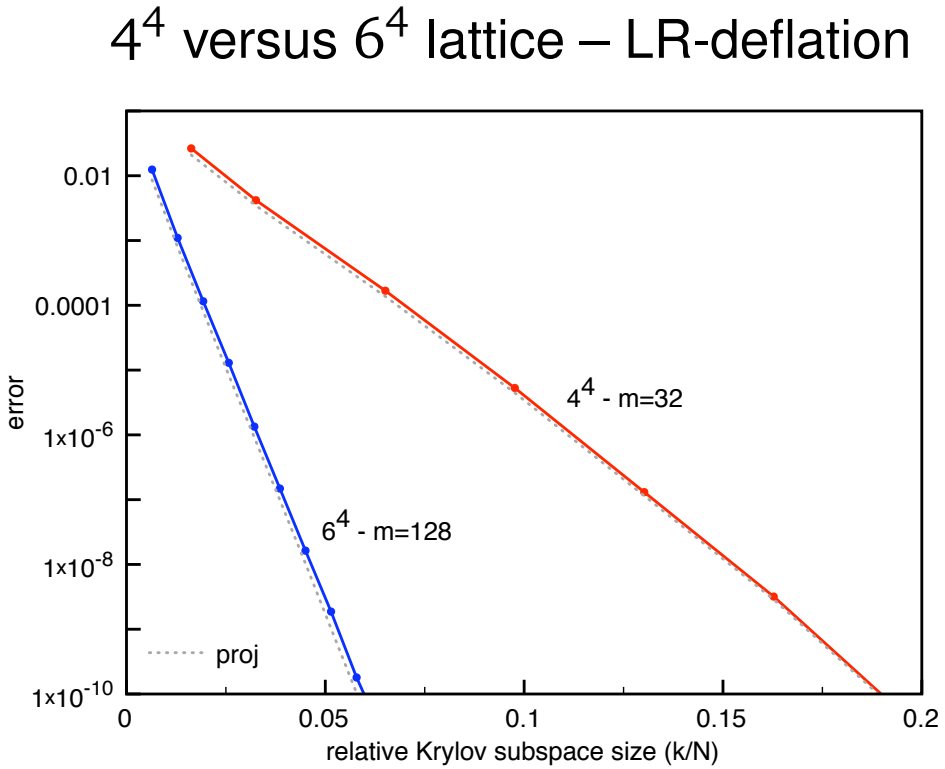
6^4 lattice (dim=15552)



- initialization phase: determine right and left eigenvectors of $\gamma_5 D_{\mathrm{w}}(\mu)$ corresponding to eigenvalues with smallest magnitude using ARPACK
- trade-off between # of deflated eigenvalues and Krylov subspace size

deflation is essential to reach satisfying efficiency

Deflation efficiency for increasing volume



deflation efficiency grows with increasing lattice volume

Two-sided Lanczos method

Arnoldi method suffers from long recurrences

$\longrightarrow$ Two-sided Lanczos: short recurrences but only bi-orthogonal

- Consider two Krylov subspaces $K_k(A, v_1)$ and $K_k(A^\dagger, w_1)$
- Construct bi-orthogonal bases V_k and W_k such that
  - $W_k^\dagger V_k = I_k$
  - $G_k \equiv W_k^\dagger A V_k$ is tridiagonal

$$G_k \equiv W_k^\dagger A V_k = \begin{pmatrix} \alpha_1 & \gamma_1 & 0 & \cdots & 0 \\ \beta_1 & \alpha_2 & \ddots & \ddots & \vdots \\ 0 & \ddots & \ddots & \ddots & 0 \\ \vdots & \ddots & \ddots & \ddots & \gamma_{k-1} \\ 0 & \cdots & 0 & \beta_{k-1} & \alpha_k \end{pmatrix}$$

  - V_k and W_k can be built with short recurrence relations:

$$\begin{cases} \beta_i v_{i+1} = (A - \alpha_i) v_i - \gamma_{i-1} v_{i-1}, \\ \gamma_i^* w_{i+1} = (A^\dagger - \alpha_i^*) w_i - \beta_{i-1}^* w_{i-1}, \end{cases}$$

where

$$\alpha_i = w_i^\dagger A v_i \quad \text{and} \quad \beta_i, \gamma_i \ \text{ from } \ w_{i+1}^\dagger v_{i+1} = 1$$

Two-sided Lanczos approximation + deflation

- $V_k W_k^\dagger$ is oblique projector on $K_k(A, v_1)$
- oblique projection of $f(A)b$ on $K_k(A, b)$:

$$y \approx y_{\text{obl}} = V_k \underbrace{W_k^\dagger f(A) V_k}\, W_k^\dagger b$$

- approximation to y_{obl} using $W_k^\dagger f(A) V_k \approx f(G_k)$

$$y_{\text{obl}} \approx \tilde{y} = |b| V_k f(G_k) e_1$$

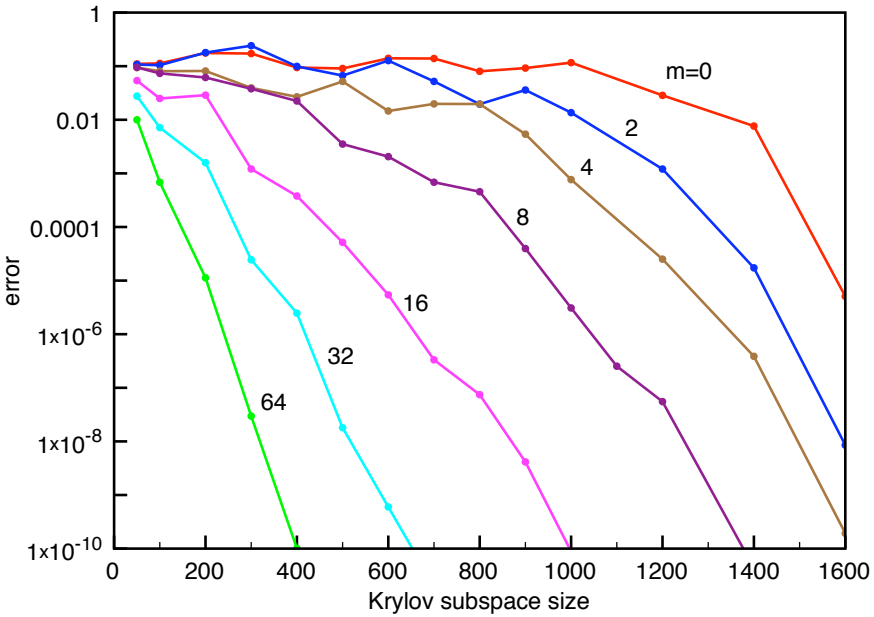
  - $\tilde{y} \in K_k(A, b)$
  - problem reduced to computation of $f(G_k)$ ($\dim G_k \ll \dim A$)

- Enhance with LR-deflation:
  construct bi-orthogonal bases V_k and W_k in $K_k(A, b_\ominus^R)$ and $K_k(A^\dagger, b_\ominus^L)$, where directions along R_m, resp. L_m, have been fully deflated from b: $b_\ominus^R = (1 - R_m L_m^\dagger) b$ and $b_\ominus^L = (1 - L_m R_m^\dagger) b$.
  Function approximation:

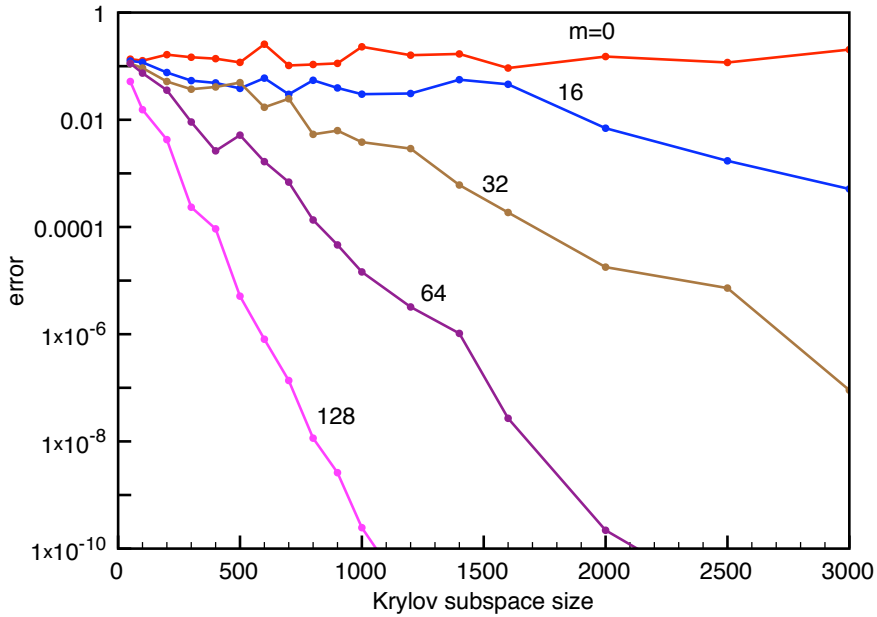
$$f(A)b \approx R_m f(\Lambda_m) L_m^\dagger b + |b_\ominus^R| V_k f(G_k) e_1$$

Two-sided Lanczos – Deflation and convergence for $D_{\mathrm{ov}}(\mu)b$

4^4 lattice (dim=3072)



6^4 lattice (dim=15552)



Arnoldi versus two-sided Lanczos – CPU-time

4^4 lattice (dim=3072)

$m = 32$ – LR-deflation

initialization time: 27.5 s

Arnoldi

k	Arnoldi	$\mathrm{sign}(H_k)$	total
200	0.45	0.20	0.66
400	1.77	1.02	2.82
600	3.94	2.77	6.74
800	6.96	6.44	13.44
1000	10.84	12.33	23.21

two-sided Lanczos

k	2s-Lanczos	$\mathrm{sign}(G_k)$	total
200	0.11	0.19	0.31
400	0.20	0.98	1.20
600	0.31	2.82	3.15
800	0.43	6.52	6.97
1000	0.51	12.45	13.00

6^4 lattice (dim=15552)

$m = 128$ – LR-deflation

initialization time: 1713 s

Arnoldi

k	Arnoldi	$\mathrm{sign}(H_k)$	total
200	2.39	0.15	2.62
400	9.01	0.94	10.06
600	20.03	2.80	22.98
800	35.09	6.49	41.78
1000	54.74	12.36	67.34

two-sided Lanczos

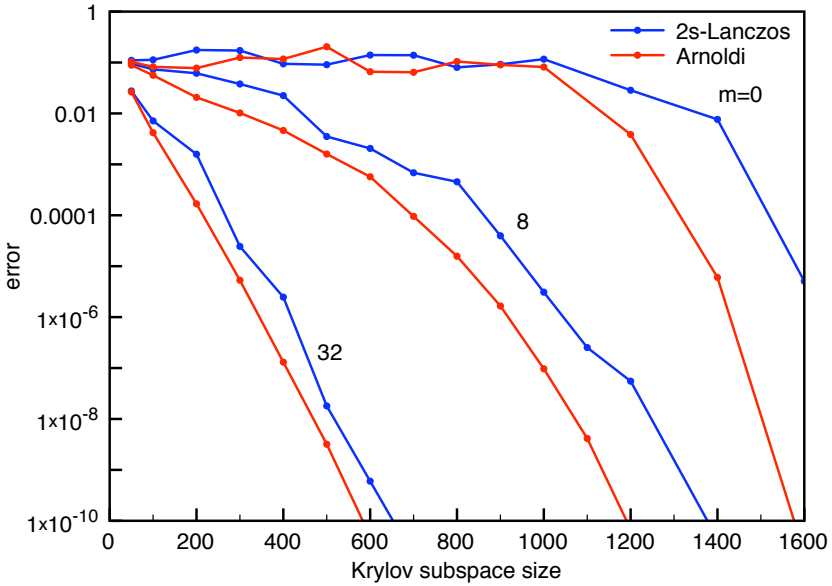
k	2s-Lanczos	$\mathrm{sign}(G_k)$	total
200	0.60	0.19	0.87
400	1.17	0.95	2.24
600	1.72	2.84	4.71
800	2.33	6.55	9.08
1000	3.02	12.45	15.69

Arnoldi basis $\sim Nk^2$

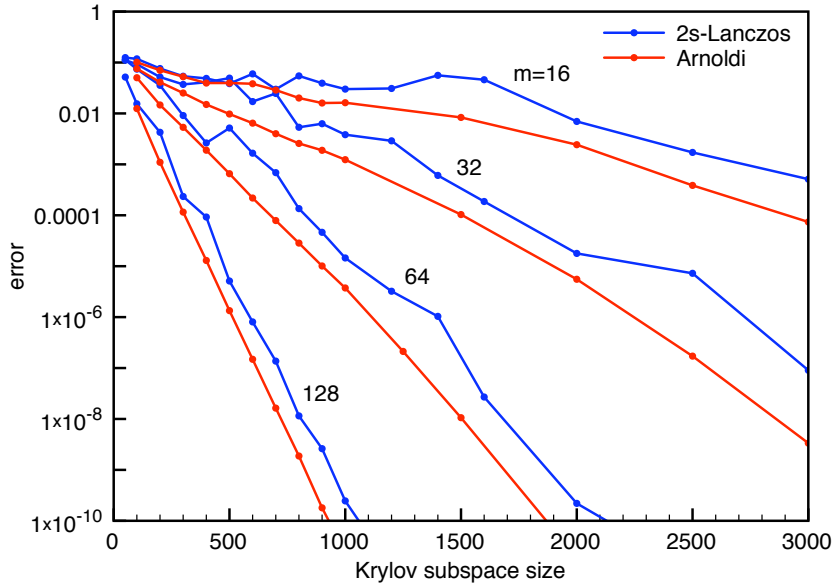
2s-Lanczos basis $\sim Nk$

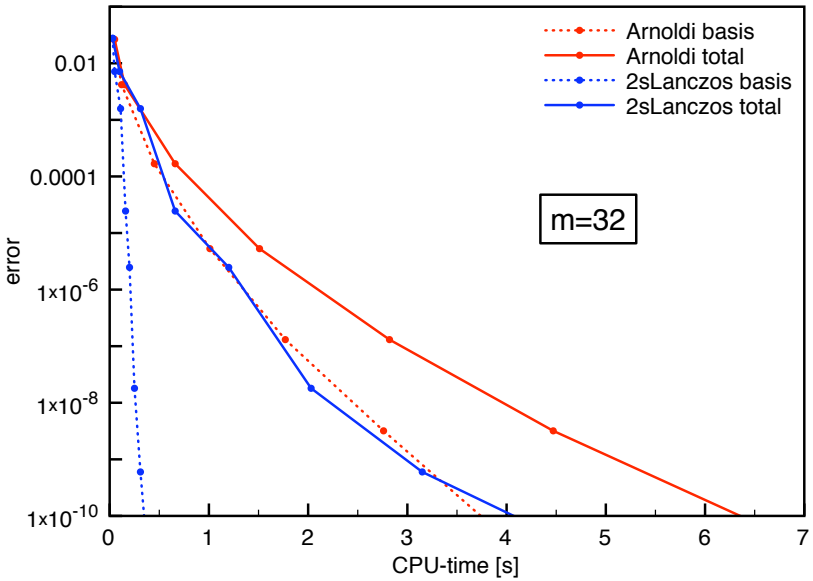
Arnoldi versus two-sided Lanczos – deflation efficiency

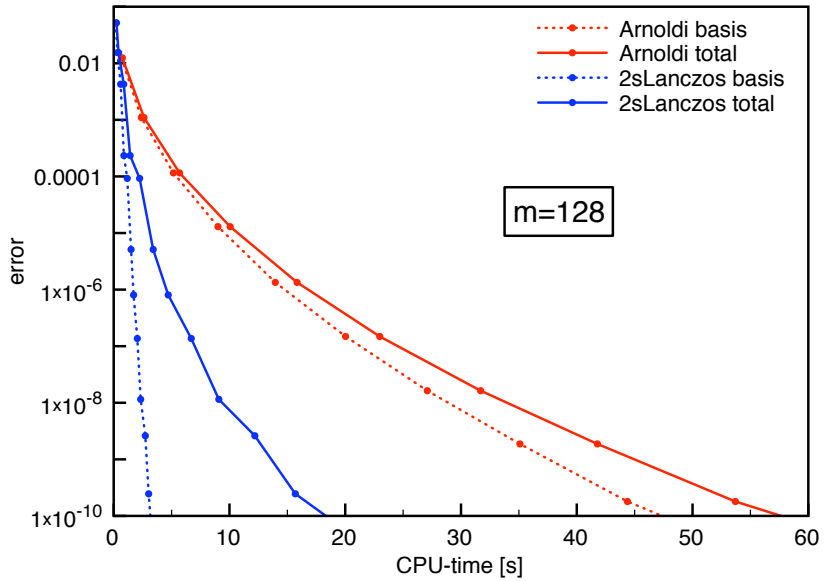
4^4 lattice (dim=3072)



6^4 lattice (dim=15552)







Outlook

- recursive Krylov subspace method for inner function computation
- alternative iterative methods:
  - restarted Arnoldi (stability problems)
  - partial fraction expansion
- improve efficiency of deflation
- apply method to larger lattices $\longrightarrow$ physics (tested for 8^4 lattice)
- use method in eigenvalue determination of overlap operator
  - test for 6^4 lattice using Arpack on Intel Core 2 Duo 2.33GHz
  - initialization: computing the 128 smallest eigenvalues of kernel $\sim$ 30 min
  - compute 16 smallest eigenvalues of overlap operator with accuracy of 10^{-4}
    - Arnoldi approximation with $k = 400 \sim$ 1h30min
    - 2S-Lanczos approximation with $k = 600 \sim$ 50min, $k = 400 \sim$ 25min
- use method in inversion of overlap operator