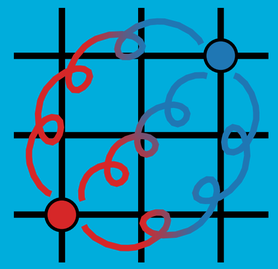

Spectral Properties of non-Hermitian Dirac Operators from the Krylov-Schur Algorithm

Peter Boyle, Chulwoo Jung, Patrick Oare, Shuhei Yamamoto

July 29th, 2026

Lattice 2026

SciDAC
Scientific Discovery through Advanced Computing

Brookhaven National Laboratory

Lattice Dirac Operators

$\mathscr{M} = N_c \times N_d \times L^3 \times T\,(\times L_s)$
dimensionality of the problem

- Each action S_{F} for lattice fermions is characterized by its **Dirac operator** D.

$$S_{\mathrm{F}} = \sum_{n,m\in\Lambda} \overline{\psi}_a^{\alpha}(n) D_{ab}^{\alpha\beta}(n,m) \psi_b^{\beta}(m) = \overline{\psi} D \psi$$

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2. γ_5 hermiticity

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$$p(\lambda) = \det(D - \lambda) = \det(D^\dagger - \lambda) = p(\lambda^*)^*$$

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See Chulwoo Jung's talk next

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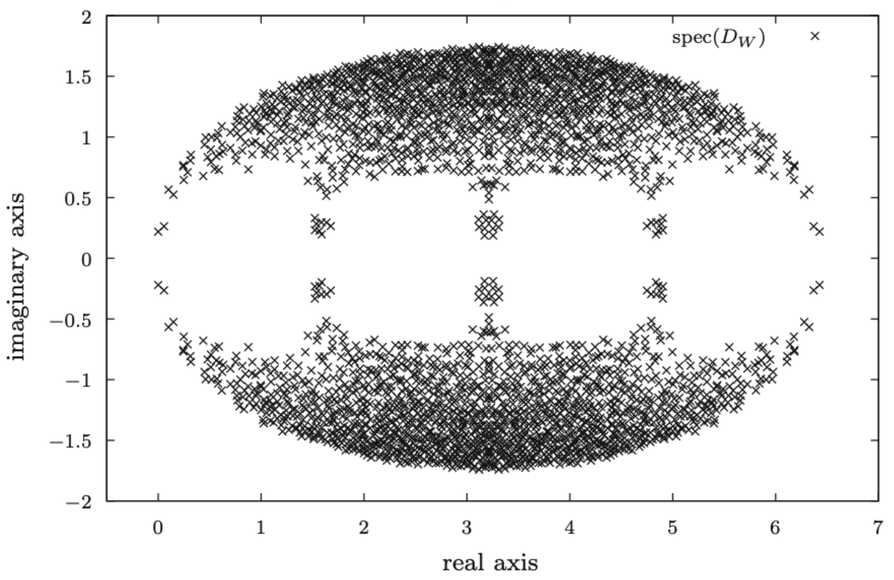
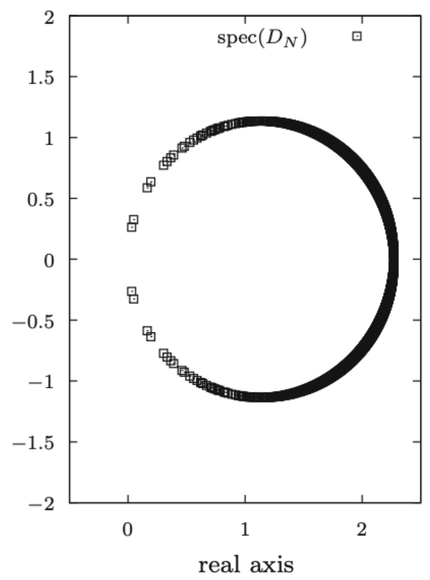
- We are primarily interested in understanding and directly computing the complex spectrum of non-Hermitian Dirac operators.

Spectrum of Dirac operators
on a 4^4 lattice.
Brannick et. al., hep-lat/1410.7170

Wilson Operator



Overlap Operator



Low Modes of D

- Typically solve the Dirac equation with Krylov methods:

$$\psi_N \in K_N(D, b) \equiv \text{span}\{b, Db, D^2b, ..., D^{N-1}b\}.$$

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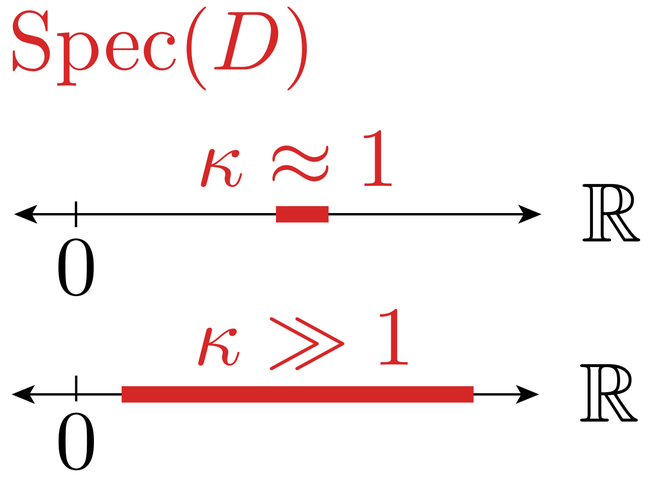
$$\kappa \equiv \left| \frac{\lambda_{\max}(D)}{\lambda_{\min}(D)} \right|$$



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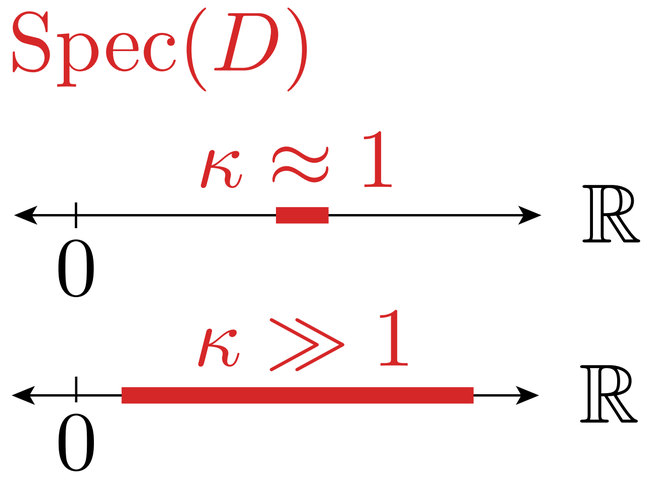

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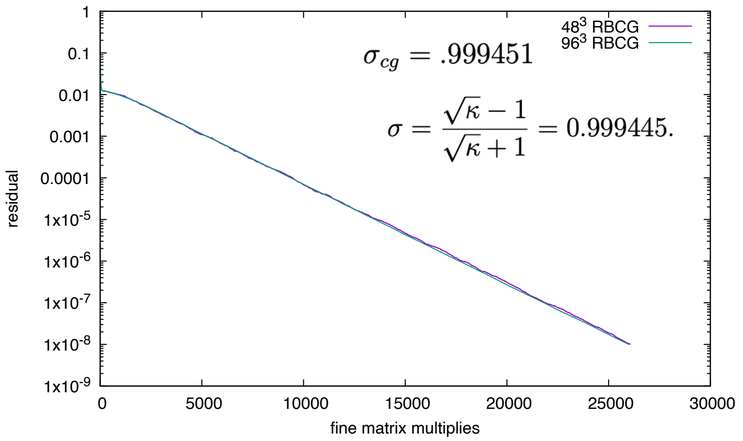
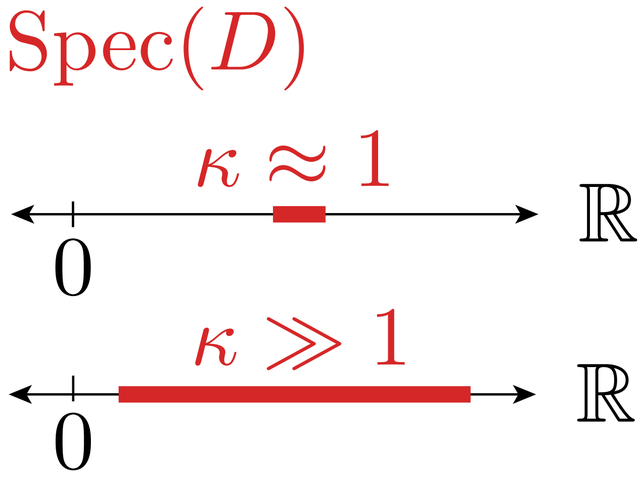
P. Boyle, hep-lat/2409.03904 (2024)



Low Modes of D

N. Nachtigal, S. Reddy, L. Trefethen
SIAM Journal on Matrix Analysis and Applications
(1992) 13:3, 778-795



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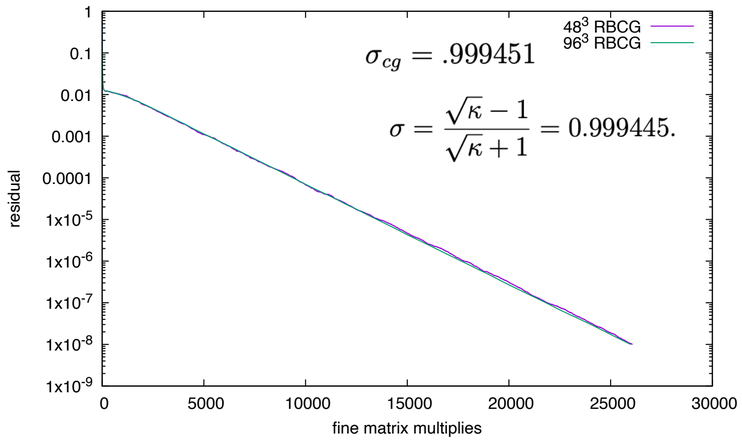

- Precise convergence of non-Hermitian D relies on pseudospectrum. But, the *slowly converging components of the residual are still the low modes of* D.

Domain-Wall Multigrid

See Peter Boyle's talk
Monday @ 15:20

R. Brower *et. al.*
Phys. Rev. D **102** (2020) 094517.

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- Knowledge of the low modes is key: near-null vectors define the coarse space, and convergence is tied to how well one furnishes the space of low modes.

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$$\mathcal{O}(m) := D^{\dagger}_{\text{mobius}}(1) D_{\text{mobius}}(m)$$

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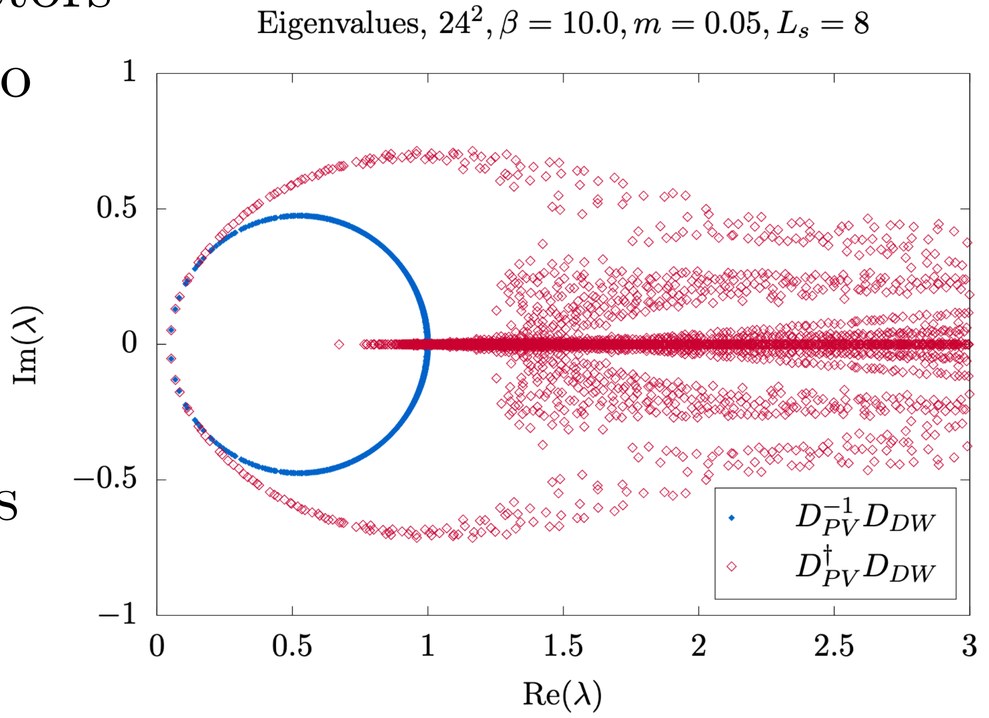

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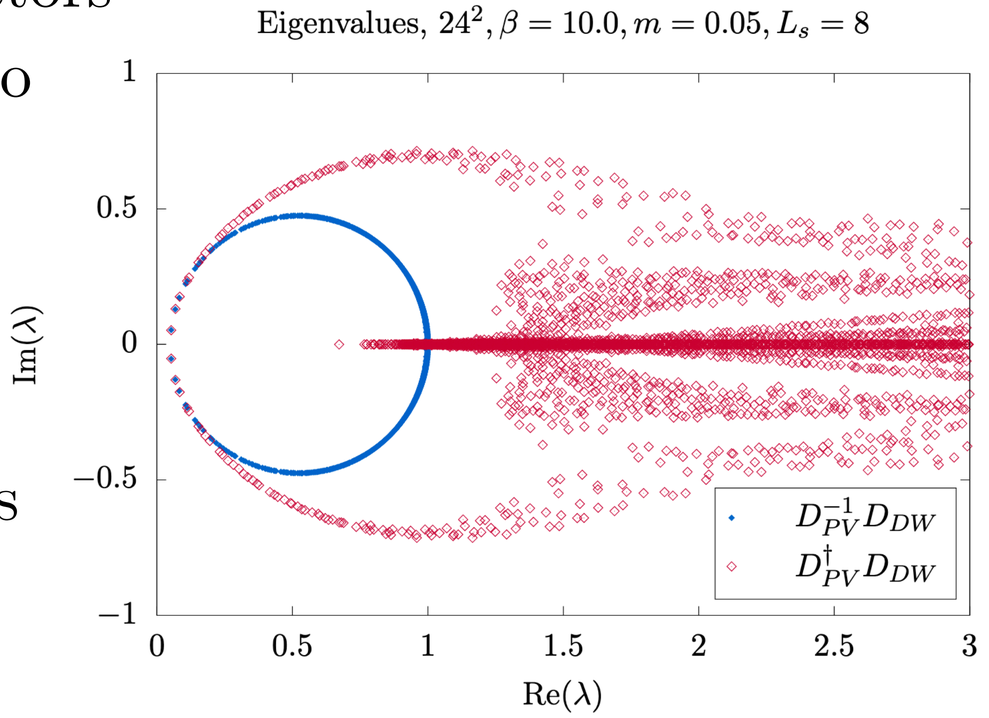

- A non-Hermitian eigensolver can directly solve for the low modes of $\mathcal{O}(m)$.

Arnoldi Iteration

- Power method: $D^N |v_0\rangle$ approaches an eigenvector of D as $N \to \infty$. Additional vectors $\{|v_0\rangle, D|v_0\rangle, \ldots, D^{N-1}|v_0\rangle\}$ also contain information about Spec(D).

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(Residual $(D - \theta)(U_N s)$ is $\perp$ to the Krylov space)

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Problem: We cannot store $\mathscr{M}$ Krylov vectors. Can we truncate the expansion?

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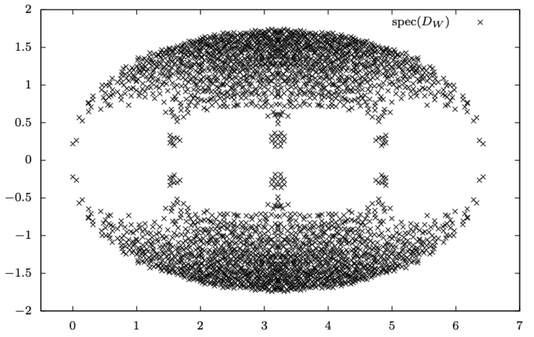

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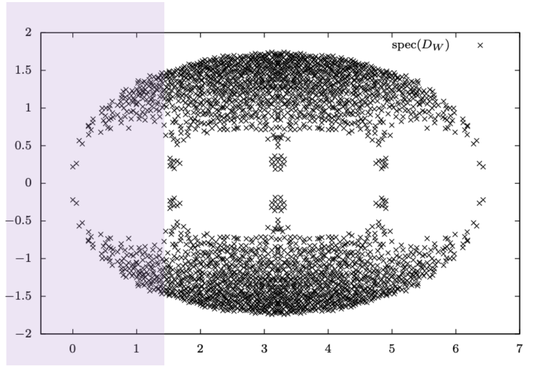

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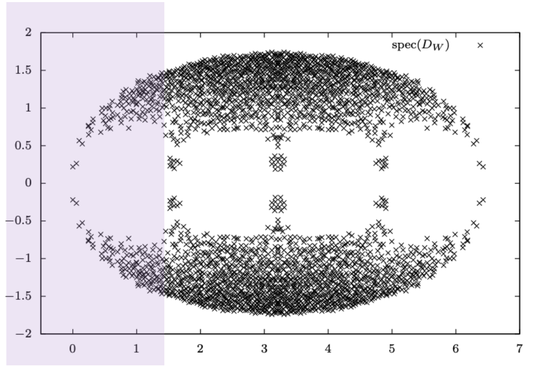

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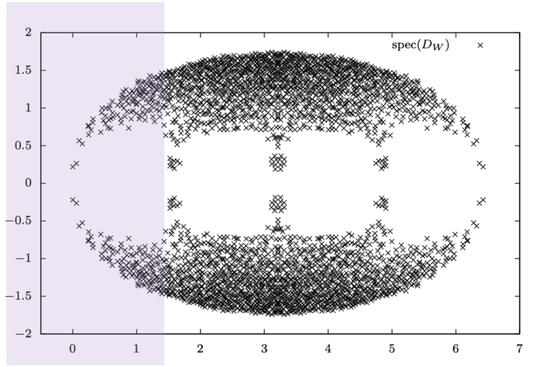

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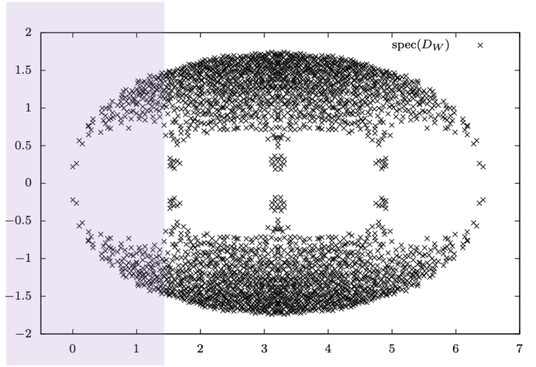

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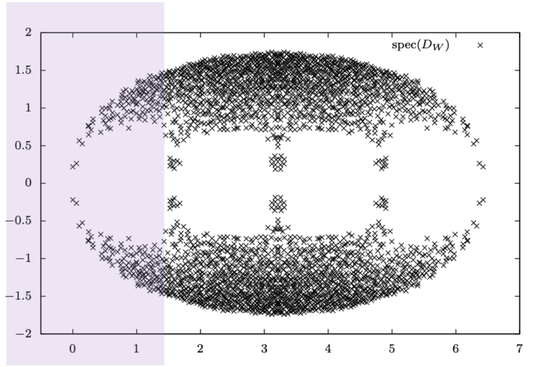

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4. Repeat until a given number of Ritz values converge.

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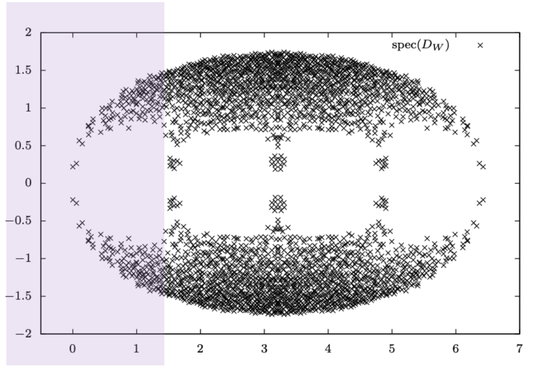

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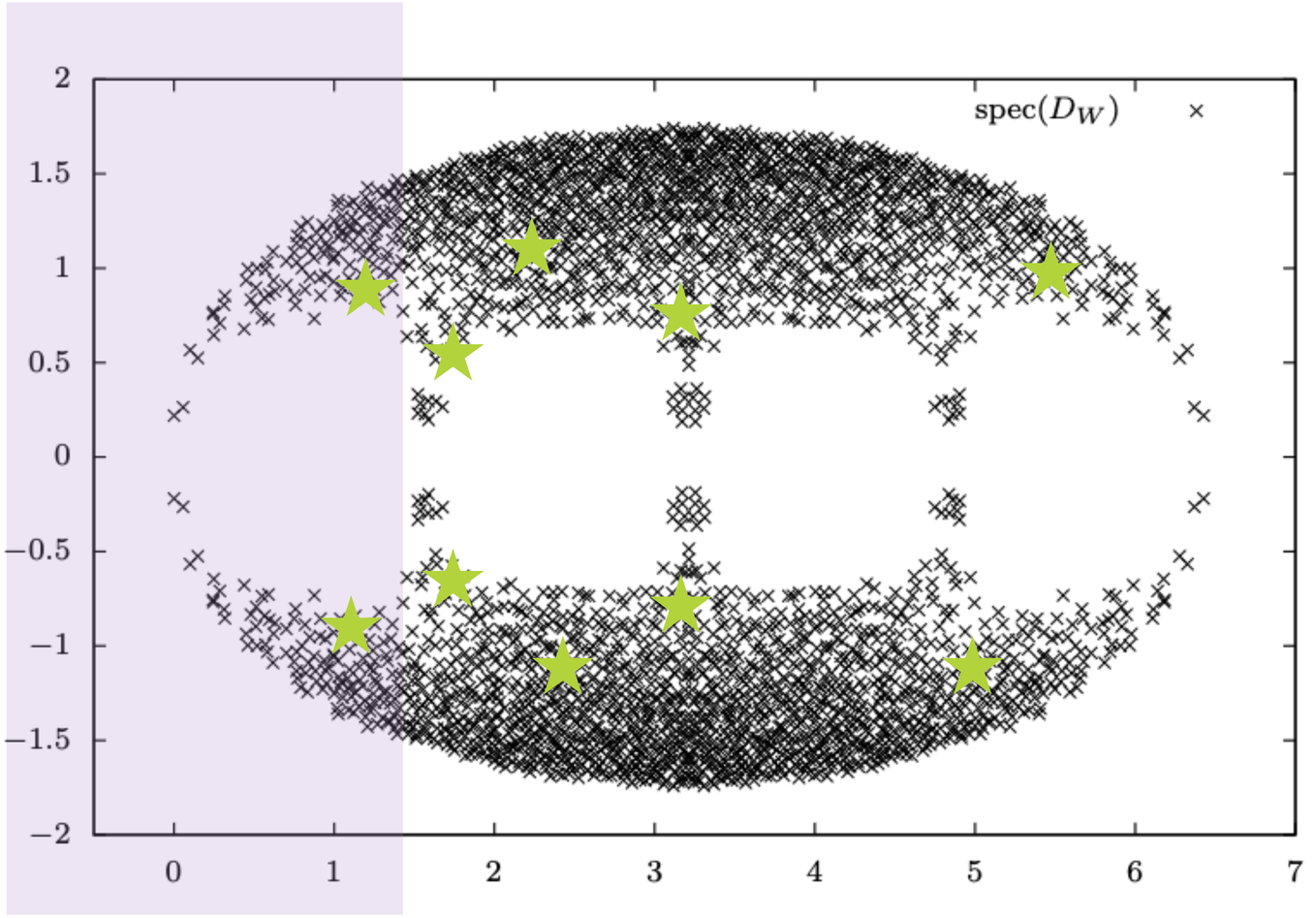
- Parameters: $K < N \ll \mathscr{M}$. N = max # evecs to store, K = # of desired evecs.

1. Expand basis to max size N.
2. Retain K "smallest eigenvalues".
3. Re-expand basis to size N.
4. Repeat until a given number of Ritz values converge.

$$Q \longrightarrow \begin{pmatrix} * & * & * & * & \dots & * \\ * & * & * & * & \dots & * \\ 0 & * & * & * & \dots & * \\ 0 & 0 & * & * & \dots & * \\ \vdots & \vdots & \vdots & \vdots & \ddots & \vdots \\ 0 & 0 & 0 & 0 & \dots & * \end{pmatrix}$$

N

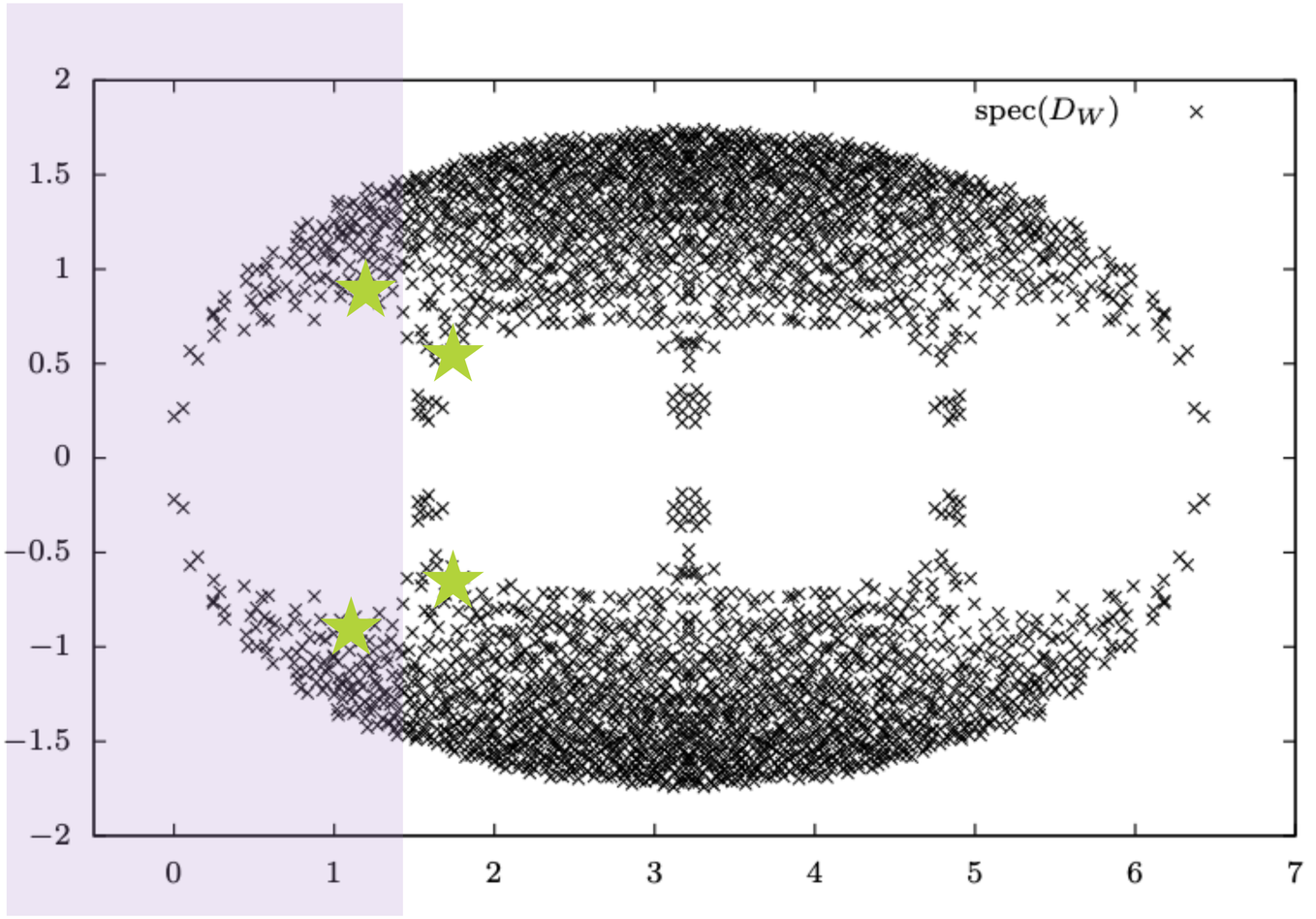
Restarting Projection Methods



Want to find spectrum in this region

Note: Symmetries not enforced until convergence

Restarting Projection Methods



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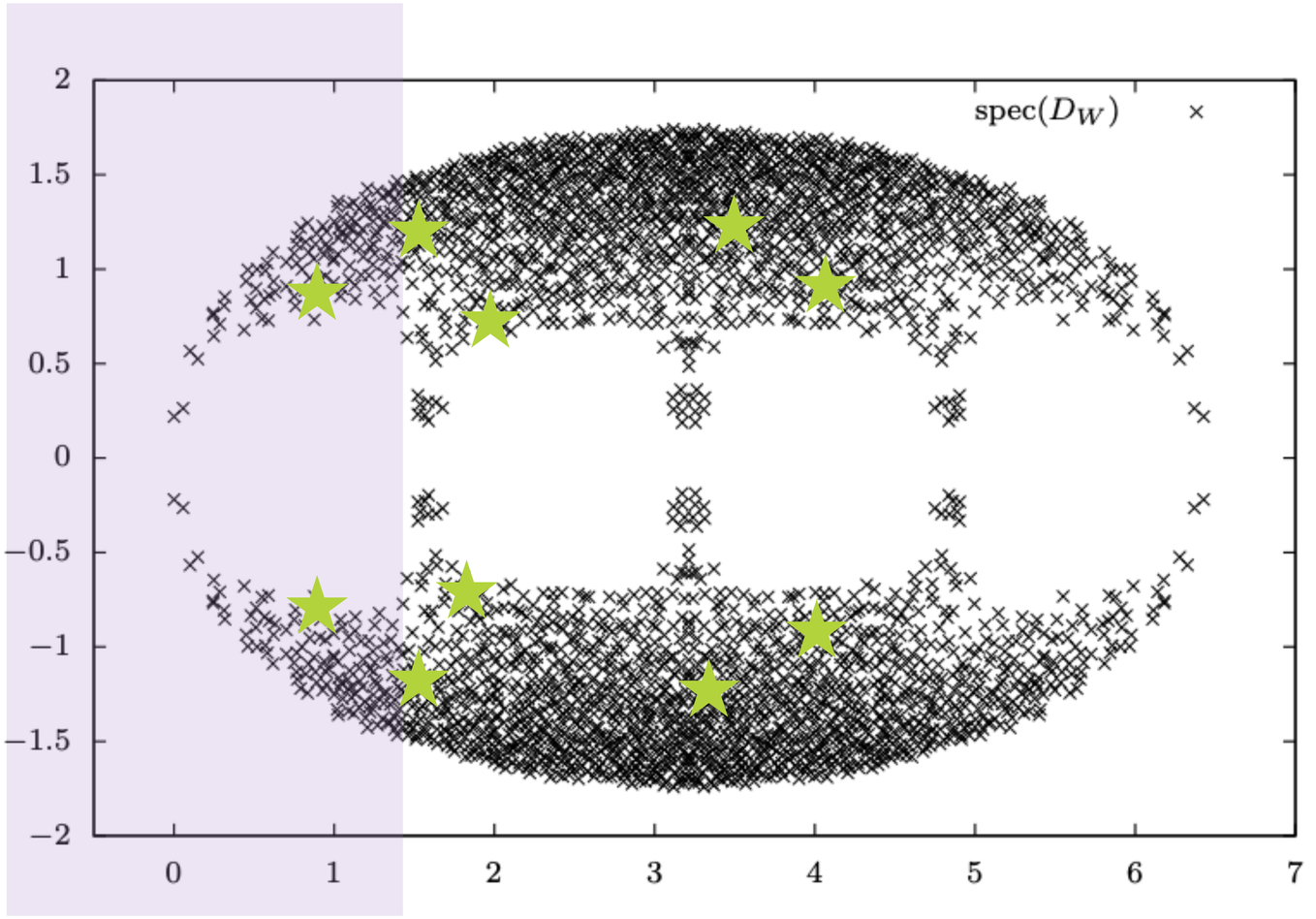
Restarting Projection Methods



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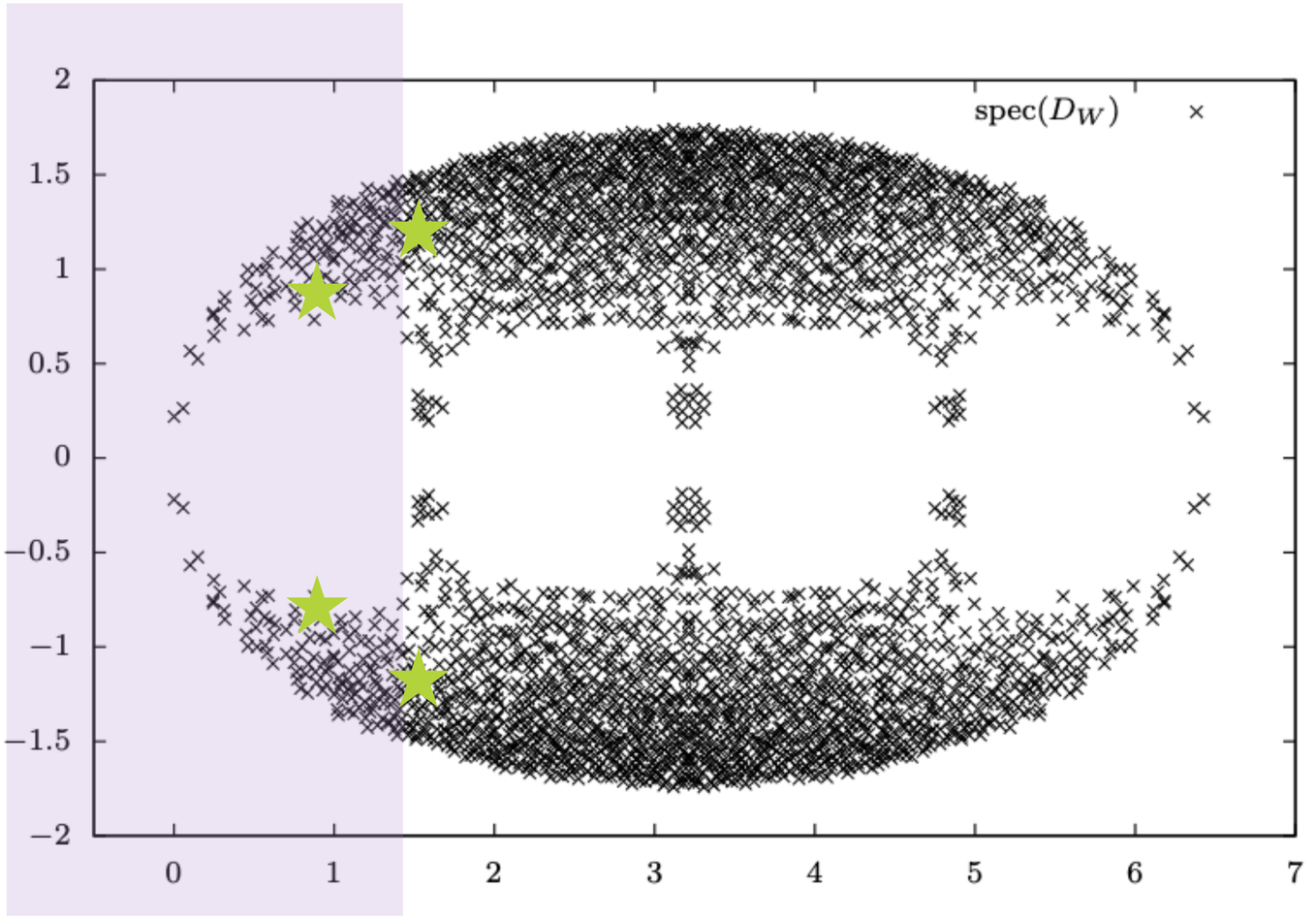

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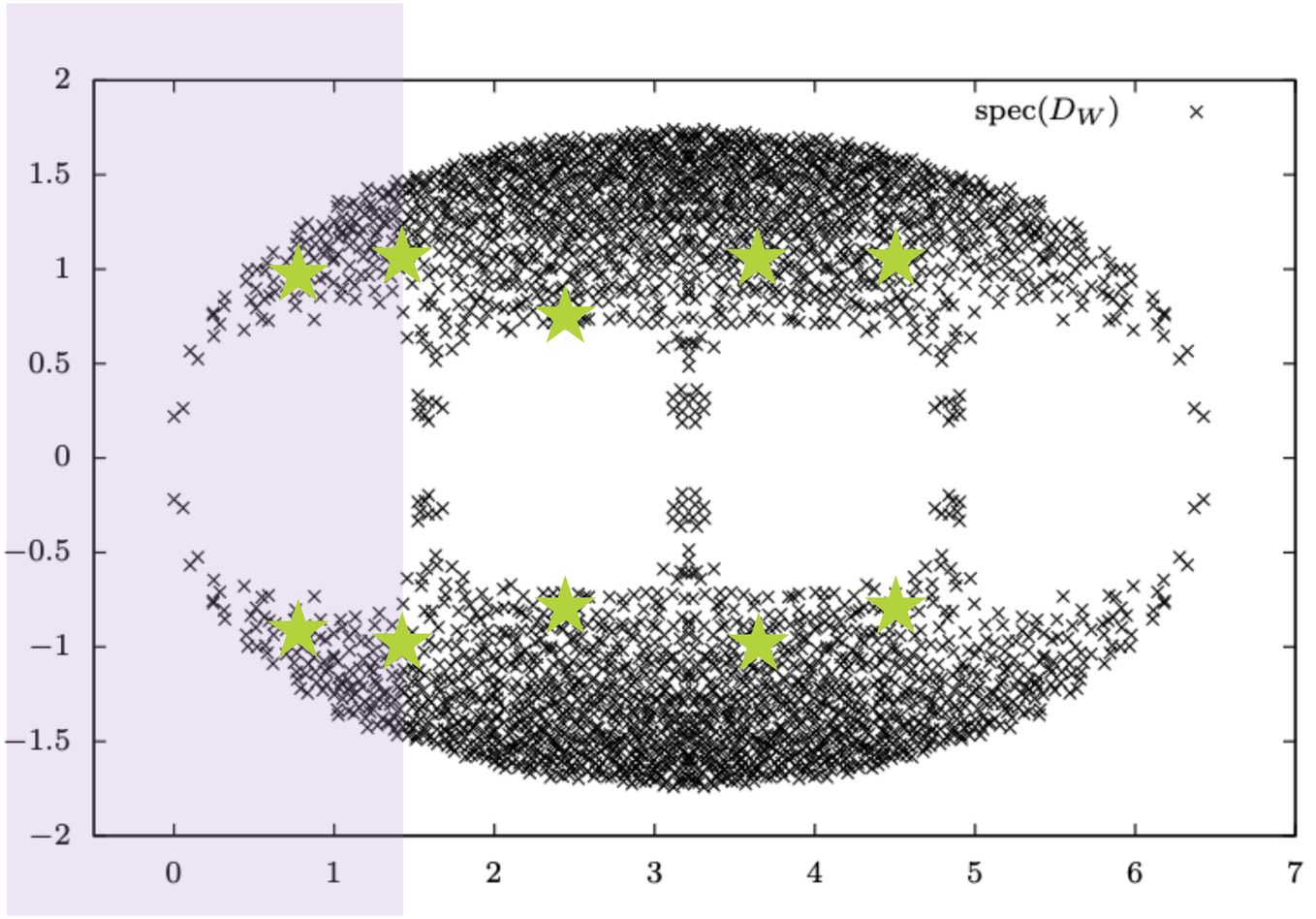
Restarting Projection Methods



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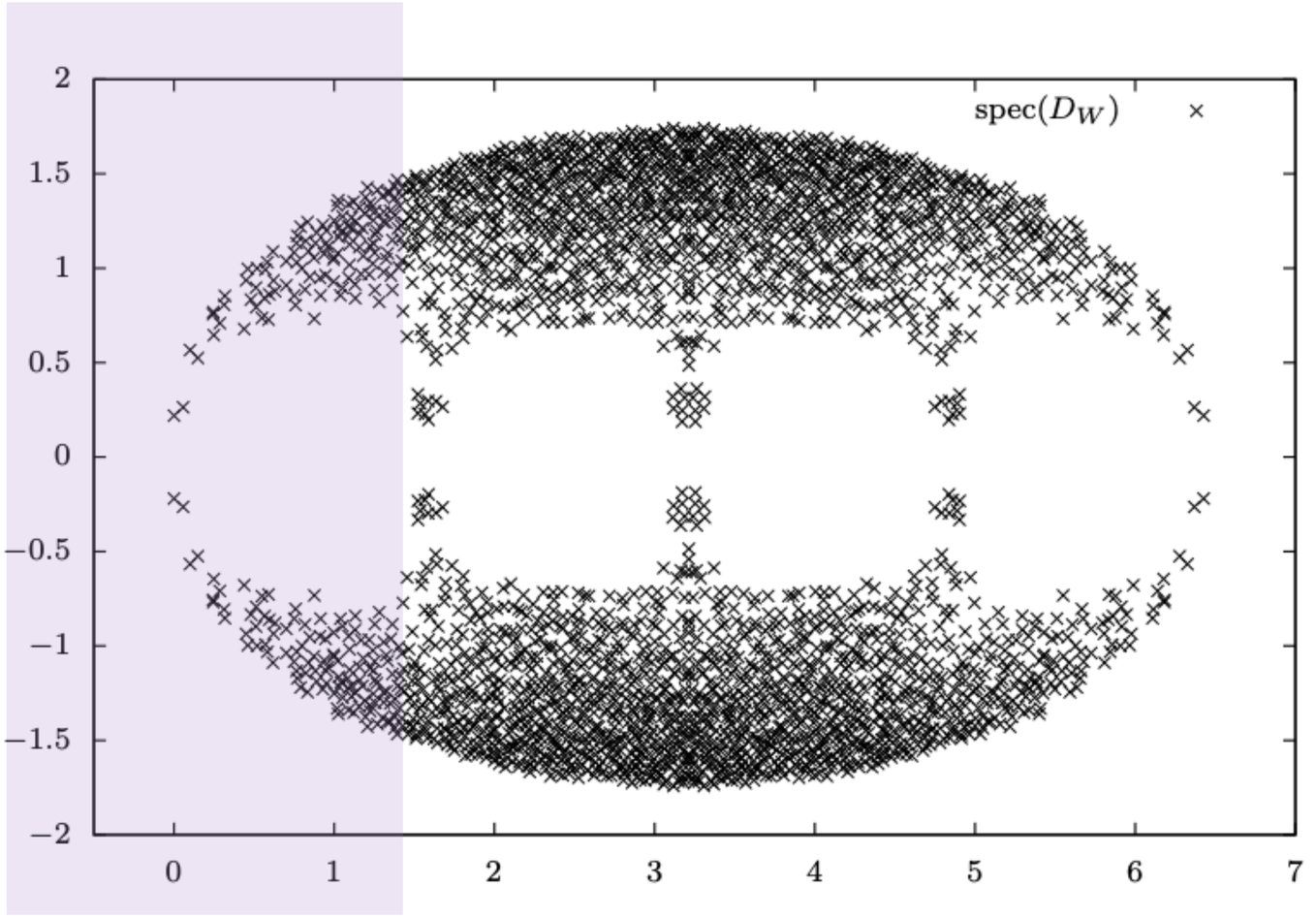

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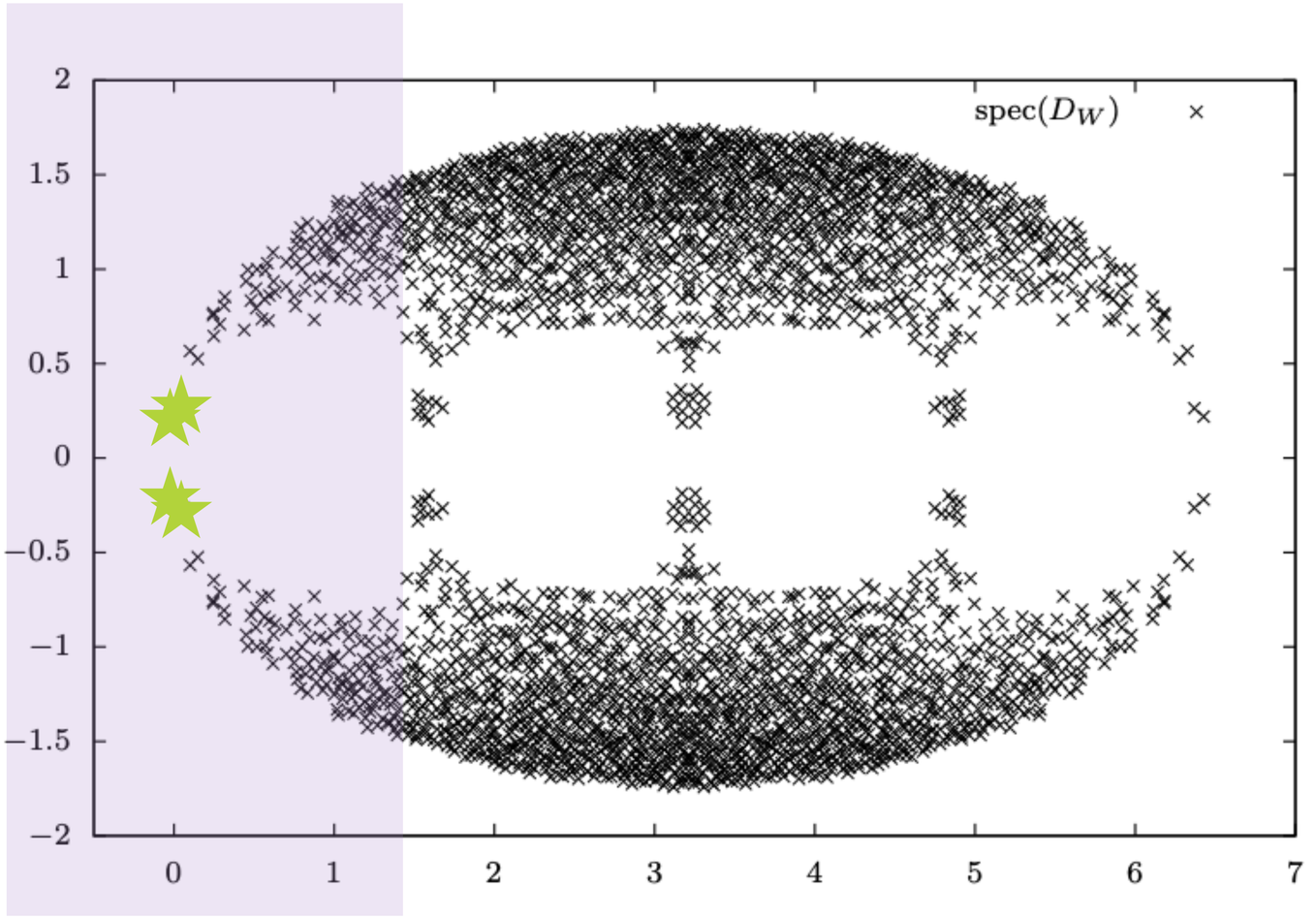
Restarting Projection Methods



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The Krylov-Schur Algorithm

G. Stewart *et. al.*, *SIAM Journal on Matrix Analysis and Applications*, 23(3):601–614 (2002).

- Arnoldi factorization imposes constraints on Q_N, b_N:

$$DU_N = U_N Q_N + u_{N+1} b_N^\dagger$$

Q_N Hessenberg

$b_N \propto e_N$

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- Takes Hessenberg form Q_N and Schur decomposes $Q_N \to V Q_N V^\dagger$ to make Q_N upper triangular; rotates $b_N \to V b_N$.
- Upper triangular decomposition for Q_N provides some advantages:
  - Easy to read off Ritz values.
  - Easier to restart than Arnoldi: just need to reorder the Schur form.

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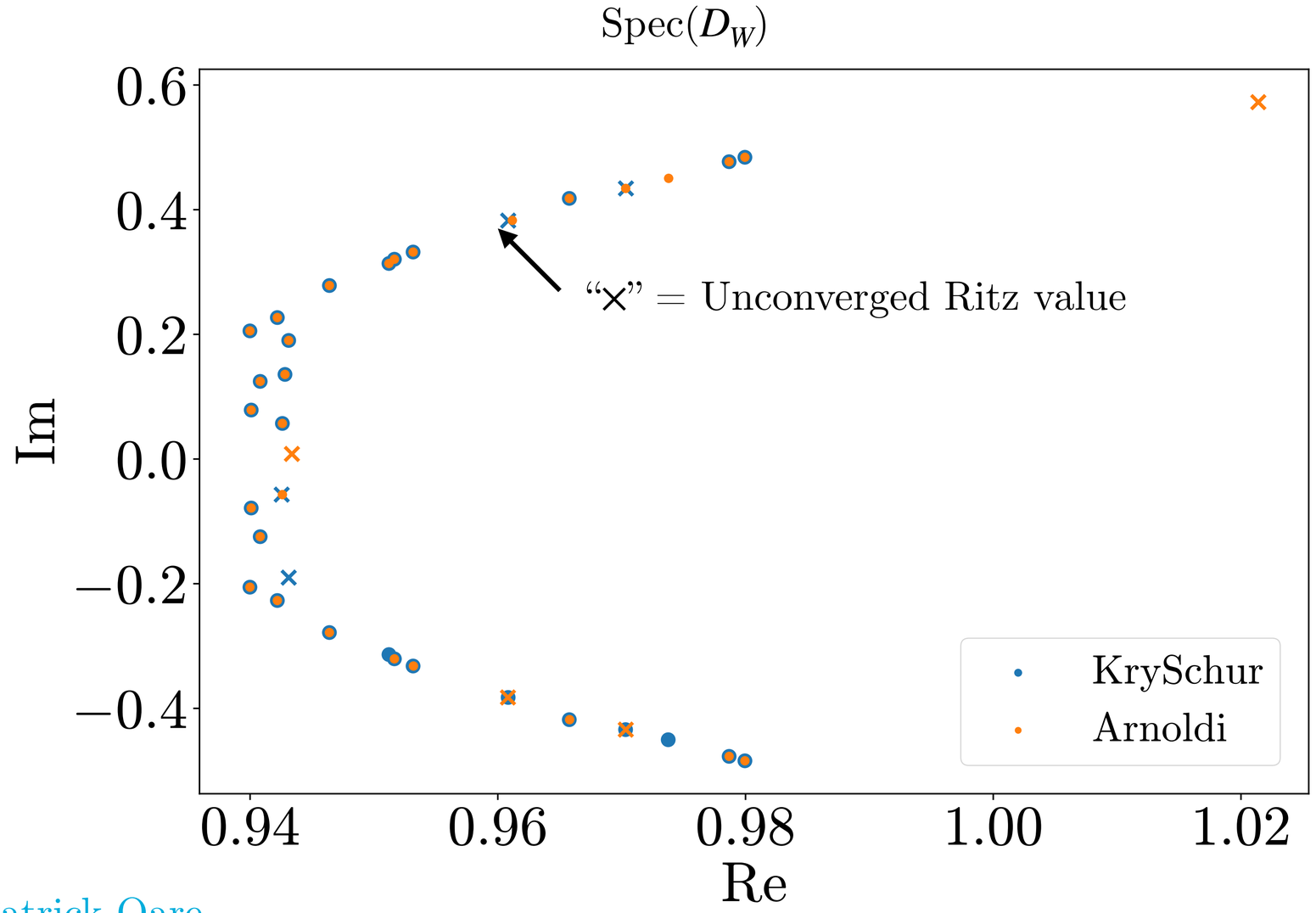
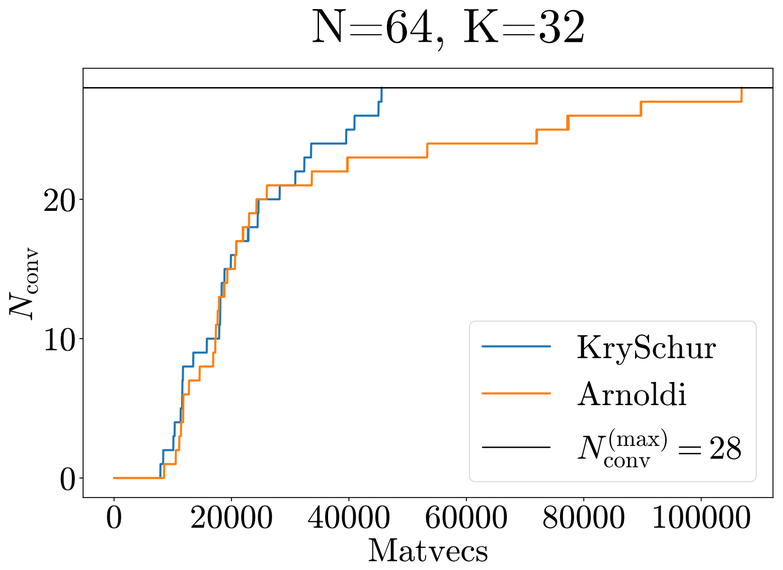
- Upper triangular decomposition for Q_N provides some advantages:
  - Easy to read off Ritz values.
  - Easier to restart than Arnoldi: just need to reorder the Schur form.
- Experimentally is similar to Arnoldi, but slightly more robust: the real advantage is that the algorithm is easy to augment with harmonic extraction.

Spec(D_W) on a sample config

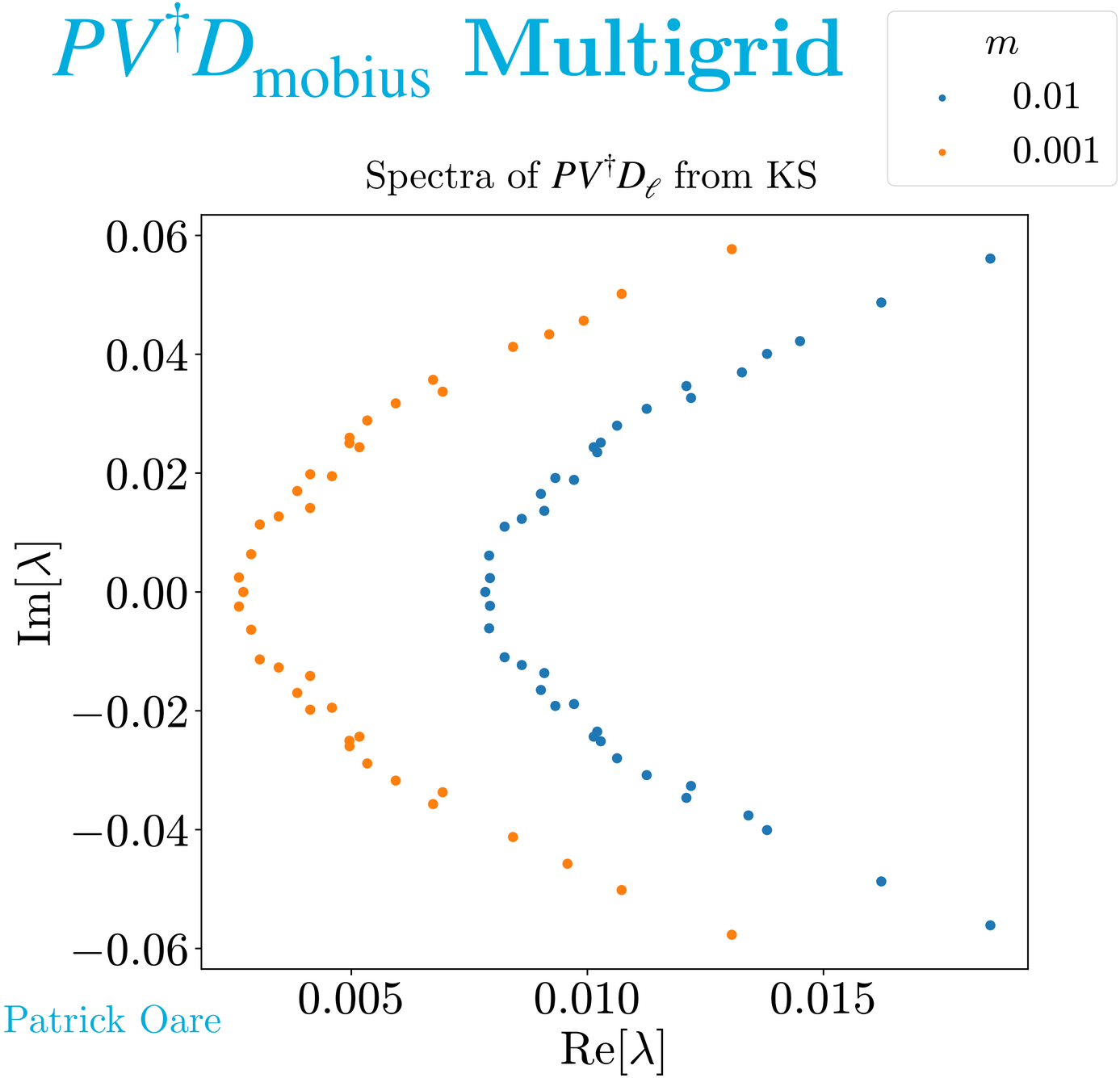
RBC/UKQCD Collaboration,
Phys.Rev.D 76 (2007) 014504.

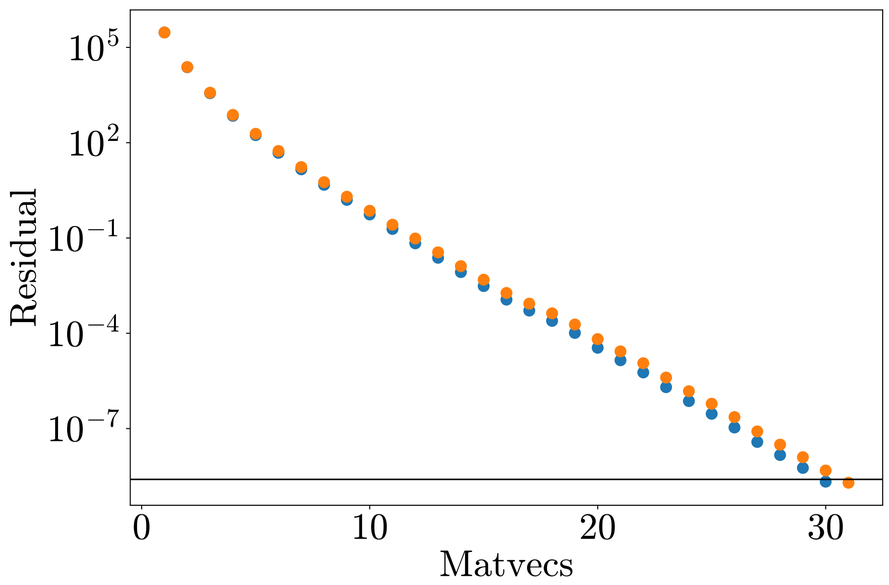


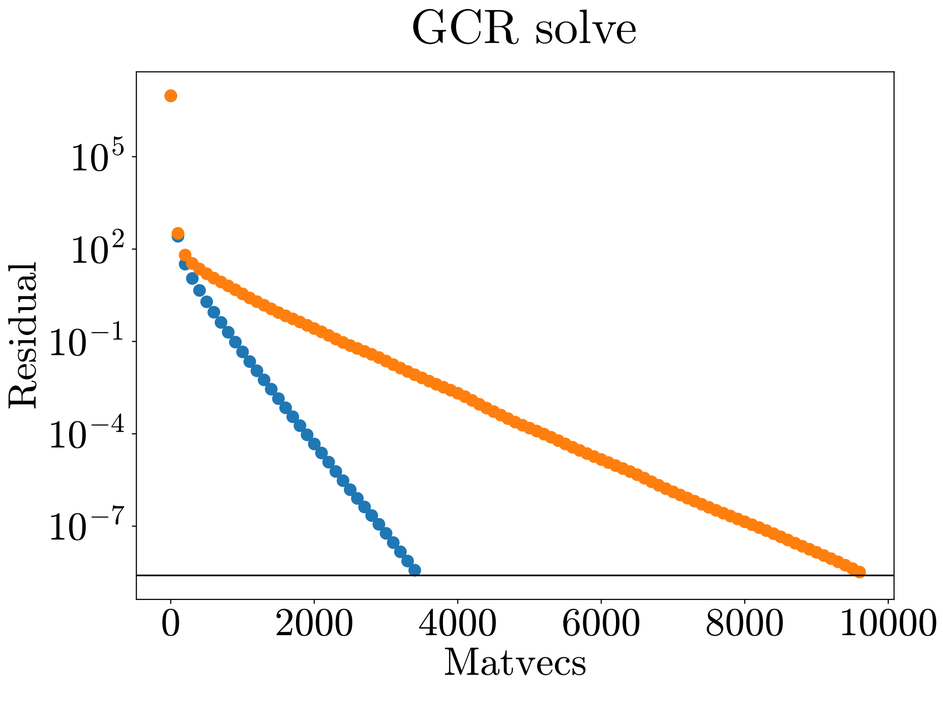
Numerical results from this talk are from a $16^3 \times 32$ gauge field configuration. Chulwoo's talk next will show results from a 32^4 ensemble.



$PV^\dagger D_{\text{mobius}}$ Multigrid

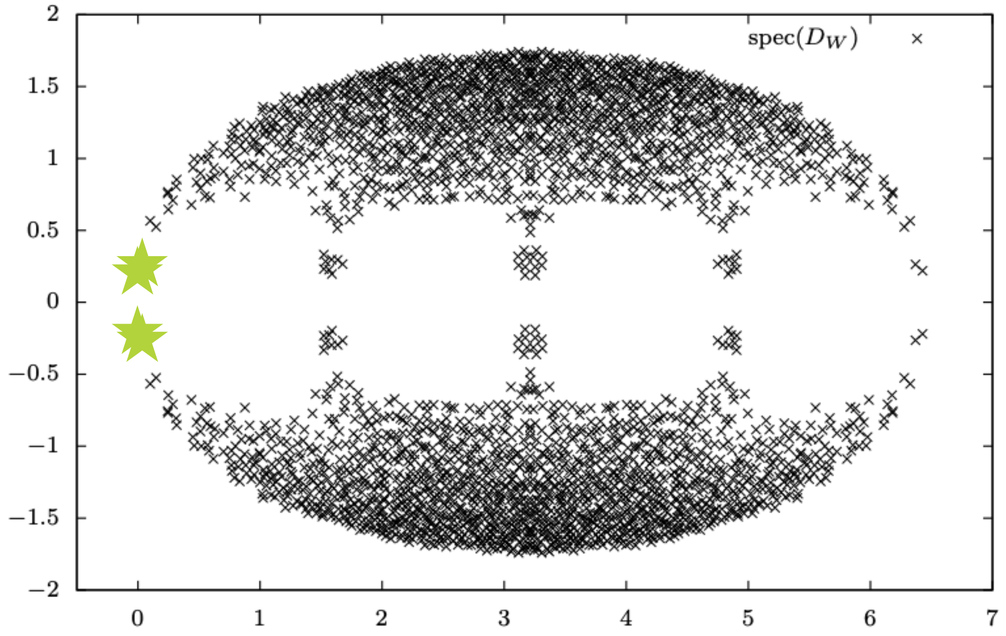






Interior Spectrum

- Krylov methods are great at accessing the spectrum near its boundary.



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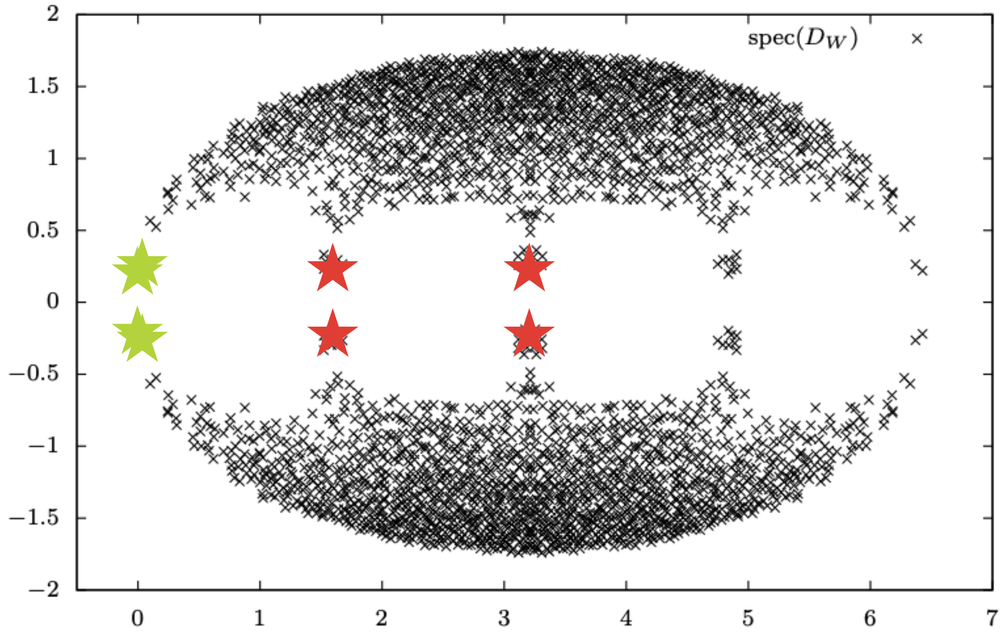

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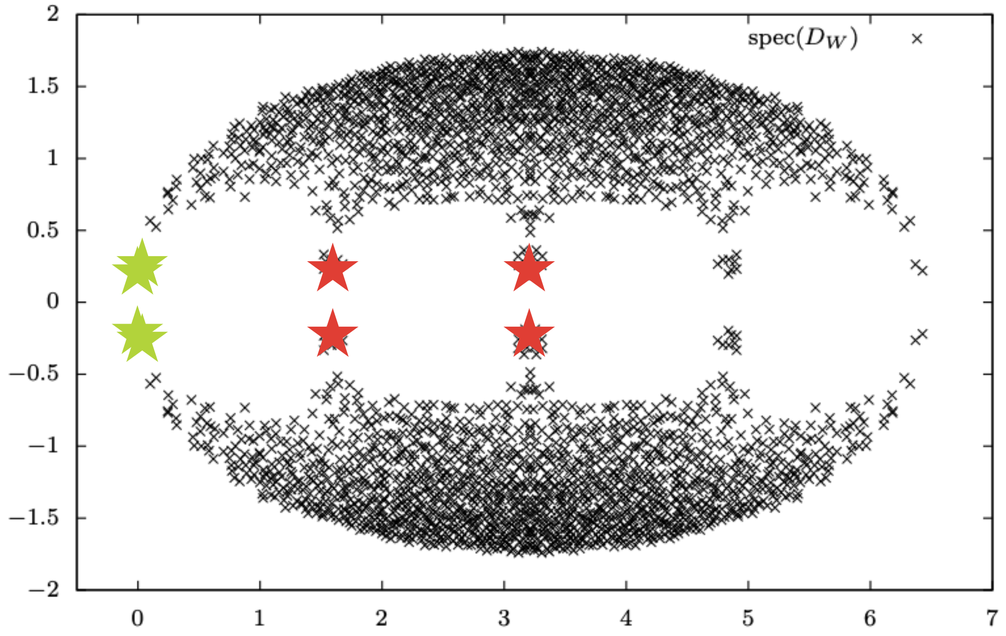

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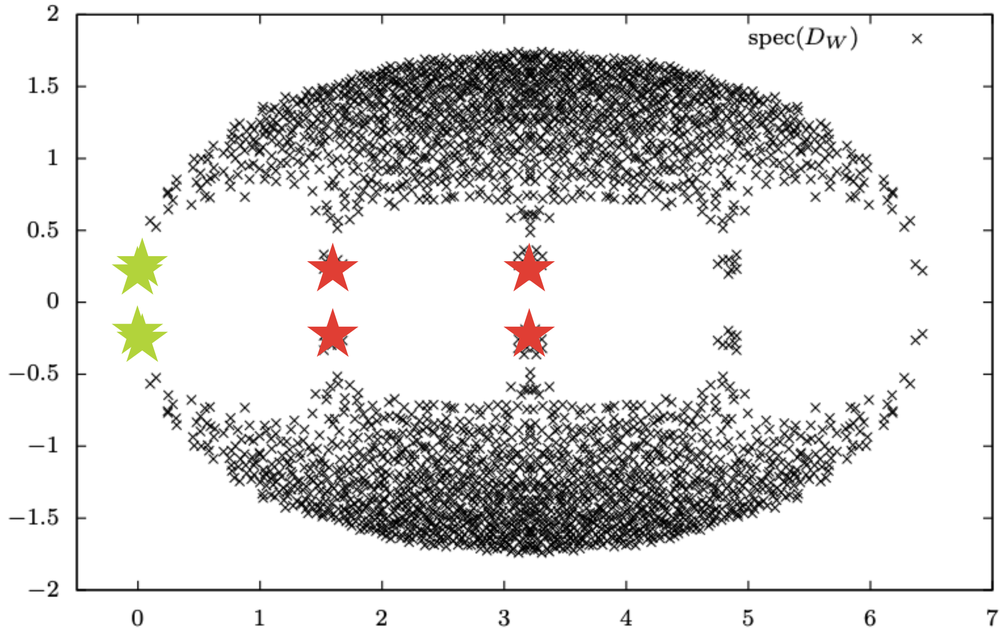

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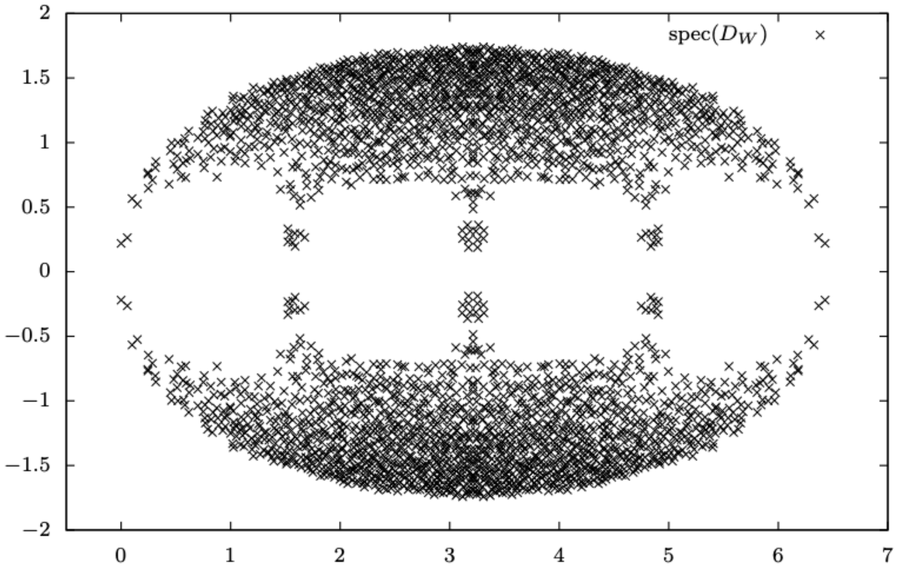
How does one determine the interior eigenvalues in the spectrum?

Shift-and-Invert Operator

- Polynomial preconditioning can suppress unwanted regions, but less control than Hermitian case.

G. Bergner, J. Wuilloud
Comput.Phys.Commun. 183 (2012).



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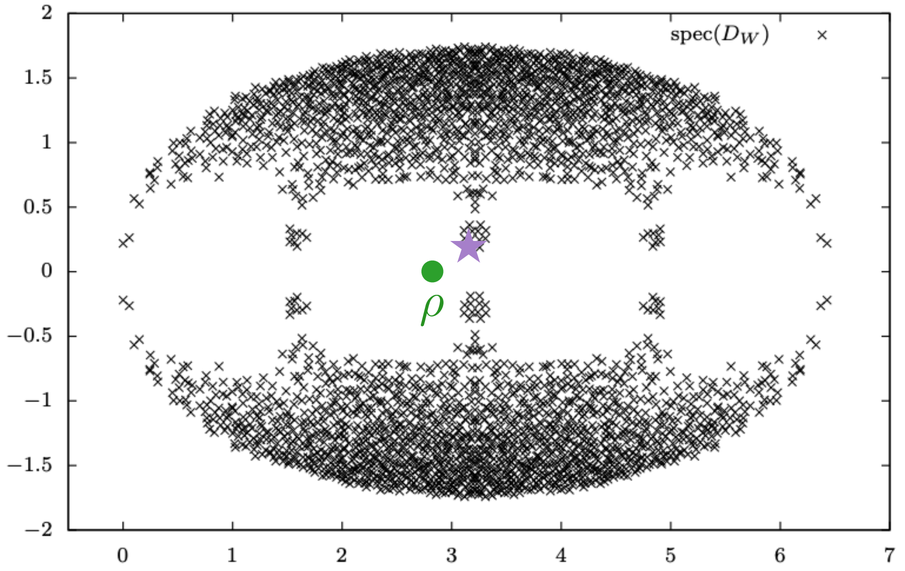

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- Fix $\rho \in \mathbb{C}$ and consider,

$$\Theta_\rho(D) \equiv (D - \rho I)^{-1}$$

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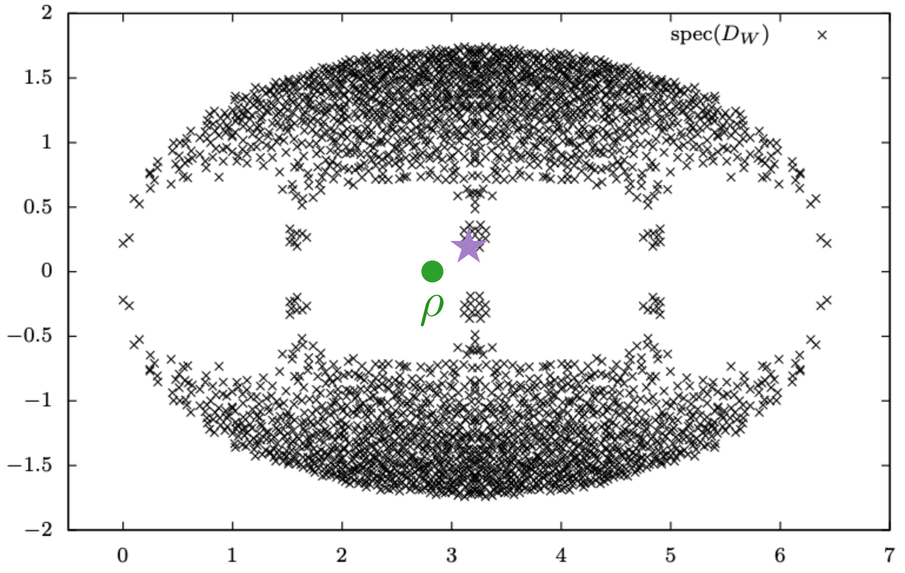
- An eigenvalue λ of D corresponds to the eigenvalue $\theta_\rho(\lambda) = (\lambda - \rho)^{-1}$ of $\Theta_\rho(D)$ with the same eigenvector.
  - The largest norm $\theta_\rho(\lambda)$ corresponds to the eigenvalue λ closest to ρ.
  - The power method applied to $\Theta_\rho(D)$ yields the closest eigenvalue of D to ρ.

Shift-and-Invert Operator



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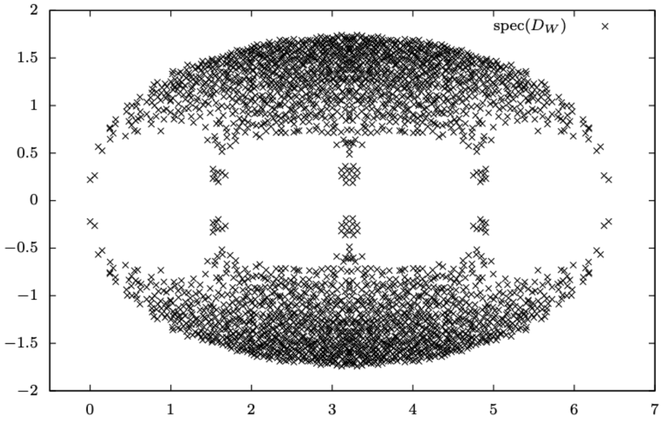
  - The largest norm $\theta_\rho(\lambda)$ corresponds to the eigenvalue λ closest to ρ.
  - The power method applied to $\Theta_\rho(D)$ yields the closest eigenvalue of D to ρ.
- Major downside: **matrix inversion is expensive**. Can use this to compute a few eigenvalues in isolation, but **not** a whole region of the spectrum.

Harmonic Krylov-Schur (HKS)

V. Herndandez *et. al.*
ACM Trans. Math. Software 31 (2005) 351.

- **Harmonic Krylov-Schur**: approximate the Galerkin condition for shift-and-invert operator $\Theta_\rho(D) = (D - \rho I)^{-1}$ by augmenting the Krylov space as $V = (D - \rho I)U$,

$$V^\dagger[\Theta_\rho(D)(Vz) - \tilde{\theta}_\rho(Vz)] = 0$$



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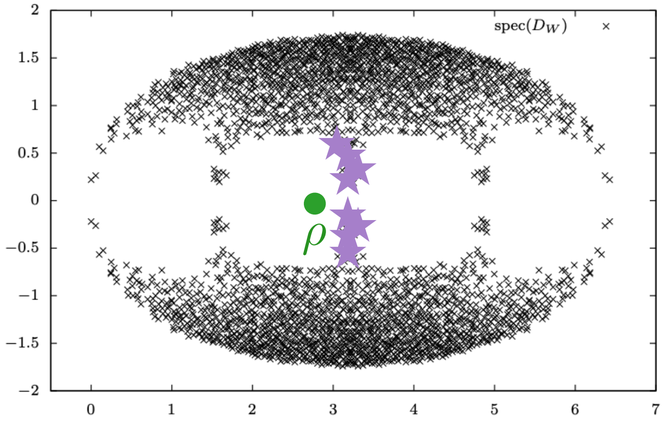

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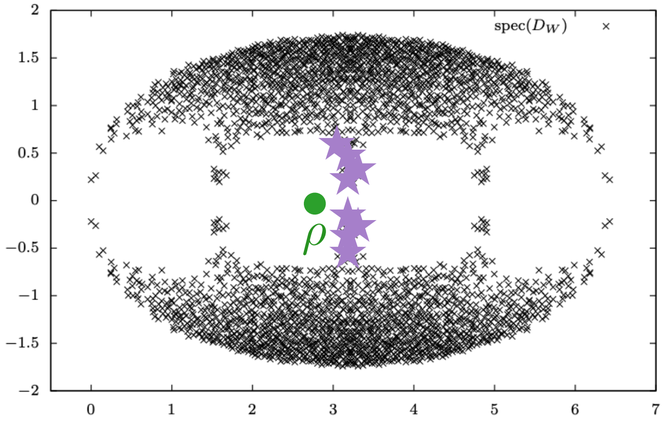

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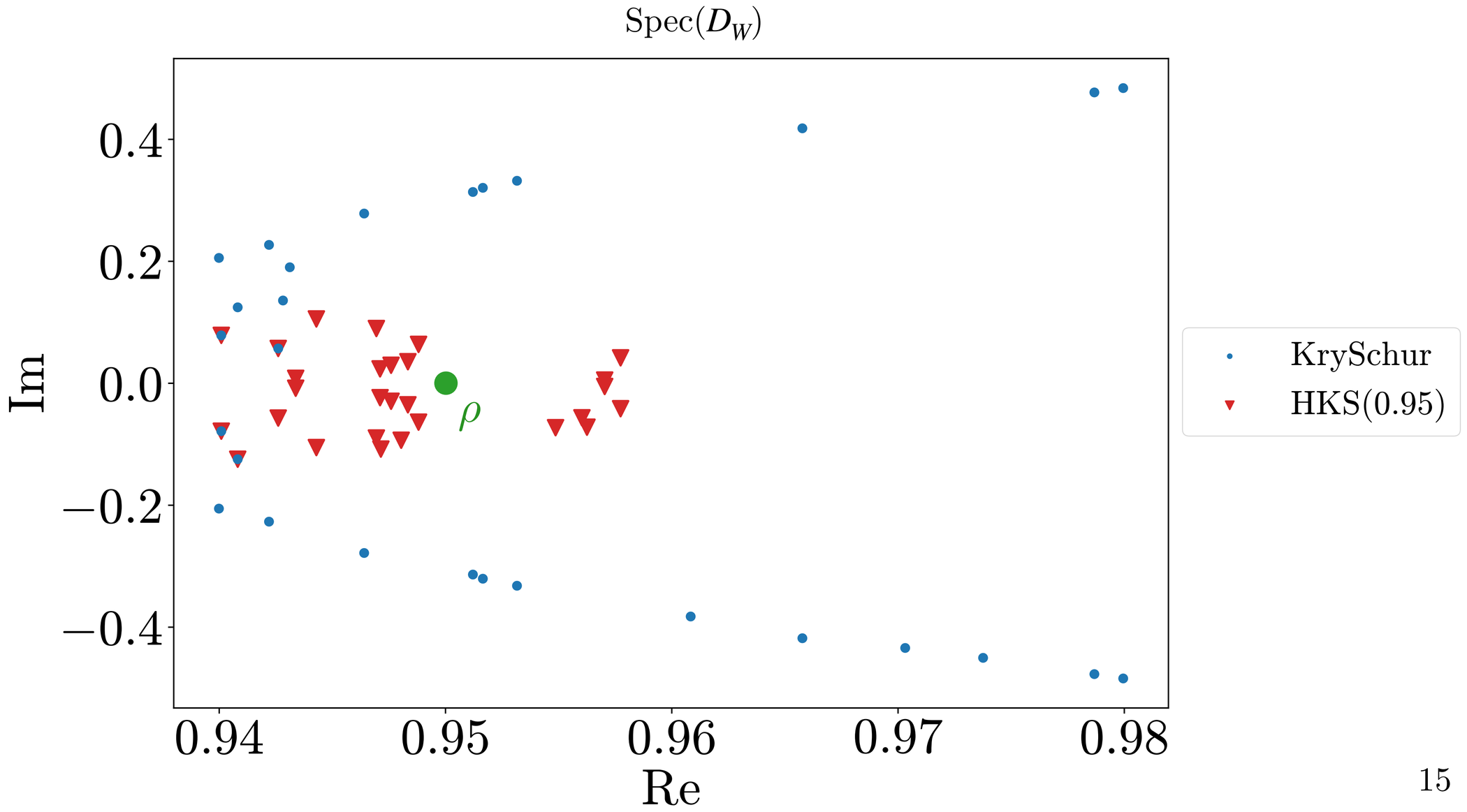
  - Gives access to eigenvalues closest to ρ by maximizing $\tilde{\theta}_\rho(\lambda) = |(\rho - \lambda)^{-1}|$.
- Modifies Krylov-Schur **without inverting the Dirac operator directly**, only translations and inversions of the Rayleigh quotient.
  - Provides the benefit of shift-and-invert by allowing us to target the interior of the spectrum without the need for direct inversion.
  - Downside: algorithm is extremely sensitive to choices of hyperparameters.

Interior spectrum with HKS



Conclusion

- The low modes of the spectrum are closely related to the slow modes of convergence for iterative linear solvers and are important to understand in order to accelerate these solvers.
- Krylov-Schur provides a more robust tool than Arnoldi to compute the spectrum of non-Hermitian Dirac operators.
- Modes in the interior of the spectrum are difficult to determine numerically.
  - The Harmonic Krylov-Schur algorithm allows us to target the spectrum's interior without inverting the Dirac operator.
- Chulwoo's talk next will discuss another application of Harmonic Krylov-Schur: directly computing real eigenmodes of the Wilson-Dirac operator.

Backup Slides

The Wilson Operator

- Canonical example of a non-normal D we'll use is the Wilson operator D_W,

$$D_W(m)_{x,y} = (4+m) - \frac{1}{2}\sum_{\mu=1}^{4}(1-\gamma_\mu)U_\mu(x)\delta_{x+\hat{\mu},y} + (1+\gamma_\mu)U_\mu^\dagger(y)\delta_{x-\hat{\mu},y}$$

  - m sets the mass gap: m small $\implies$ $D_W(m)$ poorly conditioned.
  - $D_W(m)$ is non-normal, but satisfies γ_5 hermiticity $D_W^\dagger = \gamma_5 D_W \gamma_5$.
- Its Hermitian counterpart $H_W(m) = \gamma_5 D_W(m)$ has a real spectrum.
- Characteristic poly of D_W satisfies $p(\lambda) = \det(D_W - \lambda) = \det(D_W^\dagger - \lambda) = p(\lambda^*)^*$.
- If λ is an eigenvalue, $p(\lambda) = 0$, so either:
  1. $\lambda \in \mathbb{R}$ is a real eigenvalue of D_W, or
  2. $p(\lambda^*) = 0 \implies \lambda^*$ an eigenvalue of D_W.

Eigenvalues of a γ_5-hermitian Dirac operator are either real or come in complex-conjugate pairs.

Power iteration

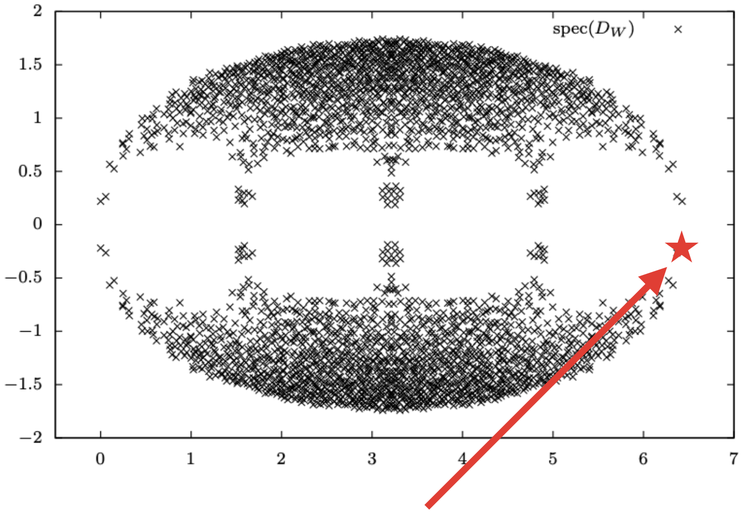
$$D = \sum_{\lambda} \lambda |\lambda\rangle\langle\lambda|$$

- Direct calculation of the eigenspectrum of an $\mathscr{M} \times \mathscr{M}$ matrix D through the characteristic polynomial $p(\lambda) = \det(D - \lambda I_{\mathscr{M}})$ is not feasible when M is large.
  - **Eigenvalue algorithms** are iterative algorithms that approximate Spec(D).
- **Power iteration**: determines eigenvalue Λ of D with maximal norm.
  - Express initial vector $|v_0\rangle$ in the eigenbasis of D as,

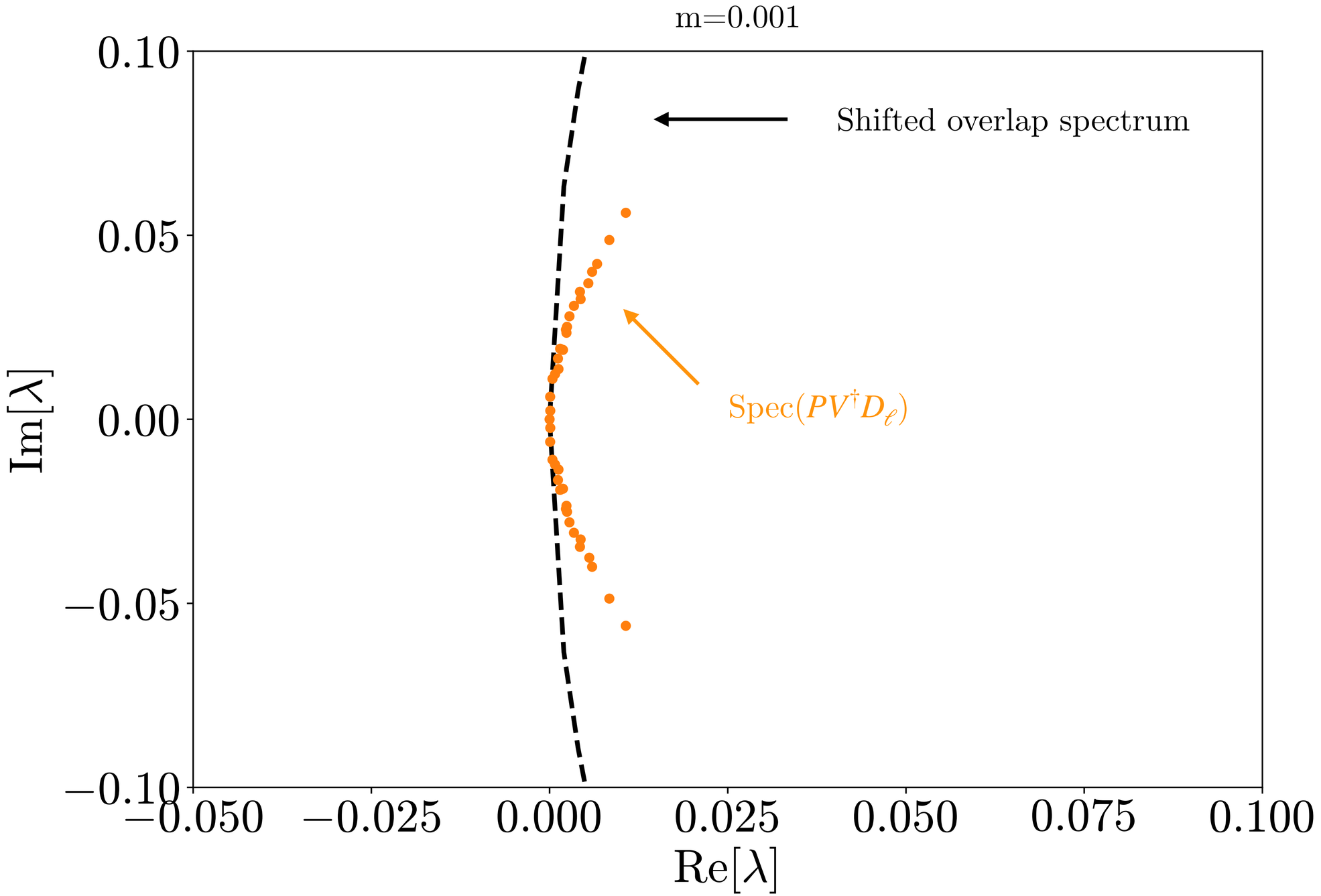
$$|v_0\rangle = \sum_{\lambda} c_\lambda |\lambda\rangle$$

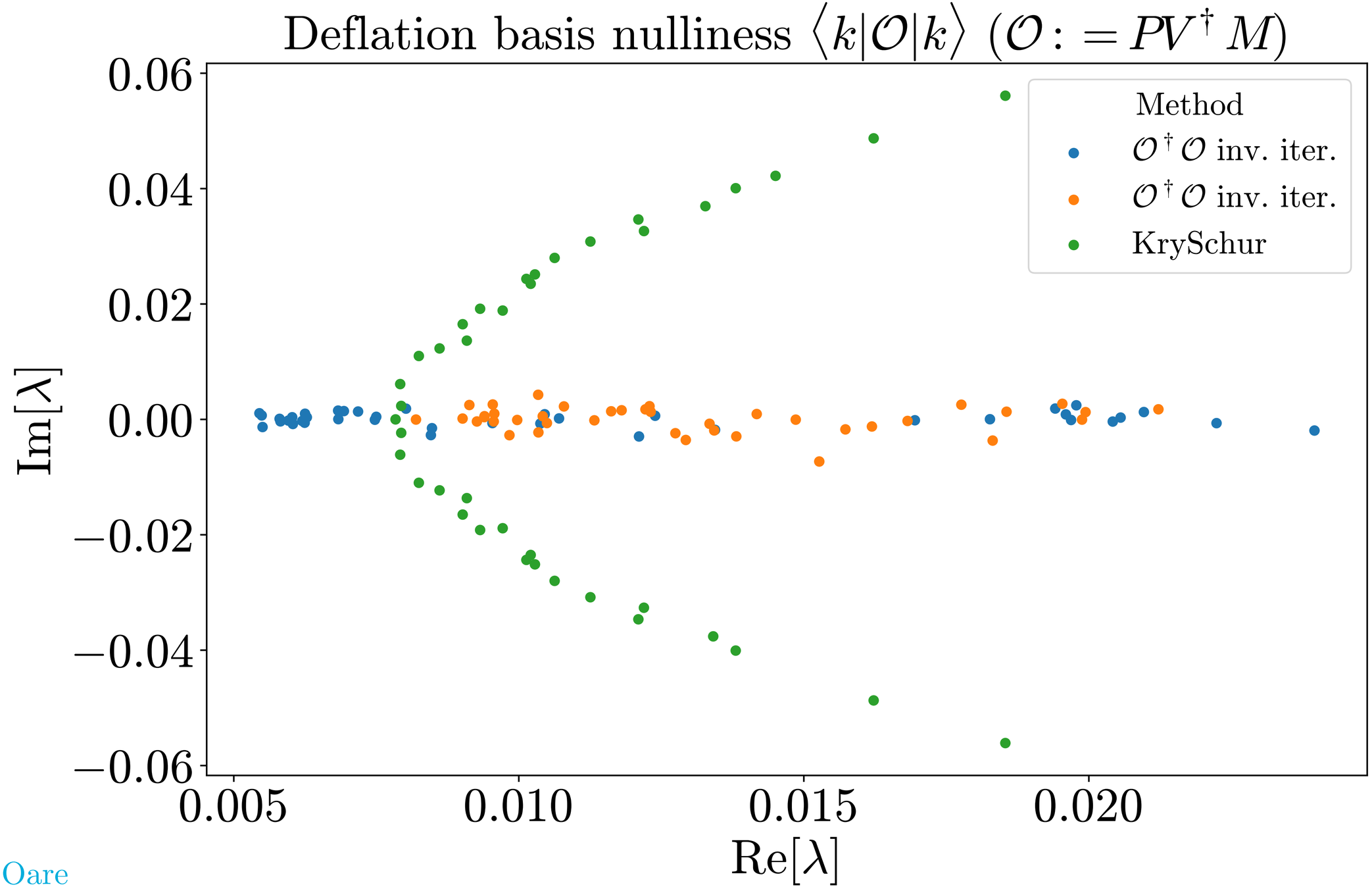
  - Repeatedly applying D to $|v_0\rangle$ converges to $|\Lambda\rangle$,

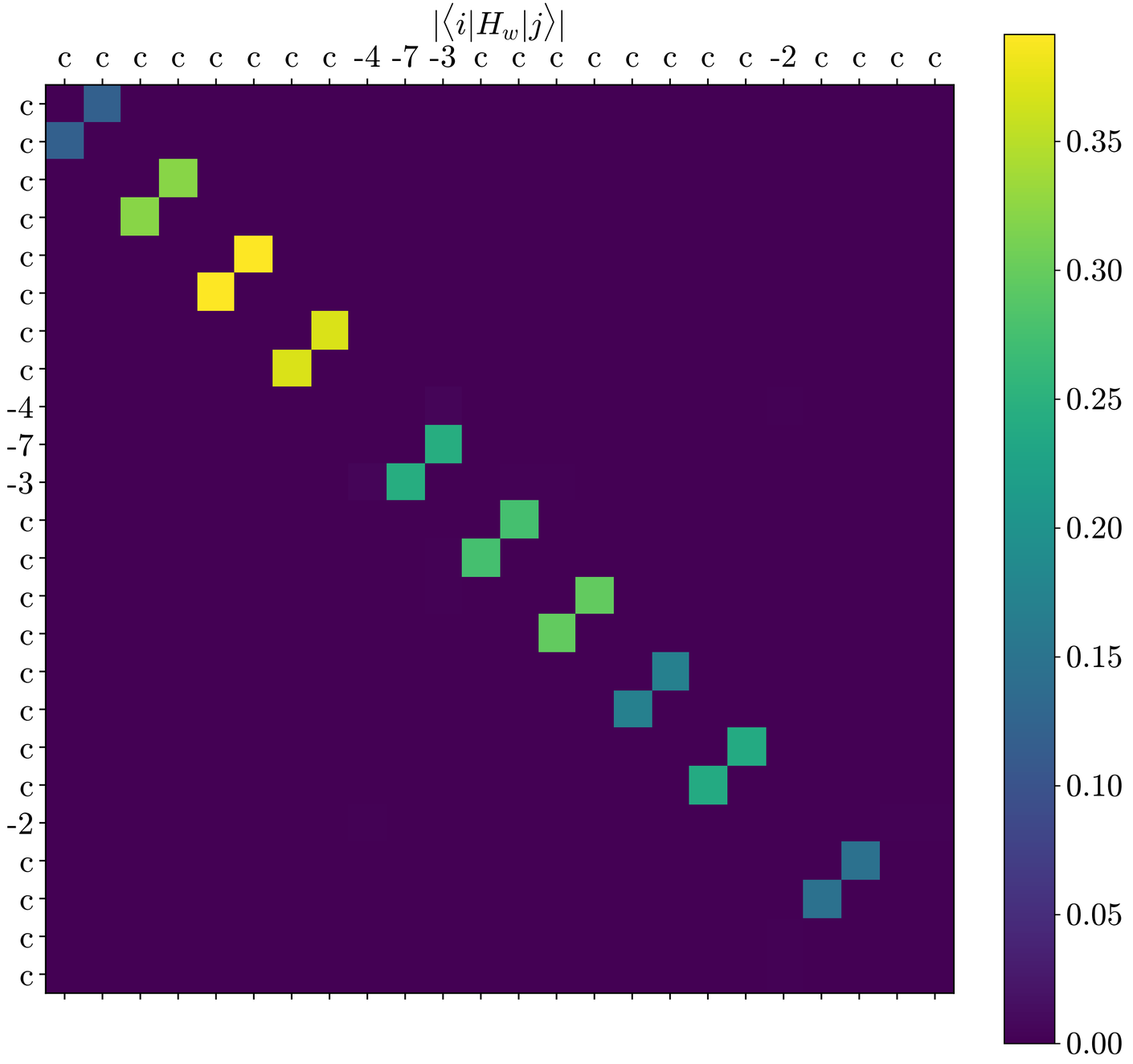
$$D^N |v_0\rangle = \sum_{\lambda} c_\lambda \lambda^N |\lambda\rangle \xrightarrow{N\to\infty} c_\Lambda \Lambda^N |\Lambda\rangle$$

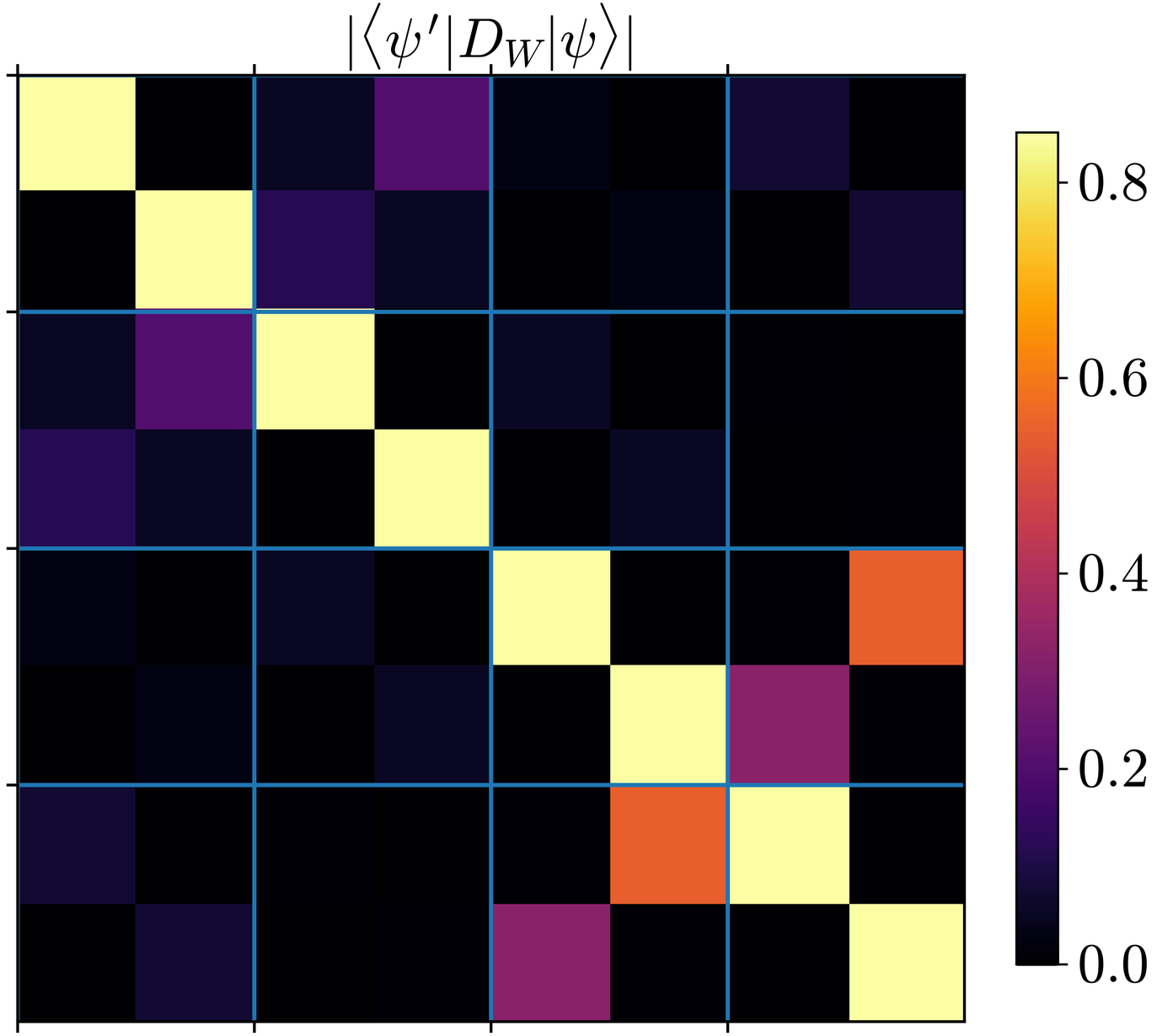


Example eigenvalue the power method can compute


m=0.001
Shifted overlap spectrum
Spec($PV^\dagger D_\ell$)
0.10
0.05
0.00
−0.05
−0.10
Im[λ]
−0.050
−0.025
0.000
0.025
0.050
0.075
0.100
Re[λ]


Deflation basis nulliness $\langle k|\mathcal{O}|k\rangle$ $(\mathcal{O} := PV^\dagger M)$
Method
$\mathcal{O}^\dagger\mathcal{O}$ inv. iter.
$\mathcal{O}^\dagger\mathcal{O}$ inv. iter.
KrySchur
0.06
0.04
0.02
0.00
−0.02
−0.04
−0.06
Im[λ]
0.005
0.010
0.015
0.020
Re[λ]


$|\langle i|H_w|j\rangle|$
c c c c c c c c -4 -7 -3 c c c c c c c c -2 c c c c
c c c c c c c c c -4 -7 -3 c c c c c c c c -2 c c c c
0.35
0.30
0.25
0.20
0.15
0.10
0.05
0.00


$|\langle\psi'|D_W|\psi\rangle|$
0.8
0.6
0.4
0.2
0.0