

A Computational Approach for Exploring Spatial Localization of Eigenvectors

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BIRS Workshop: Mathematical aspects of the physics with non-self-adjoint operators

Eigenvalue Problem

Eigenvalue Problem:

$$\mathcal{L}\psi = \lambda\psi \text{ in } \Omega \quad , \quad \mathcal{B}\psi = 0 \text{ on } \partial\Omega$$

Second-Order Linear Elliptic Operator:

$$\mathcal{L}v = -\nabla \cdot (A\nabla v) + \mathbf{b} \cdot \nabla v + cv$$

- Selfadjoint: $\mathbf{b} = \mathbf{0}$
- Morally Selfadjoint: $A^{-1}\mathbf{b}$ conservative with potential β , $\nabla\beta = A^{-1}\mathbf{b}/2$

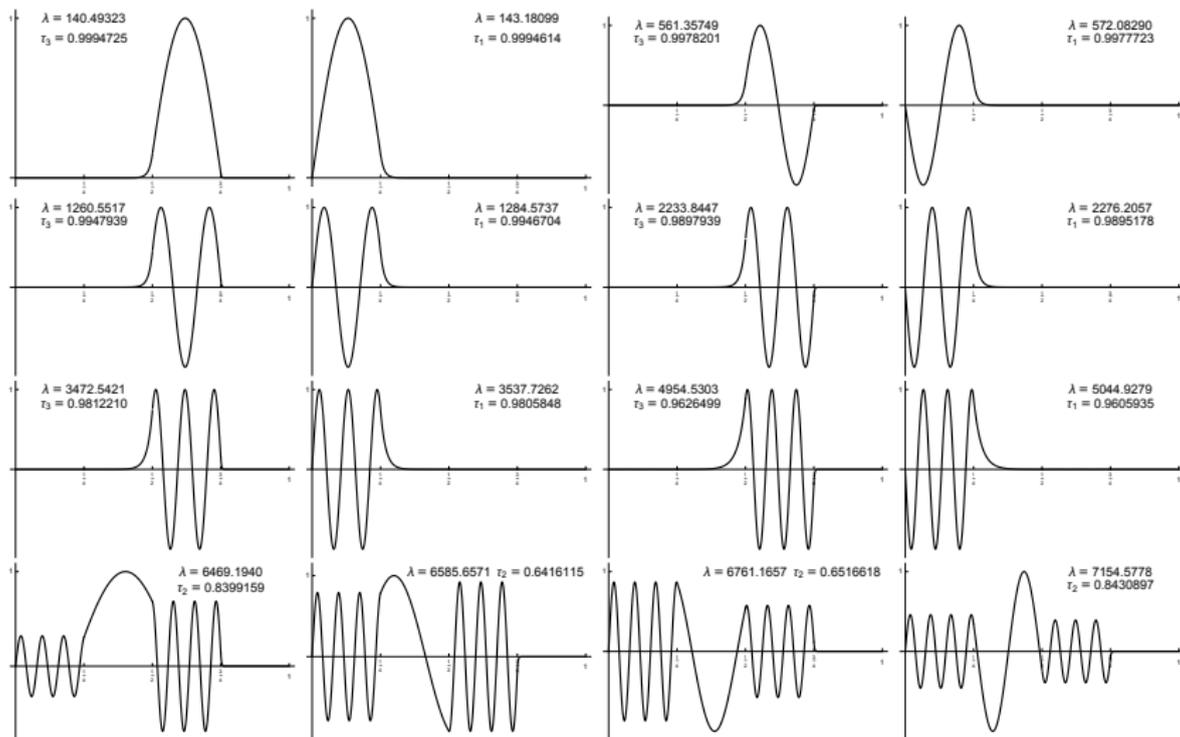
$$\tilde{\mathcal{L}}v \doteq e^{-\beta}\mathcal{L}(e^{\beta}v) = -\nabla \cdot (A\nabla v) + \left(c - \frac{\nabla \cdot \mathbf{b}}{2} + \frac{\mathbf{b} \cdot (A^{-1}\mathbf{b})}{4} \right) v$$

Eigenvector Localization:

Coefficients, domain geometry, boundary conditions can cause strong spatial localization of some eigenvectors

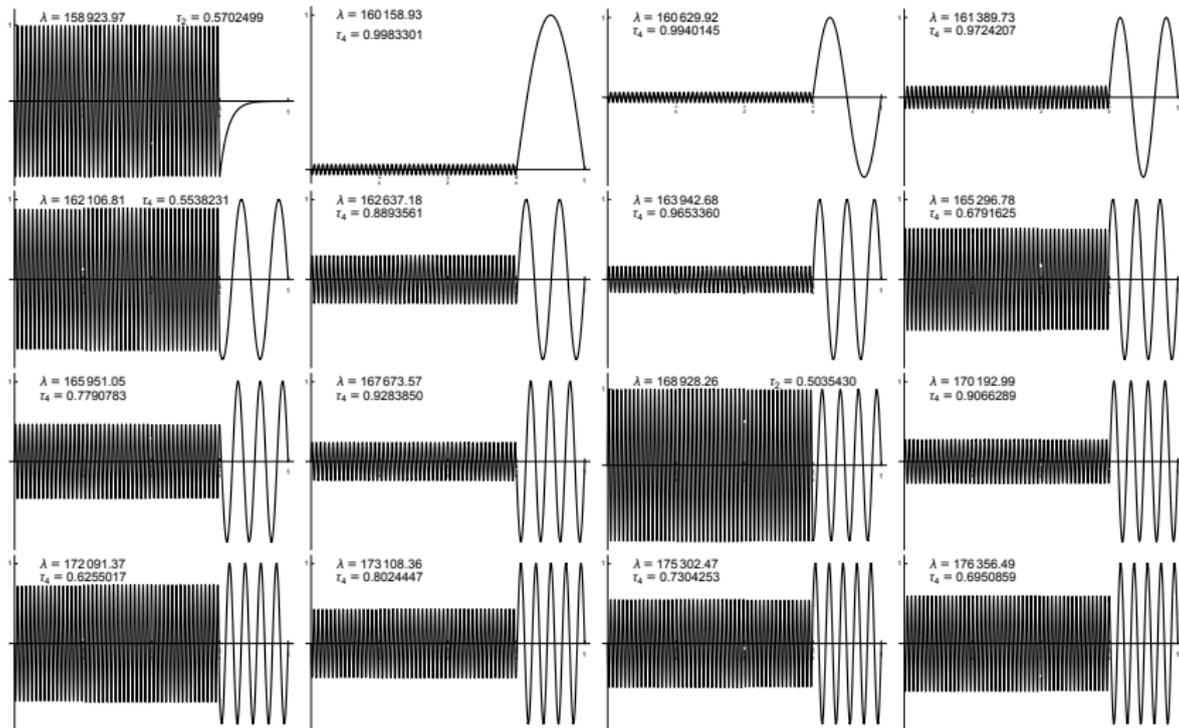
1D Model Problem: $\mathcal{L}V = -V'' + cV$, $c = (0, 80^2, 0, 400^2)$

Eigenvectors 1-16



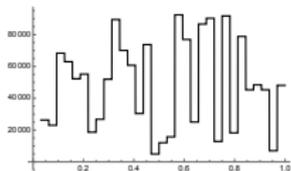
1D Model Problem: $\mathcal{L}V = -V'' + cV$, $c = (0, 80^2, 0, 400^2)$

Eigenvectors 95-110

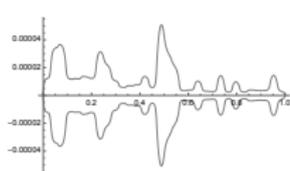


1D Localization Example, $\mathcal{L}v = -v'' - 4v' + cv$

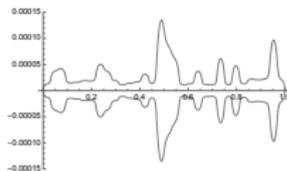
c



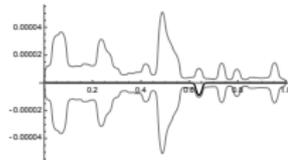
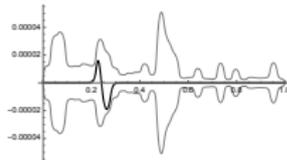
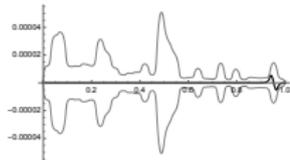
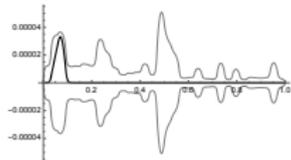
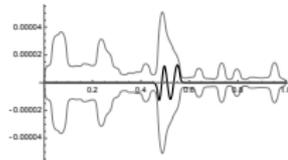
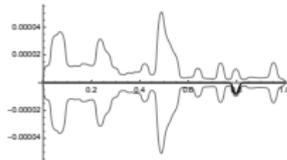
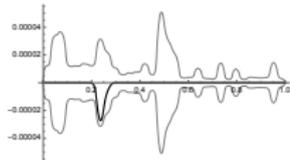
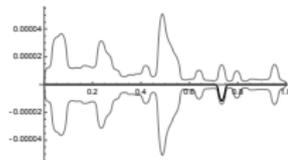
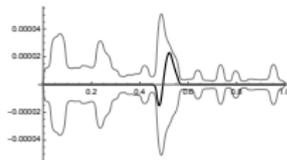
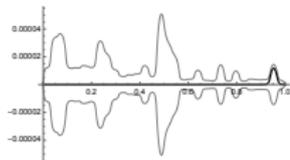
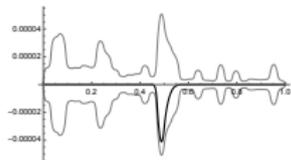
$\pm u, \mathcal{L}u = e^{-2x}$



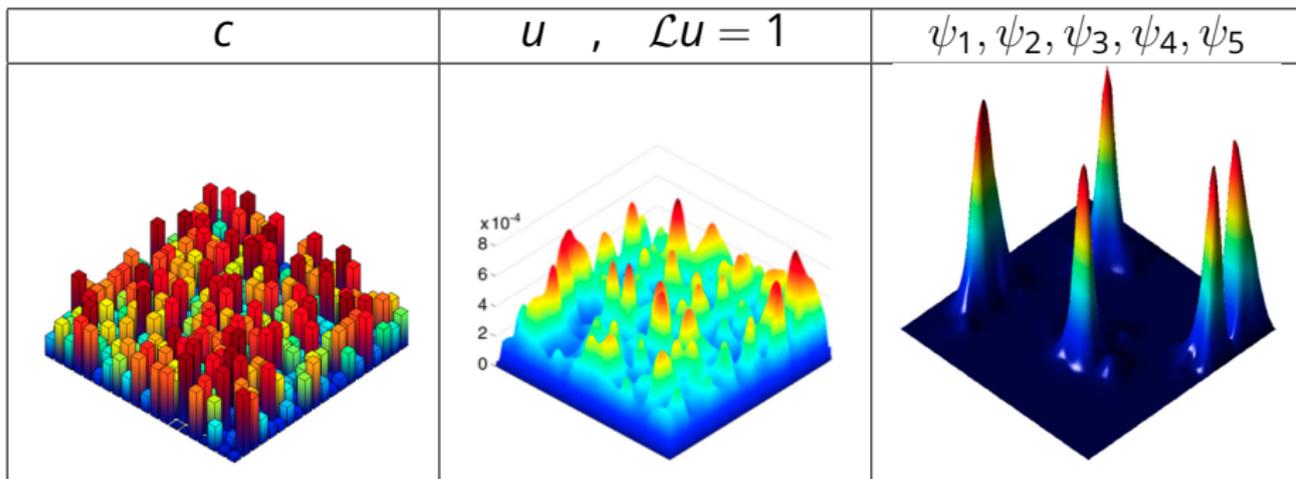
$\pm \tilde{u}, \tilde{\mathcal{L}}\tilde{u} = 1$



$$\frac{\psi_n(x)}{\lambda_n \|e^{2x} \psi_n\|_{L^\infty(\Omega)}}$$



2D Localization Example, $\mathcal{L}v = -\Delta v + cv$



Filoche/Mayboroda, PNAS 2012

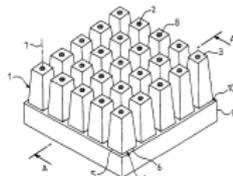
Why Might Scientists/Engineers Care?

Localization of eigenvectors ↔ localization of waves

- Semi-conductor design
- Efficient LED and solar cell operation
- Noise mitigation



(12) United States Patent Sapoval et al.		(10) Patent No.: US 7,308,965 B2
		(45) Date of Patent: Dec. 18, 2007
(54) NOISE ABATEMENT WALL	(58) Field of Classification Search	181/210, 181/203, 295, 246, 285, 286, 527/44, 145 See application file for complete search history.
(75) Inventors: Bernard Sapoval, Patric FERRÉ, Marcel Flichez, Fernand FERRÉ, Michel Chappet, Marcques FERRÉ, Didier Peyraud, Mortant FERRÉ	(56) References Cited	U.S. PATENT DOCUMENTS
(73) Assignees: Ecole Polytechnique, Palmaris FERRÉ, Ecole, Institut-Nonlinear FERRÉ	1,791,232 A * 2/19/03 Borokanin	181/209
(*) Notice: Subject to any disclaimer, the term of this patent is extended or adjusted under 35 U.S.C. 154(b) by 323 days.	2,271,164 A * 1/11/98 Scarfone	52/404.1
(21) Appl. No.: 105508,119	2,262,164 A * 5/10/97 Cardell	182/194
(22) PCT Filed: Mar. 19, 2003	2,840,179 A * 6/19/98 Angar	181/286
(86) PCT No.: PCT/FR03/010081	3,223,371 A * 2/16/06 Hildebrand et al.	181/203
§ 371 (c)(3), (2), (4) Date: Sep. 16, 2004	3,722,619 A * 3/19/93 Higgin	181/286
(87) PCT Pub. No.: WO03/078740	3,814,208 A * 6/17/04 Mortant et al.	181/203
PCT Pub. Date: Sep. 25, 2003	4,242,208 A * 12/18/98 Segura et al.	428/172
(65) Priority Publication Data	4,425,981 A * 1/1/98 Kiselevich et al.	181/286
US 2005/0103568 A1 May 19, 2005	4,515,653 A * 11/16/97 Ishizuka et al.	428/166
(30) Foreign Application Priority Data	5,824,200 A * 6/19/91 Baker	181/203
Mar. 19, 2002 (FR)	5,827,920 A * 7/19/91 D Antonio et al.	181/285
	5,908,818 A * 11/19/92 Chapp	181/285
(51) Int. Cl.	5,935,318 A * 3/19/99 D Antonio et al.	181/155
G04B 21/06 (2006-01)	5,230,763 A * 10/19/99 Brossa	
E04B 1/82 (2006-01)		(Continued)
E04B 1/84 (2006-01)		FOREIGN PATENT DOCUMENTS
E04H 17/14 (2006-01)		(Continued)
(52) U.S. Cl.	181/210, 181/203, 181/285	DE 331813 A1 * 10/1984
		(Continued)
		Priority Examiner: Edgardo San Martin (74) Attorney, Agent or Firm — Young & Thompson
		(57) ABSTRACT
		A noise-shielding device includes a substantially flat base and embossed and/or hollow elements each including at least one recess. The base recedes with the embossed and/or hollow elements, a configuration including a flexibility zone of between 1 cm and 50 cm, of fructal dimension greater than 2.5 enabling the localization of the waves over the sound frequency range, in the vicinity of the elements.
		22 Claims, 7 Drawing Sheets



Origin of the Study of (Anderson) Localization

PHYSICAL REVIEW

VOLUME 109, NUMBER 5

MARCH 1, 1958

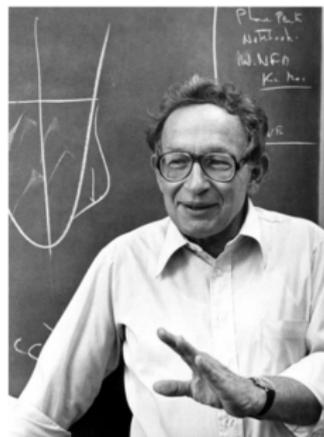
Absence of Diffusion in Certain Random Lattices

P. W. ANDERSON

Bell Telephone Laboratories, Murray Hill, New Jersey

(Received October 10, 1957)

This paper presents a simple model for such processes as spin diffusion or conduction in the "impurity band." These processes involve transport in a lattice which is in some sense random, and in them diffusion is expected to take place via quantum jumps between localized sites. In this simple model the essential randomness is introduced by requiring the energy to vary randomly from site to site. It is shown that at low enough densities no diffusion at all can take place, and the criteria for transport to occur are given.



Very few believed [localization] at the time, and even fewer saw its importance; among those who failed to fully understand it at first was certainly its author. It has yet to receive adequate mathematical treatment, and one has to resort to the indignity of numerical simulations to settle even the simplest questions about it.

—Philip W. Anderson, Nobel lecture,
8 December 1977

Four Teams of Researchers (Math Side of Things)

- 1 Filoche, Mayboroda, Arnold, David, Jerison ...
 - Filoche, Mayboroda PNAS 2012
 - Predicting localization via landscape function $\mathcal{L}u = 1$
 - Simons Collaboration on Localization of Waves
- 2 Steinerberger, Lu, Murphey, Jones
 - Steinerberger PAMS 2017
 - Predicting localization via “smoothed potentials”
- 3 Altmann, Henning, Petersheim
 - Altmann, Petersheim SISC 2019
 - Approx. localized eigenvectors/values at lower end of spectrum
- 4 Ovall, Reid
 - Ovall, Reid MCOM 2022
 - Approx. localized eigenvectors/values higher in spectrum
 - Ideas inspired by work of Marletta (IMAJNA 2009, JST 2012)

Our Approach: A More Targeted Task

$$\mathcal{L}\psi = \lambda\psi \text{ in } \Omega, \quad \mathcal{B}\psi = 0 \text{ on } \partial\Omega$$

Key Task:

Given a subdomain $R \subset \Omega$, a (small) tolerance $\delta^* > 0$ and a (large) interval $[a, b]$, find all eigenpairs (λ, ψ) of \mathcal{L} such that $\lambda \in [a, b]$ and $\delta(\psi, R) < \delta^*$.

- $\mathcal{L}w \doteq -\nabla \cdot (A\nabla w) + Vw$
- $\delta(v, R) \doteq \|v\|_{L^2(\Omega \setminus R)} / \|v\|_{L^2(\Omega)}$, $\tau(v, R) \doteq \|v\|_{L^2(R)} / \|v\|_{L^2(\Omega)}$
 - $\delta^2 + \tau^2 = 1$ localized in R if δ “near” 0 (τ “near” 1)
 - $\delta(cv, R) = \delta(v, R)$ and $\tau(cv, R) = \tau(v, R)$ for $c \neq 0$

Our Approach: Change the Problem

Old Task:

Given a subdomain $R \subset \Omega$, a (small) tolerance $\delta^* > 0$ and a (large) interval $[a, b]$, find all eigenpairs (λ, ψ) of \mathcal{L} such that

$$\lambda \in [a, b], \delta(\psi, R) < \delta^*$$

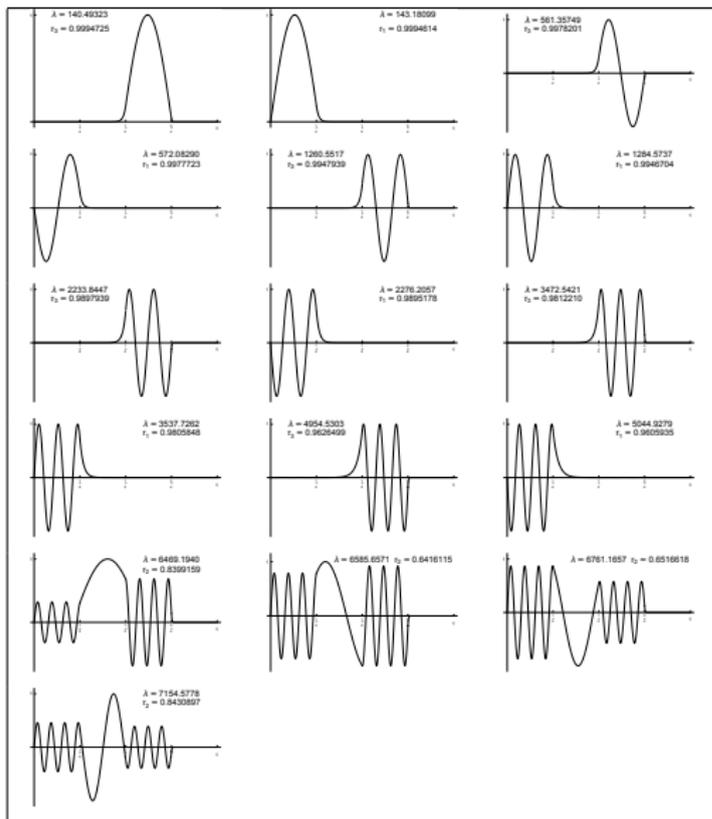
New Task:

Given a subdomain $R \subset \Omega$, a (small) tolerance $\delta^* > 0$ and a (large) interval $[a, b]$, find all eigenpairs (μ, ϕ) of \mathcal{L}_s^R such that

$$\mu \in U(a, b, s, \delta^*)$$

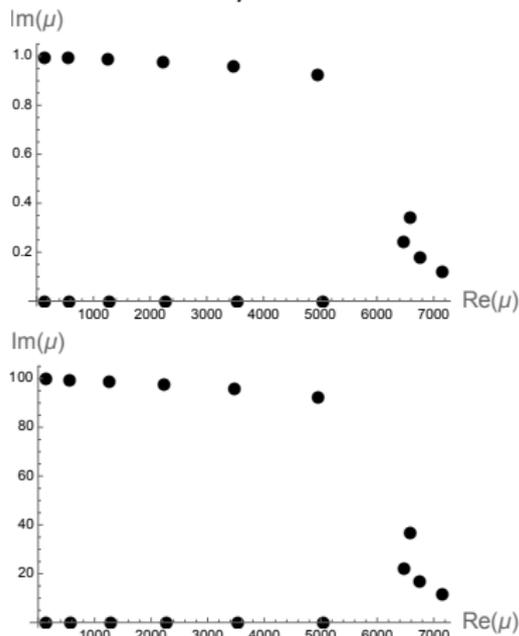
$$\mathcal{L}_s^R w \doteq (\mathcal{L} + i s \chi_R) w, s > 0$$

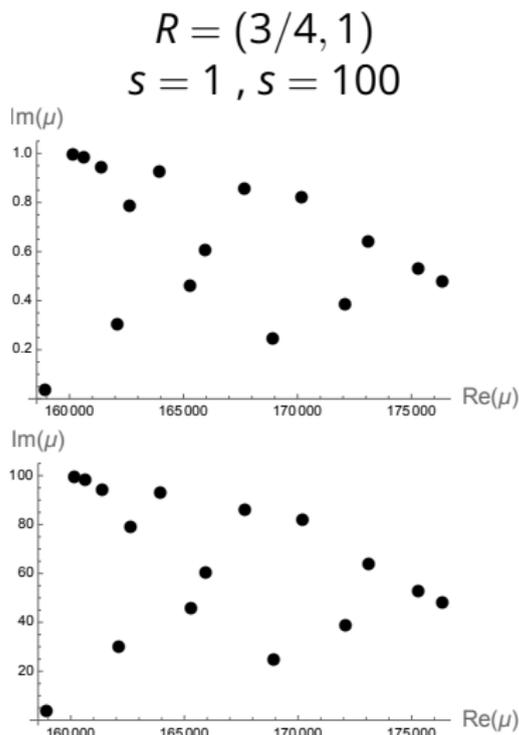
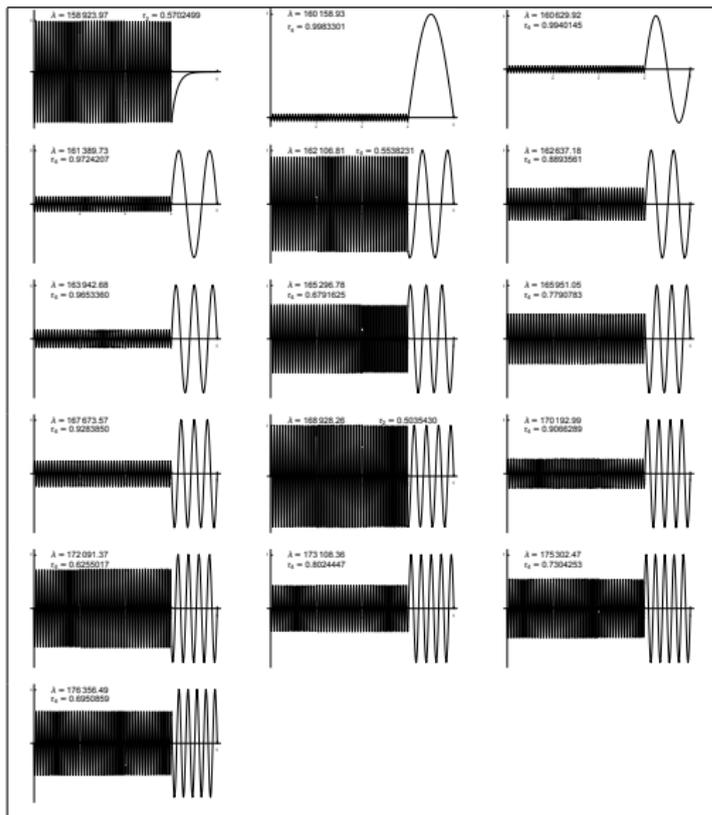




$$R = (1/2, 3/4)$$

$$s = 1, s = 100$$





Theorem: Let (λ, ψ) be an eigenpair of \mathcal{L} (selfadjoint), with $\delta(\psi, R) < \delta^*$. For $s > 0$ sufficiently small, $\text{dist}(\lambda + is, \text{Spec}(\mathcal{L}_s^R)) \leq s\delta^*$.

Proof. Let $\mathcal{L}(z) = \mathcal{L} - z\chi_{\Omega \setminus R}$, $\delta = \delta(\psi, R)$, and suppose $\|\psi\|_{L^2(\Omega)} = 1$.

- $(\lambda - \mathcal{L}(z))\psi = z\chi_{\Omega \setminus R}\psi$, $\|\chi_{\Omega \setminus R}\psi\|_{L^2(\Omega)} = \delta$
- $\|(\lambda - \mathcal{L}(z))^{-1}\|^{-1} \leq |z|\delta$ for all $z \in \mathbb{C}$ such that $\lambda \in \text{Res}(\mathcal{L}(z))$
- For **real** z , $\mathcal{L}(z)$ selfadjoint and $\text{dist}(\lambda, \text{Spec}(\mathcal{L}(z))) \leq |z|\delta$
- For $|z|$ sufficiently small, $\text{dist}(\lambda, \text{Spec}(\mathcal{L}(z))) \leq |z|\delta^*$
- For $s > 0$ sufficiently small, $\text{dist}(\lambda, \text{Spec}(\mathcal{L}(is))) \leq s\delta^*$
- For $s > 0$ sufficiently small, $\text{dist}(\lambda + is, \text{Spec}(\mathcal{L}(is) + is)) \leq s\delta$, $\mathcal{L}(is) + is = \mathcal{L}_s^R$

Question: How large can s be while still being "sufficiently small"?

Theorem: Let (μ, ϕ) be an eigenpair of \mathcal{L}_S^R , and set $\delta = \delta(\phi, R)$ and $\tau = \tau(\phi, R)$. Then

$$\Im\mu = s\tau^2 \quad , \quad \text{dist}(\Re\mu, \text{Spec}(\mathcal{L})) \leq s\delta\tau \quad ,$$

$$\|(\mathcal{L} - \Re\mu)(\Re\phi)\|_{L^2(\Omega)}^2 = s^2 \left(\delta^4 \|\Im\phi\|_{L^2(R)}^2 + \tau^4 \|\Im\phi\|_{L^2(\Omega \setminus R)}^2 \right) .$$

- For $\mu \in U(a, b, s, \delta^*)$, $[\delta(\phi, R)]^2 \leq \delta^*$
- Further normalize ϕ ($\|\phi\|_{L^2(\Omega)} = 1$), $\phi \leftarrow c\phi$,

$$c = \arg \min_{\substack{b \in \mathbb{C} \\ |b|=1}} \left(\delta^4 \|\Im(b\phi)\|_{L^2(R)}^2 + \tau^4 \|\Im(b\phi)\|_{L^2(\Omega \setminus R)}^2 \right)$$

A 2×2 hermitian eigenvalue problem

- $(\hat{\lambda}, \hat{\psi}) = (\Re\mu, \Re\phi)$ a reasonable guess at a localized eigenpair for \mathcal{L}

Algorithm Template

```
1: procedure LOCALIZE( $a, b, \delta^*, R, s$ )
2:   Get eigenpairs  $(\mu, \phi)$  of  $\mathcal{L}_s^R$  with  $\mu \in U(a, b, s, \delta^*)$  ▷ First filter
3:   for each  $(\mu, \phi)$  do
4:     Normalize:  $\phi \leftarrow c\phi$ 
5:     Post-process:  $(\Re\mu, \Re\phi) \rightsquigarrow (\tilde{\lambda}, \tilde{\psi})$ 
6:     Final check:  $\delta(\tilde{\psi}, R) < \delta^*$  and  $\tilde{\lambda} \in [a, b]$ ? ▷ Second filter
7:   end for
8:   return accepted  $(\tilde{\lambda}, \tilde{\psi})$ 
9: end procedure
```

- Line 2: Contour-integral based methods
 - FEAST, Beyn Method, SS/CIRR, SIM/RIM
 - $U(a, b, s, \delta^*) = \bigcup \{U(a_k, b_k, s, \delta^*) : 1 \leq k \leq N\}$
 - Explore $U(a_k, b_k, s, \delta^*)$ independently, in parallel
- Line 5: Few (perhaps zero) shifted-inverse iterations (in batches)

1D Model Problem: $\mathcal{L}v = -v'' + cv$, $c = (0, 80^2, 0, 400^2)$

Localization Summary:

- $[a, b] = [0, 220\,000]$, $\delta^* = 0.2$ ($\tau^* = \sqrt{0.96} \approx 0.97979590$)
- 130 eigenvalues of \mathcal{L}
- 5 eigenvectors of \mathcal{L} sufficiently localized in $R = (0, 1/4)$
- 0 eigenvectors of \mathcal{L} sufficiently localized in $R = (1/4, 1/2)$
- 5 eigenvectors of \mathcal{L} sufficiently localized in $R = (1/2, 3/4)$
- 2 eigenvectors of \mathcal{L} sufficiently localized in $R = (3/4, 1)$

“By Hand” Filtering Strategy:

- Find eigenpairs (μ, ϕ) of \mathcal{L}_s^R with $\mu \in U(a, b, s, \delta^*)$ First Filter
- Match $(\Re\mu, \Re\phi)$ with corresponding (λ, ψ) of \mathcal{L}
- Drop matched (λ, ψ) not satisfying localization criteria Second Filter

1D Model Problem: $\mathcal{L}V = -V'' + cV$, $c = (0, 80^2, 0, 400^2)$

Eigenpairs (μ, ϕ) of \mathcal{L}_s^R with $\mu \in U(a, b, s, \delta^*)$, $R = (1/2, 3/4)$

$s = 1$			$s = 100$			λ	$\delta(\psi, R)$
$\Re\mu$	$\Im\mu$	$\delta(\phi, R)$	$\Re\mu$	$\Im\mu$	$\delta(\phi, R)$		
140.49323	0.99894524	0.0324770	140.49441	99.894539	0.0324748	140.49323	0.0324770
561.35749	0.99564487	0.0659934	561.36244	99.564551	0.0659886	561.35749	0.0659934
1260.5517	0.98961499	0.1019069	1260.5640	98.961665	0.1018987	1260.5517	0.1019069
2233.8447	0.97969199	0.1425062	2233.8708	97.969580	0.1424928	2233.8447	0.1425062
3472.5421	0.96279456	0.1928871	3472.5974	96.280425	0.1928620	3472.5421	0.1928871
4954.5303	0.92669479	0.2707494	4954.6877	92.674005	0.2706658	4954.5303	0.2707494

- Automatically filtered out 124 candidates; had to drop one more

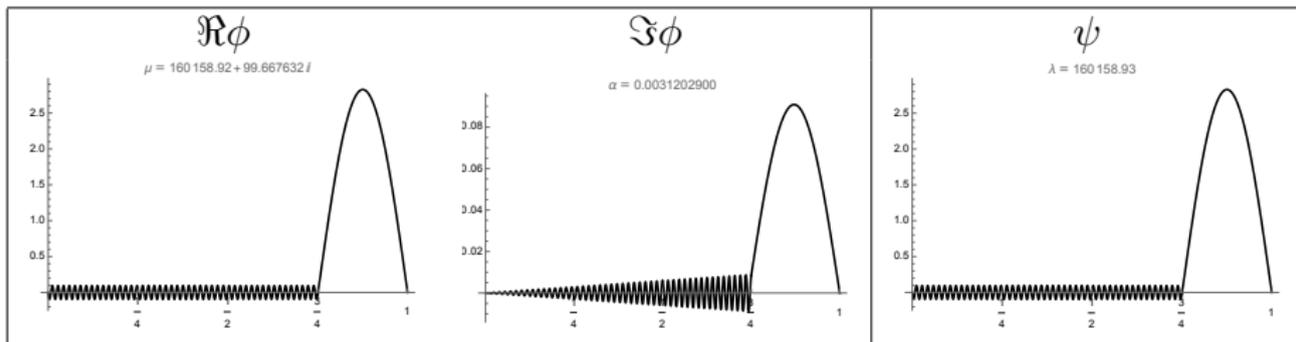
Eigenpairs (μ, ϕ) of \mathcal{L}_s^R with $\mu \in U(a, b, s, \delta^*)$, $R = (3/4, 1)$

$s = 1$			$s = 100$			λ	$\delta(\psi, R)$
$\Re\mu$	$\Im\mu$	$\delta(\phi, R)$	$\Re\mu$	$\Im\mu$	$\delta(\phi, R)$		
160158.93	0.99666301	0.0577667	160158.92	99.667632	0.0576513	160158.93	0.0577667
160629.92	0.98806481	0.1092483	160629.94	98.809982	0.1090879	160629.92	0.1092483
161389.73	0.94560213	0.2332335	161390.21	94.613050	0.2320981	161389.73	0.2332336
163942.68	0.93187361	0.2610103	163942.71	93.203093	0.2607088	163942.68	0.2610104
167673.57	0.86189881	0.3716197	167673.93	86.221341	0.3711962	167673.57	0.3716197
170192.99	0.82197599	0.4219289	170192.51	82.233071	0.4215084	170192.99	0.4219290

- Automatically filtered out 124 candidates; had to drop four more

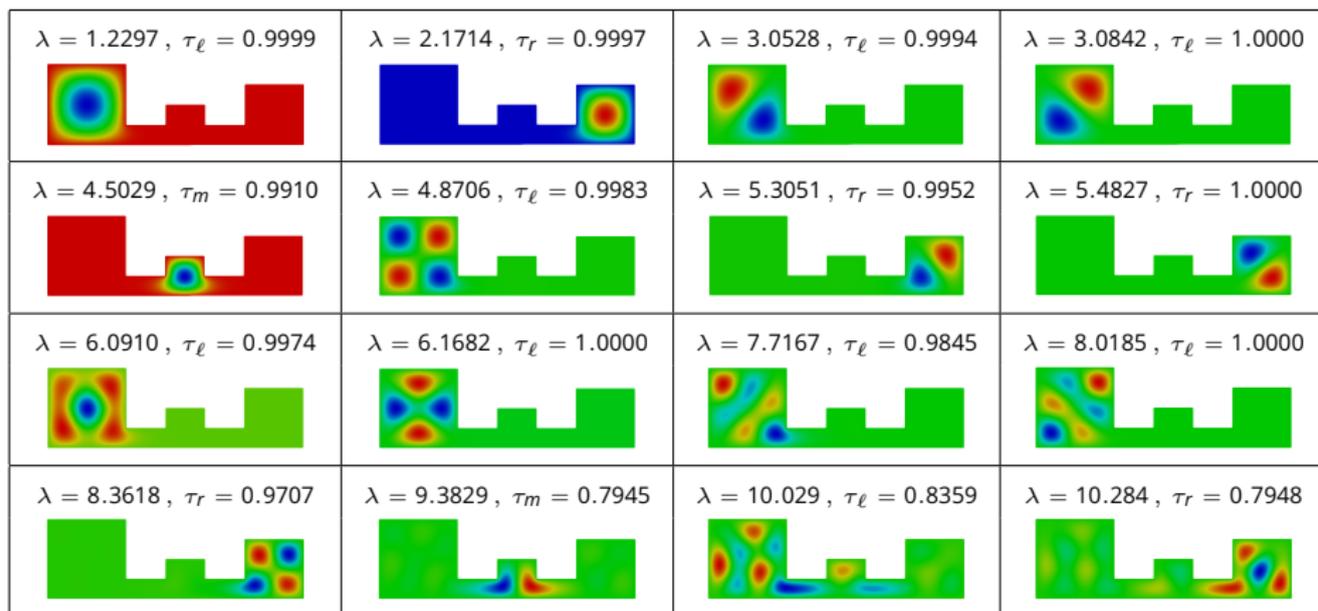
1D Model Problem: $\mathcal{L}V = -V'' + cV$, $c = (0, 80^2, 0, 400^2)$

Eigenpairs (μ, ϕ) of \mathcal{L}_S^R and (λ, ψ) of \mathcal{L} :



- $R = (3/4, 1)$ and $s = 100$
- After normalization, $\|(\mathcal{L} - \Re\mu)(\Re\phi)\|_{L^2(\Omega)} = 0.31202899606$
- Post-processing necessary?
 - $\Re\mu = 160158.92$, $\lambda = 160158.93$
 - $\|(\mathcal{L} - \Re\mu)(\Re\phi)\|_{L^2(\Omega)}/(\Re\mu) = 1.948 \times 10^{-6}$

2D Experiments: Geometry-Induced Localization



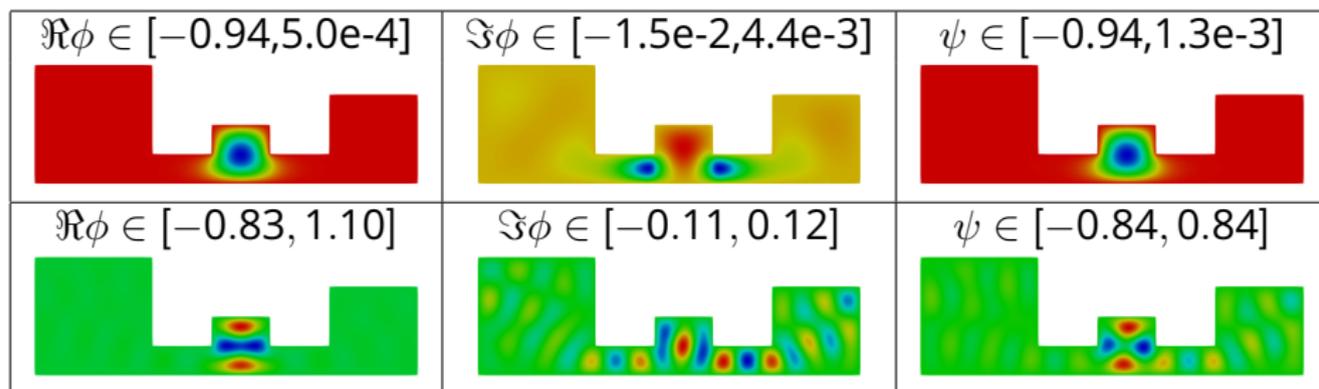
- 70 eigenpairs (λ, ψ) of \mathcal{L} with $\lambda \in [1, 33]$
 - 20 localized in left bulb within tolerance $\delta^* = 0.25$ ($\tau^* = 0.96825$)
 - 9 localized in right bulb within tolerance
 - 1 localized in middle bulb within tolerance

2D Experiments: Middle Bulb

$R = \mathbf{Middle Bulb}$, $U(1, 33, s, \delta^*)$, $s = 1$, $\delta^* = 0.25$

$\Re\mu$	$\Im\mu$	λ	$\delta(\psi, R)$
4.50447	0.98218	4.50292	0.02610
24.33196	0.96185	24.20972	0.64489

- Two candidates from \mathcal{L}_S^R : one match, one rejected

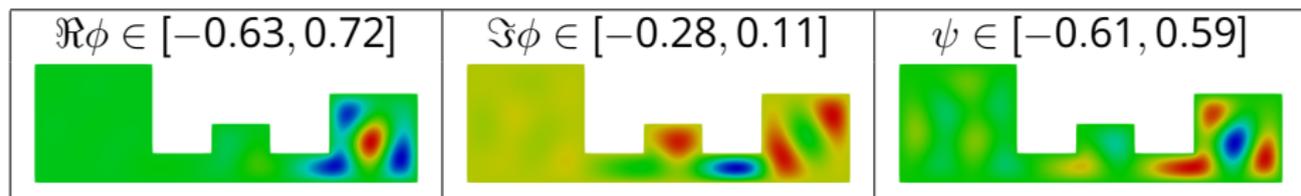


2D Experiments: Right Bulb

$R = \mathbf{Right\ Bulb}$, $U(1, 33, s, \delta^*)$, $s = 1$, $\delta^* = 0.25$

$\Re\mu$	$\Im\mu$	λ	$\delta(\psi, R)$	$\Re\mu$	$\Im\mu$	λ	$\delta(\psi, R)$
2.17146	0.99932	2.17143	0.02610	18.61842	0.99841	18.62201	0.32601
5.30605	0.99047	5.30506	0.09800	18.98014	0.83889	18.98051	0.48562
5.48270	1.00000	5.48270	0.00638	21.86147	0.99711	21.86307	0.07712
8.37589	0.94815	8.36148	0.24017	27.32128	0.99505	27.32821	0.18688
10.41327	0.82496	10.28357	0.60658	28.12641	0.90667	28.15248	0.33336
10.96057	0.99984	10.96061	0.02829	28.48136	0.99618	28.48221	0.06920
14.24624	0.99981	14.24624	0.01599	31.58901	0.97649	31.58960	0.27542

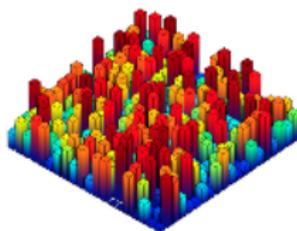
- 14 candidates from \mathcal{L}_s^R : 9 matches, five rejections
- Three rejections correspond to vectors barely missing tolerance δ^*



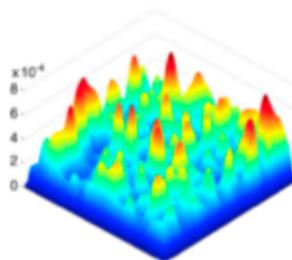
Identifying Regions R of Likely Localization?

Localization Landscape: $\mathcal{L}u = 1$ in Ω , $u = 0$ on $\partial\Omega$

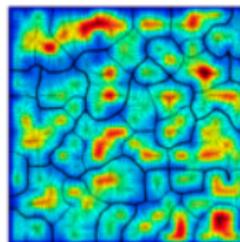
Potential V



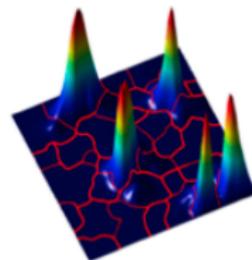
Landscape u



Partition



"In Action"



- Filoche/Mayboroda etc. approach
- Some motivating (if not fully explanatory) results

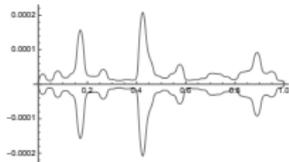
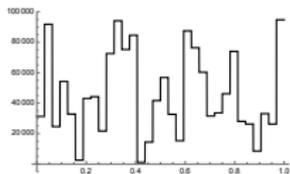
(pictures from Filoche/Mayboroda PNAS 2012)

$$\frac{|\psi_n(x)|}{\lambda_n \|\psi_n\|_{L^\infty(\Omega)}} \leq u(x) \quad , \quad u = \sum_{n \in \mathbb{N}} c_n \psi_n \quad \text{where } c_n = \frac{\int_{\Omega} \psi_n}{\lambda_n \|\psi_n\|_{L^2(\Omega)}}$$

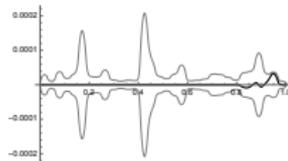
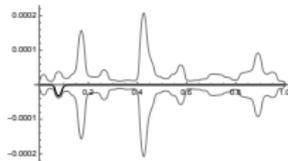
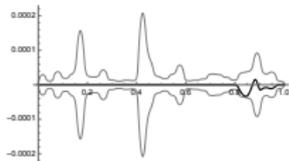
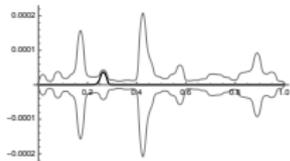
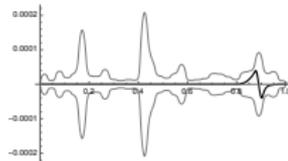
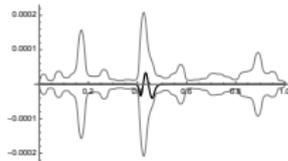
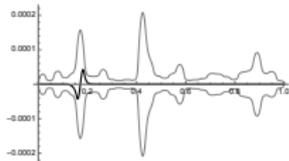
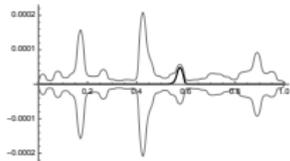
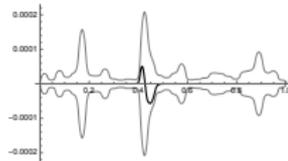
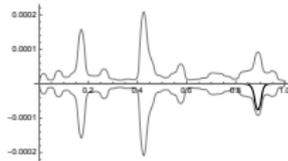
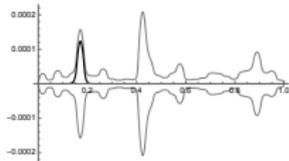
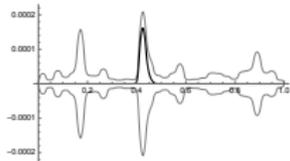
1D Localization Example, $\mathcal{L}v = -v'' + cv$, $0 \leq c \leq 10^5$

c

$\pm u, \mathcal{L}u = 1$



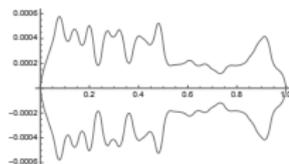
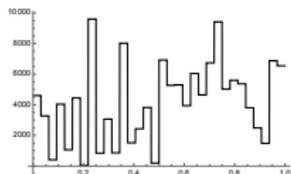
$$\frac{\psi_n(x)}{\lambda_n \|\psi_n\|_{L^\infty(\Omega)}}$$



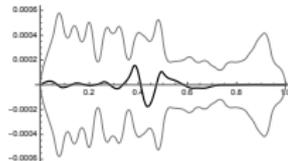
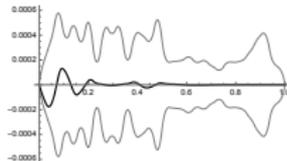
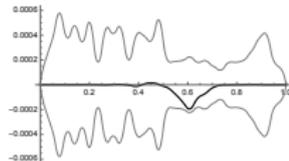
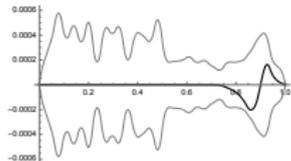
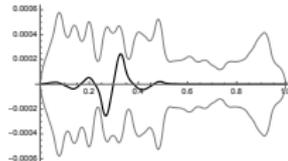
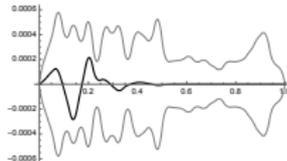
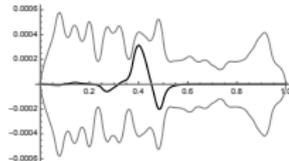
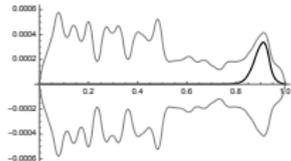
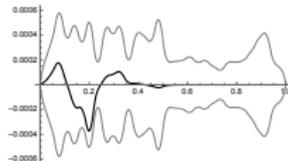
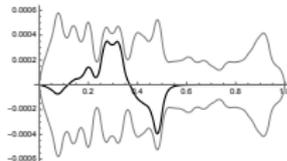
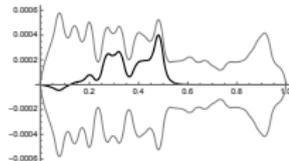
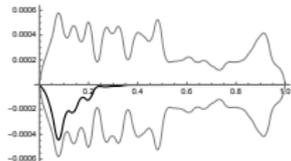
1D Localization Example, $\mathcal{L}v = -v'' + cv$, $0 \leq c \leq 10^4$

c

$\pm u, \mathcal{L}u = 1$



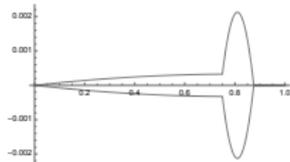
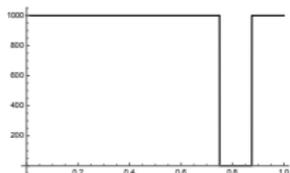
$$\frac{\psi_n(x)}{\lambda_n \|\psi_n\|_{L^\infty(\Omega)}}$$



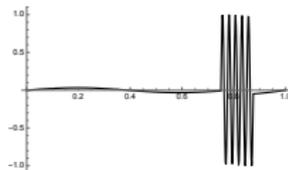
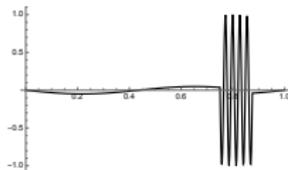
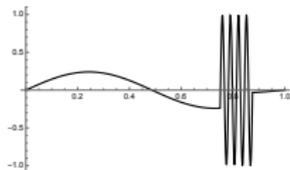
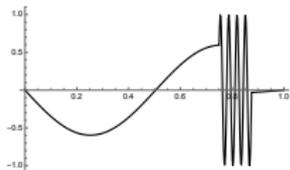
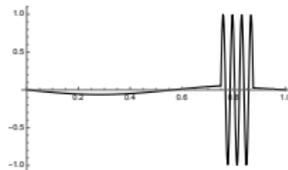
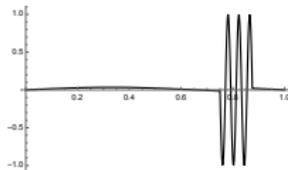
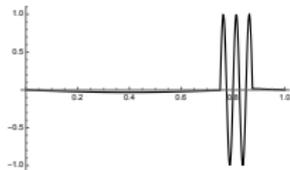
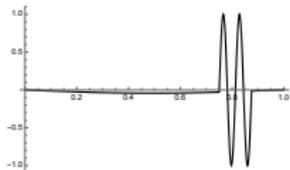
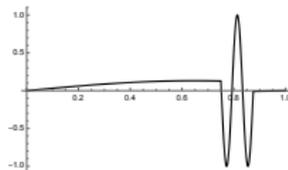
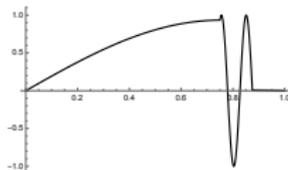
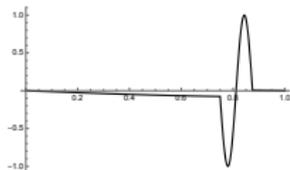
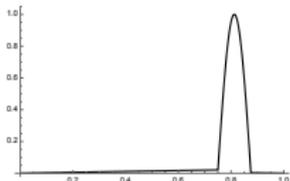
1D Localization Example, $\mathcal{L}v = -(av')'$, $1 \leq a \leq 10^3$

a

$\pm u, \mathcal{L}u = 1$



$$\frac{\psi_n(x)}{\|\psi_n\|_{L^\infty(\Omega)}}$$

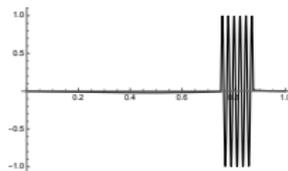
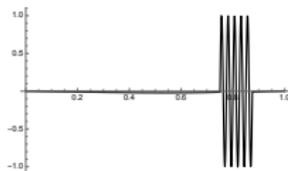
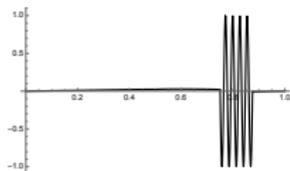
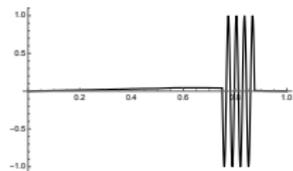
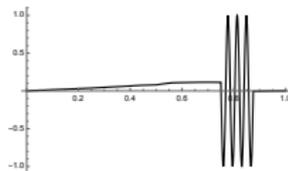
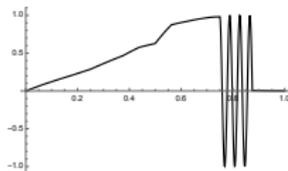
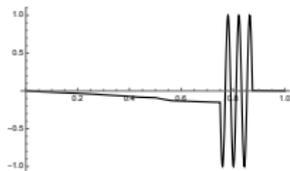
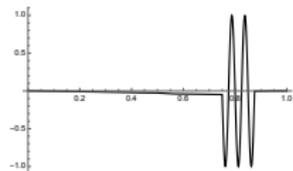
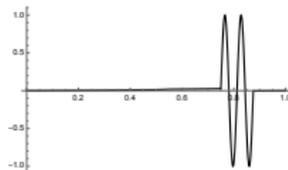
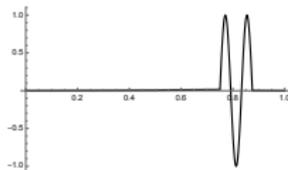
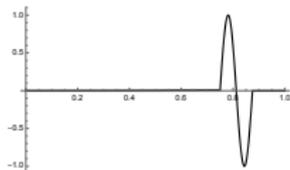
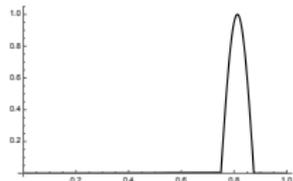
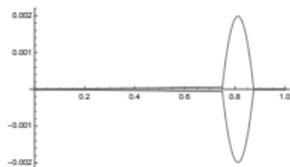
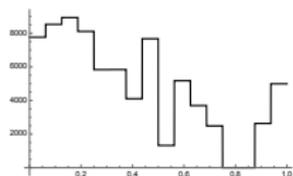


1D Localization Example, $\mathcal{L}v = -(av')'$, $1 \leq a \leq 10^4$

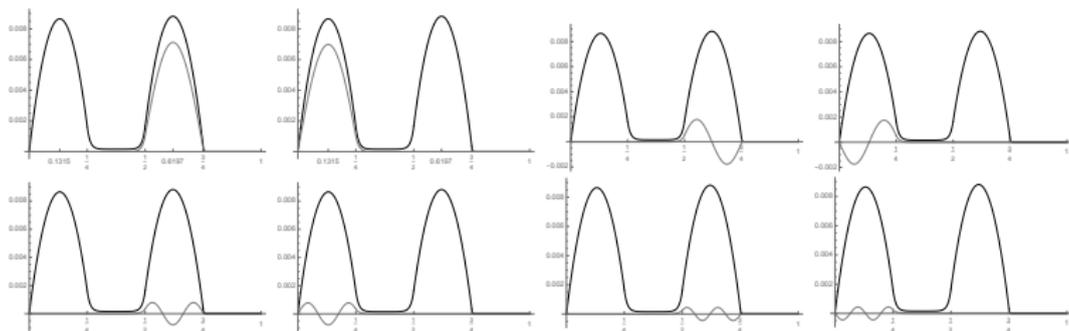
a

$\pm u, \mathcal{L}u = 1$

$$\frac{\psi_n(x)}{\|\psi_n\|_{L^\infty(\Omega)}}$$



1D Model Problem: $\mathcal{L}v = -v'' + cv$, $c = (0, 80^2, 0, 400^2)$



Estimating "Ground State" Eigenvalues and Localization Intervals a la Arnold et al (SISC 2019)

- $(x_1, W_1) = (0.61971698, 113.39424)$
 - $\tilde{\lambda}_1 = 1.25W_1 = 141.74280 \approx \lambda_1 = 140.49323$
 - $R_1 = [0.56032409, 0.67910988]$ $(E = \tilde{\lambda}_1)$
- $(x_2, W_2) = (0.13154762, 115.57503)$
 - $\tilde{\lambda}_2 = 1.25W_2 = 144.46879 \approx \lambda_2 = 143.18099$
 - $R_2 = [0.072717735, 0.19037750]$ $(E = \tilde{\lambda}_2)$

Matrix FEAST

- 2009: Polizzi. *Density-matrix-based algorithm for solving eigenvalue problems*, Phys. Rev. B.
- 2014: Polizzi, Tang. *FEAST as a subspace iteration eigensolver accelerated by approximate spectral projection*, SIMAX
- 2016: Kestyn, Polizzi, Tang. *FEAST eigensolver for non-Hermitian problems*, SISC
- 2019: Yin. *A harmonic FEAST algorithm for non-hermitian generalized eigenvalue problems*, Lin. Algebra Appl.

Operator FEAST

- 2019: Gopalakrishnan, Grubišić, Owall, Parker. *Analysis of FEAST spectral approximations using the DPG discretization*, Comput. Methods Appl. Math.,
- 2020: Gopalakrishnan, Grubišić, Owall. *Spectral discretization errors in filtered subspace iteration*, Math. Comp.
- 2020: Horning, Townsend *FEAST for differential eigenvalue problems*, SINUM
- 2021: Colbrook, Horning, Townsend. *Computing spectral measures of self-adjoint operators*, SIREV

Filtered Subspace Iteration (FEAST)

“Filtered” Operator

- f bounded, continuous on $\text{Spec}(\mathcal{L})$
- $\mathcal{B} = f(\mathcal{L})$ a bounded, selfadjoint operator

$$(\lambda, \psi) \text{ eigenpair of } \mathcal{L} \implies (f(\lambda), \psi) \text{ eigenpair of } \mathcal{B}$$

Same eigenvectors, mapped eigenvalues!

- Jordan curve $\gamma \subset \text{Res}(\mathcal{L})$ enclosing U
- Choose f so that

$$\min_{\lambda \in U \cap \text{Spec}(\mathcal{L})} |f(\lambda)| > \sup_{\lambda \in U^c \cap \text{Spec}(\mathcal{L})} |f(\lambda)|$$

- Typical choice: rational approximation of Cauchy integral

$$f(z) = \sum_{k=1}^n w_k (z_k - z)^{-1} \approx \frac{1}{2\pi i} \oint_{\gamma} (\xi - z)^{-1} d\xi = \begin{cases} 1 & , z \in U \\ 0 & , z \in U^c \setminus \gamma \end{cases}$$

Filtered Subspace Iteration (FEAST)

Subspace Iteration

- Target eigenvalues $\Lambda = U \cap \text{Spec}(\mathcal{L})$
- Target invariant subspace $E = \text{span}\{v \in \text{Dom}(\mathcal{L}) : \mathcal{L}v = \lambda v \text{ for some } \lambda \in \Lambda\}$
- Random initial subspace E_0 ($\dim E_0 \geq \dim E$, $P_E E_0 = E$)
- Subspace iteration: $E_{j+1} = \mathcal{B}E_j$ (periodically orthogonalize basis)

$$\text{gap}(E, E_j) = \mathcal{O}(\kappa^j) \quad , \quad \kappa = \frac{\sup_{\lambda \in U^c \cap \text{Spec}(\mathcal{L})} |f(\lambda)|}{\min_{\lambda \in U \cap \text{Spec}(\mathcal{L})} |f(\lambda)|}$$

- Approx. eigenvalues Λ_j extracted via Rayleigh-Ritz procedure on (small) “matrix”
 $\mathcal{L}_j = P_{E_j} \mathcal{L}|_{E_j} : E_j \rightarrow E_j$

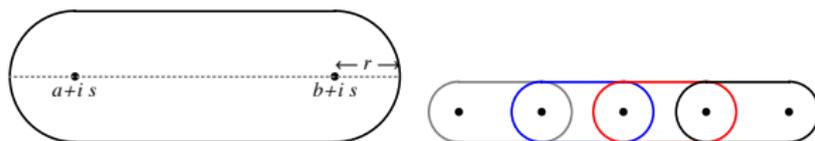
$$\text{dist}(\Lambda, \Lambda_j) = \mathcal{O}(\kappa^{2j})$$

Modifications for (merely) Diagonalizable Operators (e.g. \mathcal{L}_S)

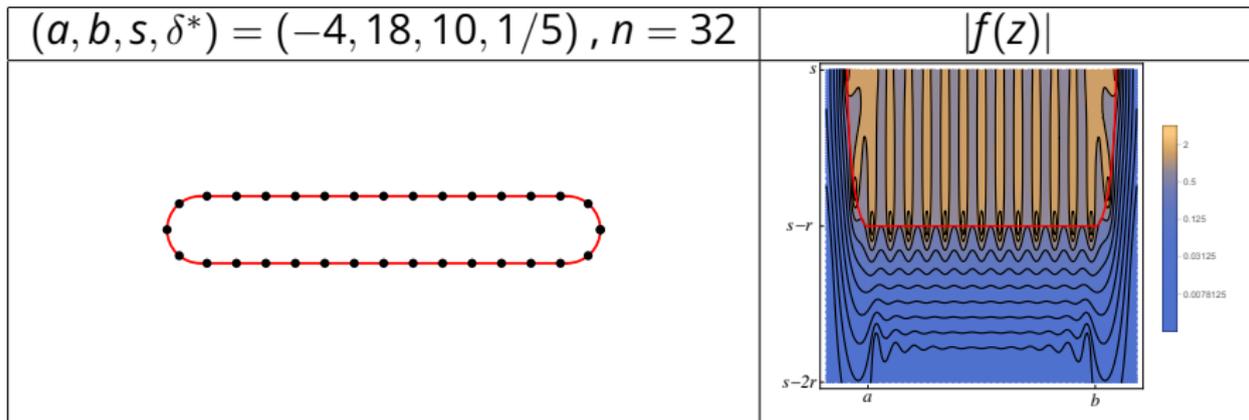
- Compute left and right approx. invariant subspaces E_j^L and E_j^R ...

FEAST Search Region and Filter Function

FEAST Search Region $\tilde{U}(a, b, s, \delta^*)$: $r = s\delta^*$



Feast Filter Function: $f(z) = \sum_{k=0}^{n-1} w_k (z_k - z)^{-1} \approx \frac{1}{2\pi i} \oint_{\partial\tilde{U}} (\xi - z)^{-1} d\xi$



Landscape Inequality Proof: Maximum Principle

- $w_{\pm} = \pm\psi - \lambda\|\psi\|_{L^{\infty}(\Omega)}u$
- $\mathcal{L}w_{\pm} = \lambda(\pm\psi - \|\psi\|_{L^{\infty}(\Omega)}) \leq 0$
- $\max_{x \in \bar{\Omega}} w_{\pm}(x) = \max_{x \in \partial\Omega} w_{\pm}(x) = 0$
- $w_{\pm}(x) \leq 0$ on Ω
- $\pm\psi(x) \leq \lambda\|\psi\|_{L^{\infty}(\Omega)}u(x)$