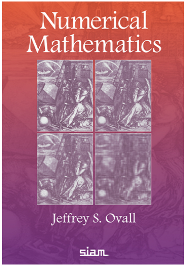
Computational (and theoretical) tools for the Magnetic Schrödinger eigenvalue problem

Jeff Ovall, David Darrow, Shivam Patel and Julie Zhu

Portland State University

jovall@pdx.edu



MIT Numerical PDE Seminar

DMS 2136228, *2208056*

Schrödinger Equation, Related Eigenvalue Problem

Magnetic Schrödinger Equation

$$\mathrm{i}\,\hbar\,\frac{\partial\Psi}{\partial t} = \frac{1}{2m}(-\mathrm{i}\,\hbar\nabla - q\,\mathbf{A})\cdot(-\mathrm{i}\,\hbar\nabla - q\,\mathbf{A})\Psi + qV\Psi$$

- Magnetic Field: $\mathbf{B} = \nabla\times\mathbf{A}$
- Electric Field: $\mathbf{E} = -\nabla V - \partial\mathbf{A}/\partial t$
- Wave function: $\Psi = \Psi(x,t)$, $|\Psi|^2$ provides probability distribution of measurement (position) [Copenhagen Interpretation]

Associated Eigenvalue Problem (Mathematician's Version)

$$\underbrace{(-\mathrm{i}\,\nabla - \mathbf{A})\cdot(-\mathrm{i}\,\nabla - \mathbf{A})\psi + V\psi}_{H(\mathbf{A},V)\psi} = \lambda\psi \text{ in } \Omega \quad , \quad \psi = 0 \text{ on } \partial\Omega$$

- Eigenpair: (λ, ψ)

Operator and Eigenvalue Facts

Looking at the Operator (Hamiltonian)

$$H(\mathbf{A},V)v = (-\mathrm{i}\nabla - \mathbf{A})\cdot(-\mathrm{i}\nabla - \mathbf{A})v + V\,v$$
$$= -\Delta v + \mathrm{i}\,(\nabla\cdot(\mathbf{A}v) + \mathbf{A}\cdot\nabla v) + \left(\|\mathbf{A}\|^2 + V\right)v$$

- (Negative) Laplacian: $H(\mathbf{0},0)$
- (Standard) Schrödinger: $H(\mathbf{0},V)$
- Magnetic Laplacian: $H(\mathbf{A},0)$

Eigenvalue/Vector Facts

- Countably many eigenvalues: $0 < \lambda_1 < \lambda_2 \leq \lambda_3 \leq \cdots$, $\lambda_n \to \infty$
- Countable orthonormal basis of eigenvectors: $(\psi_m,\psi_n) = \delta_{mn}$ and $v = \sum_{n=1}^{\infty}(v,\psi_n)\,\psi_n$ for any $v \in L^2(\Omega)$, where $(f,g) \doteq \int_\Omega f\,\overline{g}\,dx$

Localization of Waves, Localization of Eigenvectors

2026 Simons Collaboration on the Localization of Waves Annual Meeting

Date

February 19 - 20, 2026

Add to Calendar

Location

Gerald D. Fischbach
Auditorium
160 5th Ave
New York, NY 10010
United States

View Map

Thurs.: 8:30 AM—5 PM
Fri.: 8:30 AM—2 PM

Organizers:

Svitlana Mayboroda, University of Minnesota
Marcel Filoche, ESPCI Paris – PSL University

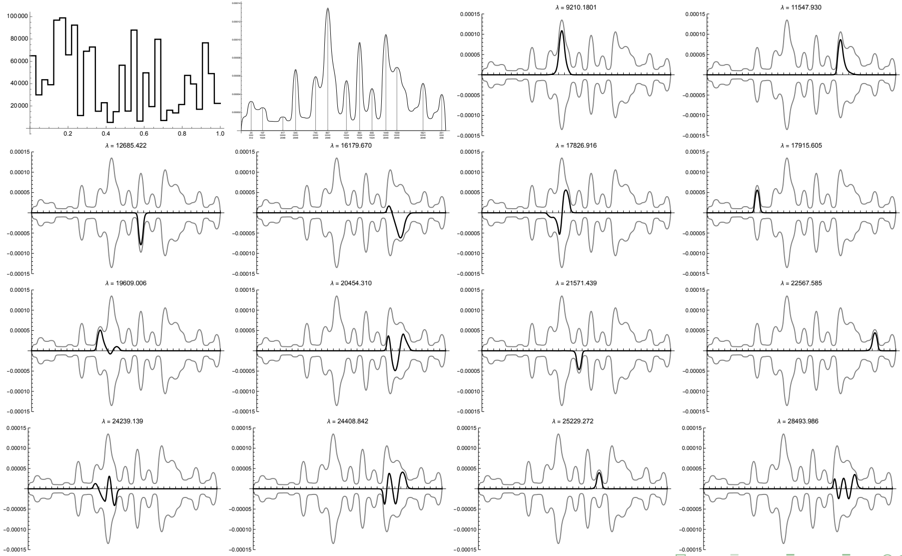
Meeting Goals:

The 2026 Annual Meeting of the Simons Collaboration on Localization of Waves gathers leading mathematicians and physicists working to advance the understanding of wave propagation and localization in disordered media and complex geometries.

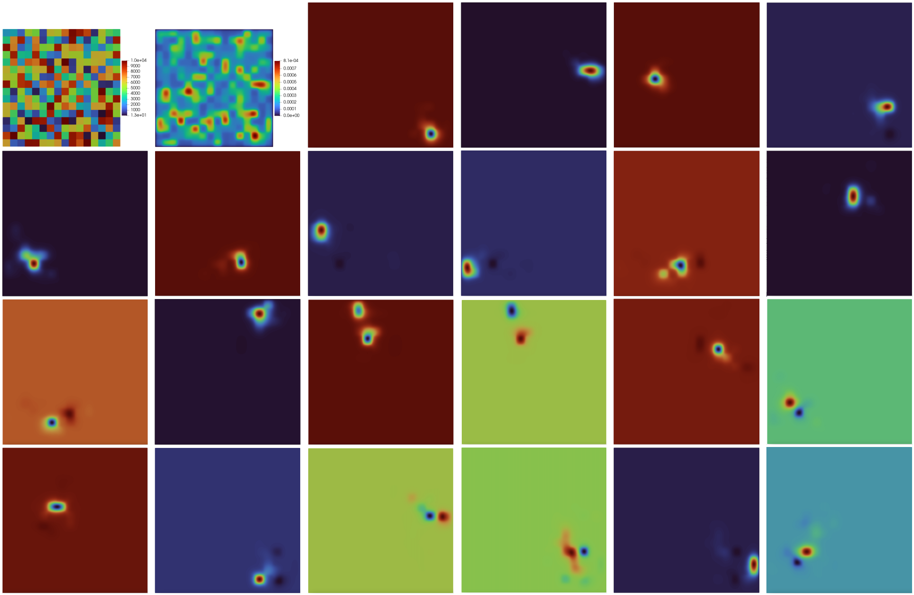
Across two days of presentations, speakers will highlight significant progress at the intersection of mathematics, physics, and engineering of localization of waves. Topics range from the counterexample to the hot spots conjecture to quasicrystals and associated properties of water waves, to theoretical breakthroughs in Anderson localization, to experimental achievements in the realm of disordered semiconductors and systems of cold atoms in the presence of a random speckle potential.

Illustrating Eigenvector Localization: $H(\mathbf{0}, V)$

Potential | $H(\mathbf{0}, V)u = 1$ | $|\psi(x)|/(\lambda\,\|\psi\|_{L^\infty(\Omega)}) \leq u(x)$

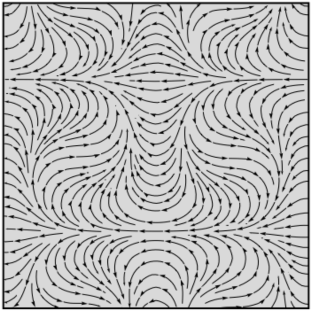


Illustrating Eigenvector Localization: $H(\mathbf{0}, V)$

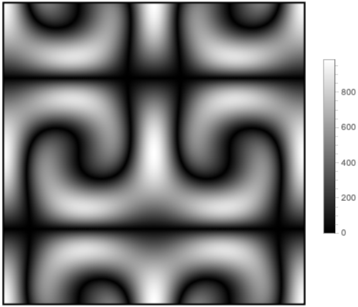


Illustrating Eigenvector Localization: $H(\mathbf{A}, 0)$

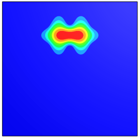
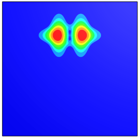
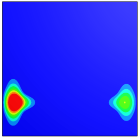
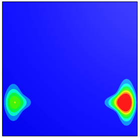
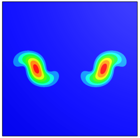
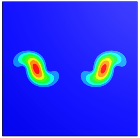
$\mathbf{A}$



$|\mathrm{curl}(\mathbf{A})|$

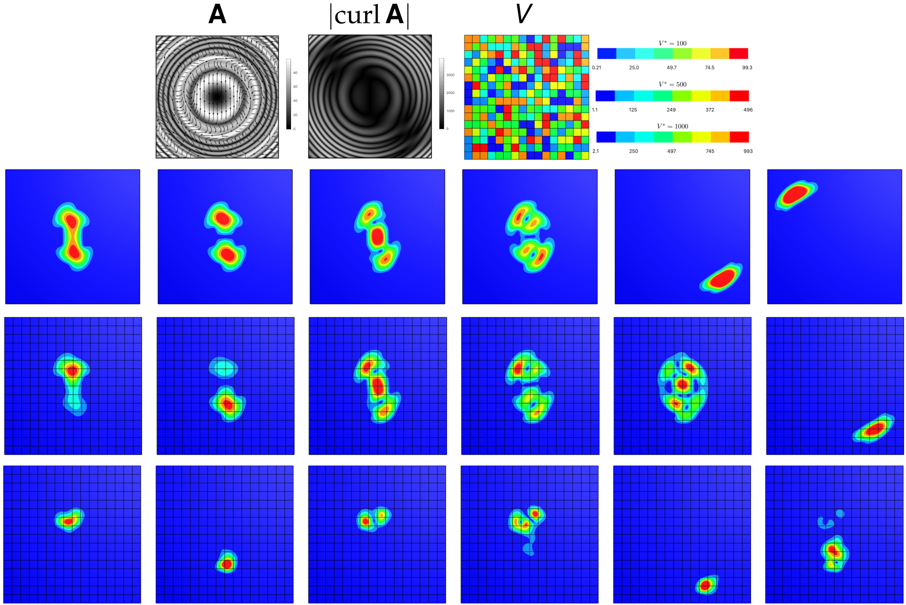


94.240	117.860	120.568	120.568	134.993	134.993

- Scalar curl: $\mathrm{curl}(\mathbf{A}) = \mathrm{rot}(\mathbf{A}) = \partial A_2/\partial x - \partial A_1/\partial y$

Illustrating Eigenvector Localization: $H(\mathbf{A}, V)$



Some Theoretical Insight for $H(\mathbf{A}, 0)$

Theorem (OQRS, 2024)

Let (λ, ψ) be an eigenpair of $H(\mathbf{A}, 0)$, where $\mathbf{A} = \nabla a + \mathbf{F}$ and $\nabla \cdot \mathbf{F} = 0$. It holds that,

$$\frac{|\psi(x)|}{\lambda \|\psi\|_{L^\infty(\Omega)}} \leq \int_0^\infty \int_\Omega \left| \mathbb{E}_{\omega(0)=x, \omega(t)=y}\, e^{-\mathrm{i} \int_0^t \mathbf{F}(\omega(s)) \cdot d\omega(s)} \right| K_\Omega(t, x, y)\, dy\, dt \;.$$

Vol. 94 (2024) *REPORTS ON MATHEMATICAL PHYSICS* No. 2

ON LOCALIZATION OF EIGENFUNCTIONS OF THE MAGNETIC LAPLACIAN

Jeffrey S. Ovall*

Portland State University, Portland, OR 97201, USA
(e-mail: ovall@pdx.edu)

Hadrian Quan

University of Washington, Seattle, WA 98195, USA
(e-mail: hadrianq@uw.edu)

Robyn Reid

Portland State University, Portland, OR 97201, USA
(e-mail: reid3@pdx.edu)

and

Stefan Steinerberger

University of Washington, Seattle, WA 98195, USA
(e-mail: steinerb@uw.edu)

(*May 10, 2024 — Revised August 16, 2024*)

Let $\Omega \subset \mathbb{R}^d$ and consider the magnetic Laplace operator given by $H(A) = (-i\nabla - A(x))^2$, where $A : \Omega \to \mathbb{R}^d$, subject to Dirichlet boundary conditions. For certain vector fields A, this operator can have eigenfunctions, $H(A)\psi = \lambda\psi$, that are highly localized in a small region of Ω. The main goal of this paper is to show that if $|\psi|$ assumes its maximum at $x_0 \in \Omega$, then A behaves 'almost' like a conservative vector field in a $1/\sqrt{\lambda}$–neighborhood of x_0 in a precise sense. In particular, we expect localization in regions where $|\mathrm{curl}\, A|$ is small. The result is illustrated with numerical examples.

Keywords: localization, eigenfunction, Schrödinger operator, regularization.

The Short Story

Look where $\mathrm{curl}\,\mathbf{F}$ ($= \mathrm{curl}\,\mathbf{A}$) is relatively small for a good guess as to where eigenvectors low in the spectrum will localize

- Recall $B = \mathrm{curl}\,\mathbf{A}$, scalar magnetic field (up to scaling)
- Localization well-understood for $H(\mathbf{0}, V)$
- More to learn for $H(\mathbf{A}, 0)$ and $H(\mathbf{A}, V)$

Taylor Expansion of F about $\hat{x}$

$$\mathbf{F}(x) = \nabla v(x) + \frac{\mathrm{curl}\,\mathbf{F}(\hat{x})}{2} \begin{pmatrix} -(x_2 - \hat{x}_2) \\ x_1 - \hat{x}_1 \end{pmatrix} + \mathrm{H.O.T.}$$

$$v(x) = \left(\mathbf{F}(\hat{x}) + \frac{1}{2} J(\hat{x})\,(x - \hat{x}) \right) \cdot (x - \hat{x})$$

Improving Computational Efficiency Via Conjugation

SIAM J. Sci. Comput.
Vol. 47, No. 5, pp. B1026–B1044

A CANONICAL GAUGE FOR COMPUTING OF EIGENPAIRS OF THE MAGNETIC SCHRÖDINGER OPERATOR*

JEFFREY S. OVALL† and LI ZHU†

Abstract. We consider the eigenvalue problem for the magnetic Schrödinger operator and take advantage of a property called gauge invariance to transform the given problem into an equivalent problem that is more amenable to numerical approximation. More specifically, we propose a canonical magnetic gauge that can be computed by solving a Poisson problem that yields a new operator having the same spectrum but eigenvectors that are less oscillatory. Extensive numerical tests demonstrate that accurate computation of eigenpairs can be done more efficiently and stably with the canonical magnetic gauge.

Key words. eigenvalues, eigenvectors, magnetic Schrödinger, finite elements, gauge transform, eigenvector localization

MSC codes. 35P15, 47A75, 65N25

DOI. 10.1137/24M1692228

Code and Data Available

See reproducibility of computational results at end of the article.

Gauge Invariance, Conugation = “Preconditioning” ?

Lemma (Conjugation, Gauge Invariance)

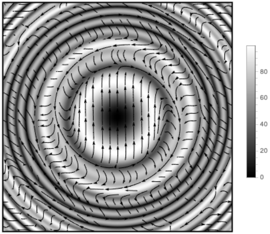
Suppose that $\mathbf{A} = \nabla a + \mathbf{F}$ *in* Ω *for some scalar field* a *and vector field* $\mathbf{F}$. *Then* $e^{-ia} H(\mathbf{A}, V) e^{ia} = H(\mathbf{F}, V)$. *Furthermore,* (λ, ψ) *is an eigenpair of* $H(\mathbf{A}, V)$ *if and only if* $(\lambda, e^{-ia}\psi)$ *is an eigenpair of* $H(\mathbf{F}, V)$.

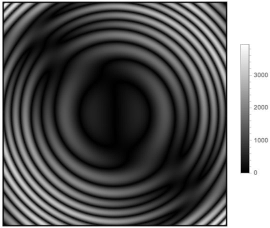
- Same eigevalues, remodulated eigenvectors:
  (λ, ψ) for $H(\mathbf{A}, V)$ iff (λ, ϕ) for $H(\mathbf{F}, V)$, $\phi = e^{-i a}\psi$, $|\phi| = |\psi|$
- Physically irrelevant which eigenpairs we compute $H(\mathbf{A}, V)$ vs. $H(\mathbf{F}, V)$

Research Question (“Preconditioning”)

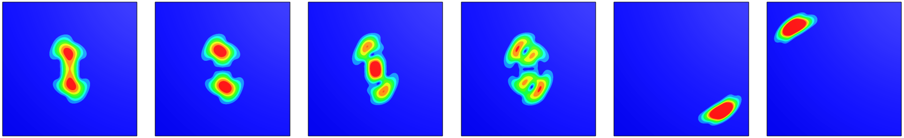
Given **A**, can we efficiently produce equivalent **F** for which computing eigenpairs of $H(\mathbf{F}, V)$ is **easier** than computing eigenpairs of $H(\mathbf{A}, V)$?

$H(\mathbf{A}) = H(\mathbf{A}, 0)$ versus $H(\mathbf{F}) = H(\mathbf{F}, 0)$





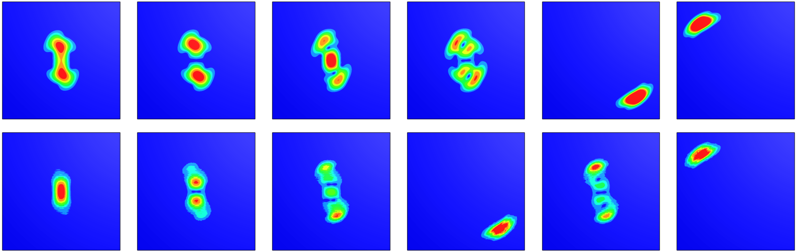
h	DOF
0.01	417451
0.03	46996
0.05	17017



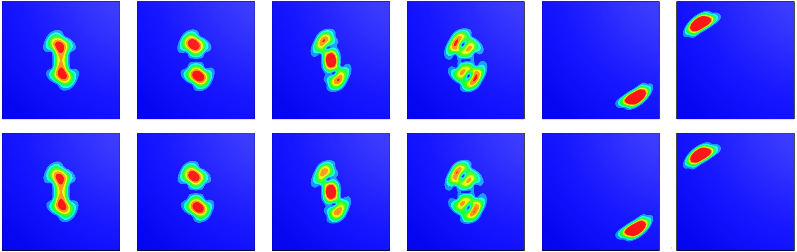
	h	Time	λ_1	λ_2	λ_3	λ_4	λ_5	λ_6
	0.01	310.55s	104.069	111.630	154.607	177.494	196.589	196.590
$H(\mathbf{A})$	0.03	77.08s	109.963	119.903	159.500	184.112	200.066	200.089
	0.05	25.93s	134.774	176.245	219.781	237.908	238.637	238.910
	0.01	354.08s	104.057	111.613	154.598	177.481	196.583	196.583
$H(\mathbf{F})$	0.03	25.07s	104.075	111.642	154.638	177.554	196.607	196.608
	0.05	7.46s	104.444	112.211	155.502	179.126	197.103	197.141

$H(\mathbf{A})$ versus $H(\mathbf{F})$

$H(\mathbf{A})$, $h = 0.01$ (top) and $h = 0.05$



$H(\mathbf{F})$, $h = 0.01$ (top) and $h = 0.05$



How the **F** did we get that kind of improvement?

Theorem (Canonical Gauge)

Let $\mathbf{A}$ *be a given magnetic potential. The solution* $a \in H^1(\Omega;\mathbb{R})$ *of the minimization problem*

$$\|\mathbf{A} - \nabla a\|_{L^2(\Omega;\mathbb{R})} = \min_{v \in H^1(\Omega;\mathbb{R})} \|\mathbf{A} - \nabla v\|_{L^2(\Omega;\mathbb{R})} \;,$$

which is unique up to an additive constant, is also a weak solution of the Neumann problem

$$\Delta a = \nabla \cdot \mathbf{A} \text{ in } \Omega \quad , \quad \nabla a \cdot \mathbf{n} = \mathbf{A} \cdot \mathbf{n} \text{ on } \partial\Omega \,.$$

Setting $\mathbf{F} = \mathbf{A} - \nabla a$, *we have* $\nabla \cdot \mathbf{F} = 0$.

- Among all vector fields equivalent to $\mathbf{A}$, $\mathbf{F}$ has the smallest L^2-norm on Ω.
- The scalar and vector fields a and $\mathbf{F}$ provide a Helmoltz-Hodge decomposition of $\mathbf{A}$, $\mathbf{A} = \nabla a + \mathbf{F}$, with $\int_\Omega \mathbf{F} \cdot \nabla a \, dx = 0$.
- The vector field $\mathbf{F}$ satisfies Coulomb's constraint, $\nabla \cdot \mathbf{F} = 0$ in Ω.
- The vector field $\mathbf{F}$ has vanishing boundary flux, $\mathbf{F} \cdot \mathbf{n} = 0$ on $\partial\Omega$.

Algorithm Template

Algorithm Template

On current discrete (finite element) space,

1. Approximate solution a of Neumann problem

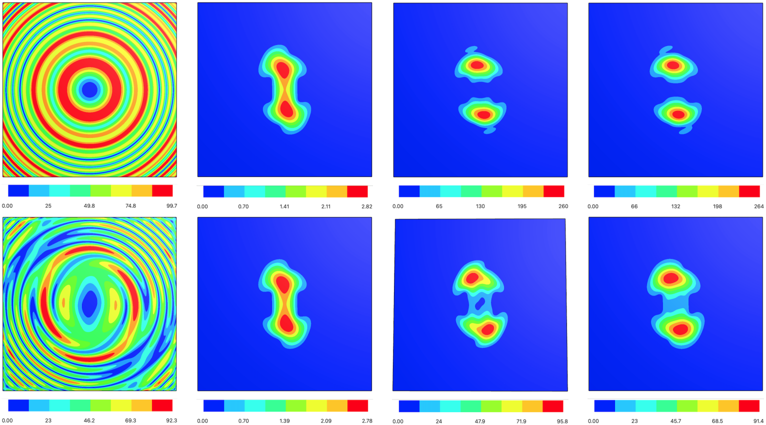
$$\Delta a = \nabla \cdot \mathbf{A} \text{ in } \Omega \quad , \quad \nabla a \cdot \mathbf{n} = \mathbf{A} \cdot \mathbf{n} \text{ on } \partial\Omega \, .$$

2. Use this to approximate $\mathbf{F} = \mathbf{A} - \nabla a$
3. Set up (generalized) linear algebraic eigenvalue problem for $H(\mathbf{F}, V)\psi = \lambda\psi$
4. Use favorite eigensolver (e.g. ARPACK, FEAST)

NGSolve + Pythonic FEAST

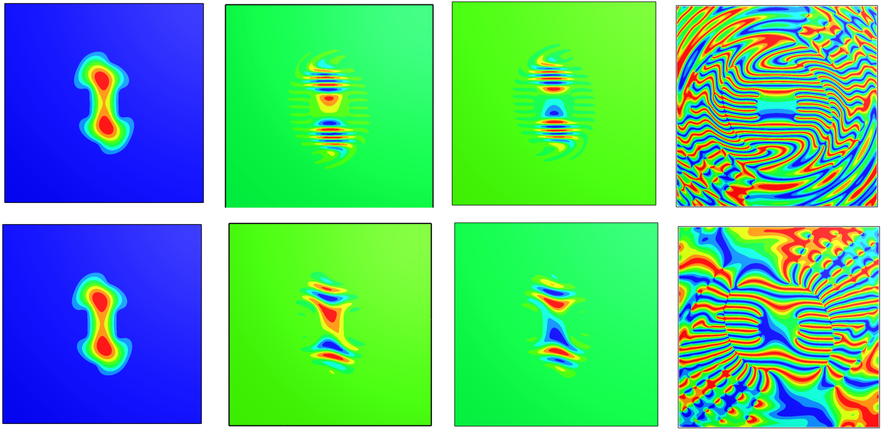
- Finite elements of uniform degree $p = 3$
- Quasi-uniform mesh with characteristic edge length h

$H(\mathbf{A})$ versus $H(\mathbf{F})$: Evidence for Heuristics 1-3



	$j=1$	$j=2$	$j=3$	$j=4$	$j=5$	$j=6$
$\lVert\nabla\psi_j\rVert_{L^2(\Omega)}$	71.0007	79.5820	60.4883	75.4745	51.9968	51.9967
$\lVert\mathbf{A}\psi_j\rVert_{L^2(\Omega)}$	70.7587	79.2955	59.8389	74.8731	51.4847	51.4847
$\lVert\nabla\phi_j\rVert_{L^2(\Omega)}$	31.0322	35.5500	33.6866	40.9010	22.0141	22.0141
$\lVert\mathbf{F}\phi_j\rVert_{L^2(\Omega)}$	30.4731	34.9024	32.5051	39.7792	20.7749	20.7749

$H(\mathbf{A})$ versus $H(\mathbf{F})$: Evidence for Heuristic 4



- Top: $|\psi_1|$, $\Re\psi_1$, $\Im\psi_1$, and phase of ψ_1
- Bottom: $|\phi_1|$, $\Re\phi_1$, $\Im\phi_1$, and phase of ϕ_1
- ϕ_1 less oscillatory than ψ_1; well-resolved on coarser mesh

Heuristics

$$H(\mathbf{A}, V)\psi = \lambda\psi \quad , \quad H(\mathbf{F}, V)\phi = \lambda\phi \quad , \quad \phi = e^{-\mathrm{i}a}\psi$$

- $\nabla\psi - \mathrm{i}\,\mathbf{A}\psi = e^{\mathrm{i}a}(\nabla\phi - \mathrm{i}\,\mathbf{F}\phi)$, so $|\nabla\psi - \mathrm{i}\,\mathbf{A}\psi| = |\nabla\phi - \mathrm{i}\,\mathbf{F}\phi|$
- $|\mathbf{F}\phi| = |\mathbf{F}\psi|$ and $|\mathbf{A}\phi| = |\mathbf{A}\psi|$
- $\|\mathbf{F}\| < \|\mathbf{A}\|$ unless $\mathbf{A} = \mathbf{F}$; expect $|\mathbf{F}| < |\mathbf{A}|$ for much of Ω
- Heuristic 1:

  $$\|\mathbf{F}\phi\|_{L^2(\Omega)} < \|\mathbf{A}\psi\|_{L^2(\Omega)}, \text{ and } |\mathbf{F}\phi| < |\mathbf{A}\psi| \text{ for much of } \Omega$$

- Heuristic 2:

  $$\|\nabla\phi\|_{L^2(\Omega)} < \|\nabla\psi\|_{L^2(\Omega)}, \text{ and } |\nabla\phi| < |\nabla\psi| \text{ for much of } \Omega$$

- Heuristic 3: $\nabla\psi \approx \mathrm{i}\mathbf{A}\psi$, $\nabla\phi \approx \mathrm{i}\mathbf{F}\phi$

  $$\|\nabla\phi\| \approx \|\mathbf{F}\phi\| \text{ and } \|\mathbf{A}\psi\| \approx \|\nabla\psi\|$$

- Heuristic 4: $|\nabla\phi| < |\nabla\psi|$ implies ϕ less oscillatory than ψ!

Heuristics, Part II

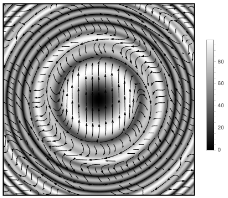
$$H(\mathbf{A},V)\psi=\lambda\psi \quad , \quad H(\mathbf{F},V)\phi=\lambda\phi \quad , \quad \phi=e^{-\mathrm{i}a}\psi$$

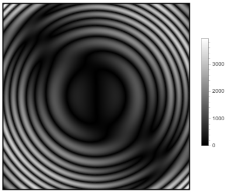
- $\|\psi\|_{L^2(\Omega)}=\|\phi\|_{L^2(\Omega)}=1$
- $\lambda_n=\|\nabla\psi_n-\mathrm{i}\,\mathbf{A}\psi_n\|^2_{L^2(\Omega)}+\|V^{1/2}\psi_n\|^2_{L^2(\Omega)}=\|\nabla\phi_n-\mathrm{i}\,\mathbf{F}\phi_n\|^2_{L^2(\Omega)}+\|V^{1/2}\phi_n\|_{L^2(\Omega)}$

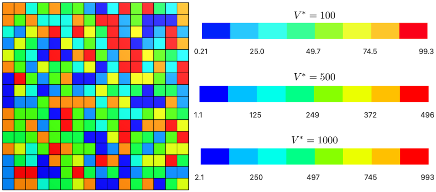
$$\begin{aligned}\lambda_n &= \inf_{\substack{v\in H^1_0(\Omega)\,,\,\|v\|_{L^2(\Omega)}=1\\ v\in\{\psi_1,\ldots,\psi_{n-1}\}^\perp}} \|\nabla v-\mathrm{i}\,\mathbf{A}v\|^2_{L^2(\Omega)}+\|V^{1/2}v\|^2_{L^2(\Omega)}\\ &= \inf_{\substack{v\in H^1_0(\Omega)\,,\,\|v\|_{L^2(\Omega)}=1\\ v\in\{\phi_1,\ldots,\phi_{n-1}\}^\perp}} \|\nabla v-\mathrm{i}\,\mathbf{F}v\|^2_{L^2(\Omega)}+\|V^{1/2}v\|^2_{L^2(\Omega)}\end{aligned}$$

- $\|V^{1/2}\psi_n\|_{L^2(\Omega)}=\|V^{1/2}\phi_n\|_{L^2(\Omega)}$, so $\|\nabla\psi_n-\mathrm{i}\,\mathbf{A}\psi_n\|_{L^2(\Omega)}=\|\nabla\phi_n-\mathrm{i}\,\mathbf{F}\phi_n\|_{L^2(\Omega)}$
- $\nabla\psi_n\approx\mathrm{i}\mathbf{A}\psi_n$, $\nabla\phi_n\approx\mathrm{i}\mathbf{F}\phi_n$

$H(\mathbf{A}, V)$ versus $H(\mathbf{F}, V)$







$H(\mathbf{A}, V)$, $V^* = 500$	0.01	401.57s	224.158	273.235	313.723	334.855	374.314	387.587
	0.03	11.66s	242.230	294.788	344.036	351.915	397.155	400.898
	0.05	6.27s	260.100	320.014	361.198	383.091	408.173	432.155
$H(\mathbf{F}, V)$, $V^* = 500$	0.01	431.87s	224.140	273.215	313.694	334.843	374.290	387.581
	0.03	11.97s	224.237	273.563	314.400	335.186	374.712	387.637
	0.05	5.75s	224.433	274.276	315.946	335.992	375.607	387.792

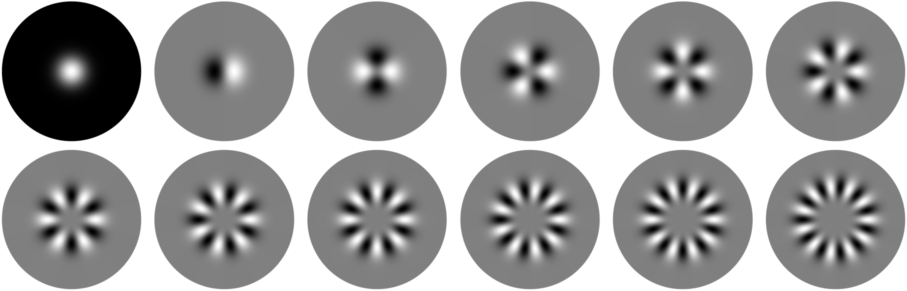
$\|\nabla\psi_j\|_{L^2(\Omega)}$	72.8499	73.1349	83.2860	64.7322	71.1297	52.4223
$\|\mathbf{A}\psi_j\|_{L^2(\Omega)}$	72.3454	72.6661	82.5599	63.8395	69.9942	51.8223
$\|\nabla\phi_j\|_{L^2(\Omega)}$	30.3262	39.2781	43.9434	34.4332	35.8518	18.3745
$\|\mathbf{F}\phi_j\|_{L^2(\Omega)}$	29.0915	38.3966	42.5488	32.7229	33.5400	16.5846

Strong (Constant) Magnetic Field, $\mathbf{A} = \frac{B}{2}(-x_2, x_1)$

Strong(!) Clustering of Eigenvalues near $B = 100$, Unit Disk

m	n	λ_{mn}	m	n	λ_{mn}
0	1	100.000000000000000019	-6	1	100.000000000358522353
-1	1	100.000000000000000925	-7	1	100.000000002499287314
-2	1	100.000000000000022631	-8	1	100.000000015234998522
-3	1	100.000000000000368942	-9	1	100.000000082493117125
-4	1	100.000000000004508745	-10	1	100.000000401715705360
-5	1	100.000000000044055783	-11	1	100.000001777011768016

Real parts of eigenvectors below



Boundary Integral Formulation, $(-\Delta - \kappa^2)_y G_\kappa(x, y) = \delta_x(y)$

- For any $\phi \in C(\partial\Omega)$ and any $\kappa > 0$,

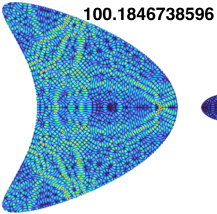
$$u(x) = \int_{\partial\Omega} G_\kappa(x, y)\phi(y)\, dS(y)\ ,\ x \in \Omega \rightsquigarrow -\Delta u = \kappa^2 u \text{ in } \Omega$$

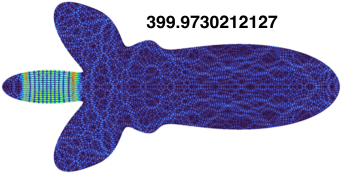
- Find $\kappa > 0$ such that

$$\int_{\partial\Omega} G_\kappa(x, y)\phi(y)\, dS(y) = 0 \text{ on } \partial\Omega \quad , \quad G_\kappa(x, y) = \frac{i}{4} H_0^{(1)}(\kappa|x - y|)$$

  for some non-trivial $\phi \in C(\Omega)$

- *Evaluation of resonances: adaptivity and AAA rational approximation of randomly scalarized boundary integral resolvents*, O.P. Bruno, M.A. Santana, L.N. Trefethen, `arXiv:2405.19582v2`





Toward A High-Order BIE Technique $\mathbf{A} = \frac{B}{2}(-x_2, x_1)$

Boundary Integral Formulation, $(H(\mathbf{A}) - \lambda)_y G_\lambda(x,y) = \delta_x(y)$

- For any $\phi \in C(\partial\Omega)$ and any $\kappa > 0$,

$$u(x) = \int_{\partial\Omega} G_\lambda(x,y)\phi(y)\, dS(y)\ ,\ x \in \Omega \rightsquigarrow H(\mathbf{A})u = \lambda u \text{ in } \Omega$$

- Find $\lambda > 0$ such that

$$\int_{\partial\Omega} G_\lambda(x,y)\phi(y)\, dS(y) = 0 \text{ on } \partial\Omega$$

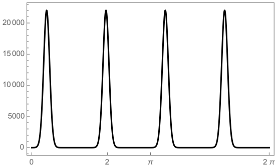
  for some non-trivial $\phi \in C(\Omega)$
- For $a = (1 - \lambda/B)/2$, $R = \pi/2$-clockwise rotation matrix,

$$G_\lambda(x,y) = \frac{\Gamma(a)}{4\pi}\, e^{\mathrm{i}(B/2)(Rx)\cdot y}\, e^{-(B/4)|x-y|^2}\, U(a, 1, (B/2)|x-y|^2)$$

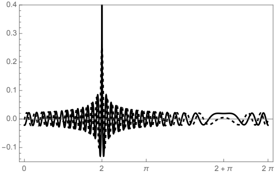
- $G_\kappa(x,y) = \frac{\mathrm{i}}{4} H_0^{(1)}(\kappa|x-y|)$ and $G_\lambda(x,y)$ have logarithmic singularities at $y = x$ and are increasingly oscillatory as κ or B increases.

$$\psi(t) = \int_0^{2\pi} K(t,s)\phi(s)\, ds$$

$f(s)$



$K(2,s)\,,\ \kappa = 50$



- $I_0 = \int_0^{2\pi} f(s)\, ds$
- $I_1 = \int_0^{2\pi} K(2,s) f(s)\, ds$

n	I_0	$I_1(50)$	$I_1(100)$	$I_1(200)$
8	9.558e-01	7.097e-01	5.444e-01	1.956e+00
16	8.246e-02	6.315e-02	3.416e-01	4.328e-01
32	2.134e-05	1.137e-02	1.223e-02	6.110e-02
64	2.056e-16	2.274e-06	8.937e-07	9.680e-06
128	6.169e-16	3.238e-15	1.843e-14	5.017e-14
256	2.056e-16	5.142e-15	1.322e-14	3.669e-14

Magic Quadrature

Quadrature on Unit Disk for Hankel Kernel

$$\int_0^{2\pi} K_\kappa(t,s)f(s)\,ds \approx \sum_{j=0}^{n-1} w_j(\kappa,t)f(s_j)$$

- $s_j = j(2\pi/n)$ trapezoid rule quadrature points!
- $w_j(\kappa,t)$ incorporates nasty behavior of $K_\kappa(t,\cdot)$ proprietary for now

The Plan

1. Extend to quadrature on more general smooth boundaries
2. Compute higher-frequency eigenmodes for Laplace
3. Develop similar quadrature for magnetic Laplace “Helmholtz” kernel
4. Adjust to treat domains with corners

Hunting for Eigenvectors Near a Subspace

MATHEMATICS OF COMPUTATION
Volume 92, Number 341, May 2023, Pages 1005–1031
https://doi.org/10.1090/mcom/3734
Article electronically published on January 6, 2023

AN ALGORITHM FOR IDENTIFYING EIGENVECTORS EXHIBITING STRONG SPATIAL LOCALIZATION

JEFFREY S. OVALL AND ROBYN REID

MATHEMATICS OF COMPUTATION
Volume 00, Number 0, Pages 000–000
S 0025-5718(XX)0000-0

DETECTING EIGENVECTORS OF AN OPERATOR THAT ARE NEAR A SPECIFIED SUBSPACE

DAVID DARROW AND JEFFREY S. OVALL

Quantifying Closeness to a Subspace $W \subset L^2(\Omega)$

Orthogonal Projector

- $Q : L^2(\Omega) \to L^2(\Omega)$ linear, $\mathrm{Ran}(Q) = W$
- $Q^2 = Q$, $Q^* = Q$
- $Q = \chi_R$ for $R \subset \Omega$ — Ovall/Reid MCOM 2023, Reid. Diss. 2024
- More general Q — Darrow/Ovall MCOM 2025

Two Complementary Measures

$$\tau(v) = \frac{\|Qv\|_{L^2(\Omega)}}{\|v\|_{L^2(\Omega)}} \quad , \quad \delta(v) = \frac{\|(I-Q)v\|_{L^2(\Omega)}}{\|v\|_{L^2(\Omega)}} = \mathrm{rel\,dist}(v, W)$$

- $\delta(v)^2 + \tau(v)^2 = 1$
- $(\tau(v), \delta(v)) = (\cos(\theta), \sin(\theta))$, $\theta = \theta(v)$ is angle between v and W
- For any $c \in \mathbb{C}$, $\tau(cv) = \tau(v)$ and $\delta(cv) = \delta(v)$

Key Computational Task: $\mathcal{L} = H(\mathbf{A}, V)$

Key Task

Given a subspace $W \subset L^2(\Omega)$, a (small) tolerance $\delta^* > 0$ and a (large) interval $[a, b]$, find all eigenpairs (λ, ψ) of $\mathcal{L}$ such that

$$\lambda \in [a, b] \;\; \textit{and} \;\; \delta(\psi) \leq \delta^*$$

or determine that there are not any.

Heuristic

- $\mathcal{L}$ selfadjoint, real eigenvalues
- "Encode" constraints $\lambda \in [a, b]$ and $\delta(\psi) \leq \delta^*$ in a modified problem

  If $\delta(\psi)$ small for eigenpair (λ, ψ) of $\mathcal{L}$, then $Q\psi \approx \psi$, so $\mathcal{L}(s)\,\psi \approx (\lambda + \mathrm{i}\, s)\psi$, where $\mathcal{L}(s) = \mathcal{L} + \mathrm{i}\, s\, Q$
- There should be an eigenpair (μ, ϕ) of $\mathcal{L}(s)$ with $\mu \approx \lambda + \mathrm{i}\, s$

“Encoding” Theorem: $\mathcal{L}(s) \doteq \mathcal{L} + \mathrm{i}\, s\, Q$

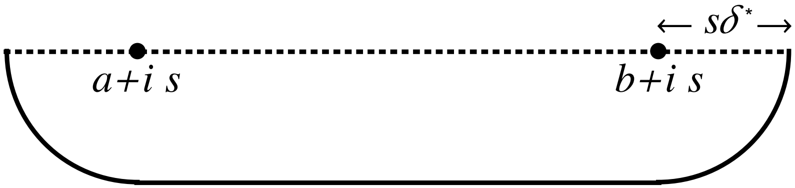
Theorem (OR 2023, DO 2024)

Let (λ, ψ) *be an eigenpair of* $\mathcal{L}$. *For* $s > 0$ *sufficiently small, there is an eigenpair* $(\mu(s), \phi(s))$ *of* $\mathcal{L}(s)$ *such that*

$$|\lambda + \mathrm{i}\, s - \mu(s)| \le s\delta(\psi)\ .$$

In this case, if $\lambda \in [a, b]$ *and* $\delta(\psi) \le \delta^*$, *then* $\mu(s) \in U = U(a, b, s, \delta^*)$ *(pictured below). Furthermore,*

$$\lim_{s\to 0} \frac{\mu(s) - \lambda}{\mathrm{i}s} = [\tau(\psi)]^2 \quad , \quad \lim_{s\to 0} \frac{\lambda + \mathrm{i}s - \mu(s)}{\mathrm{i}s} = [\delta(\psi)]^2\ .$$



Algorithm Template

procedure Localize(a, b, δ^*, W, s)

  Get eigenpairs (μ, ϕ) of $\mathcal{L}(s)$ with $\mu \in U(a, b, s, \delta^*)$ ▷ First filter

  for each (μ, ϕ) **do**

    Re-normalize: $\phi \longleftarrow c\phi$ if $\mathcal{L}$ a real operator

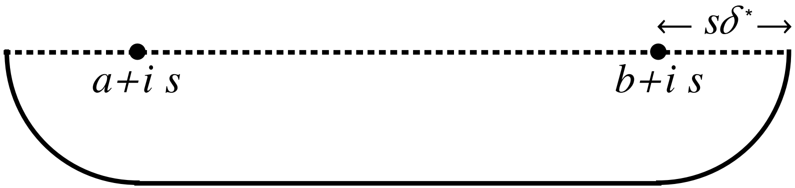
    Post-process: $(\Re\mu, \Re\phi) \rightsquigarrow (\tilde{\lambda}, \tilde{\psi})$ OR $(\Re\mu, \phi) \rightsquigarrow (\tilde{\lambda}, \tilde{\psi})$

    Final check: $\delta(\tilde{\psi}) < \delta^*$ and $\tilde{\lambda} \in [a, b]$? ▷ Second filter

  end for

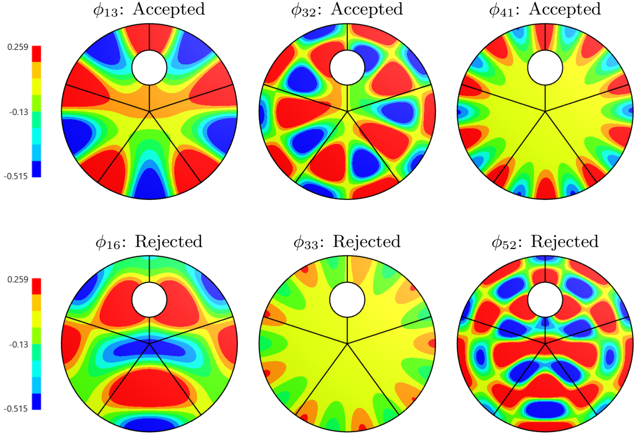
  return accepted $(\tilde{\lambda}, \tilde{\psi})$

end procedure



2D Illustration: $\mathcal{L} = H(\mathbf{0}, 0)$, W ="five-fold symmetry"

$s = 0.1$, $\delta^* = \sqrt{1/10} \approx 0.316$ ($\tau^* = \sqrt{9/10} \approx 0.949$)



- Accepted from first 100: $\{\psi_0, \psi_{12}, \psi_{13}, \psi_{32}, \psi_{40}, \psi_{41}\}$
- Q = projection onto subset Zernike poly. w/ five-fold symmetry