Toward a high-order method for the magnetic Laplace eigenvalue problem with strong magnetic field

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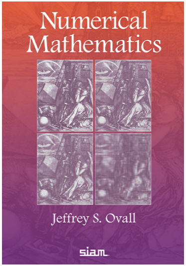
AMS Western Sectional Meeting



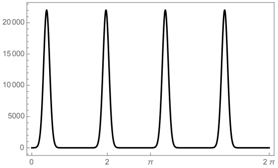
DMS 2136228, *2208056*

Magic Quadrature for Hankel Kernel

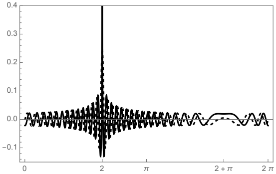
with S. Patel

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

$f(s)$



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



- $I_0 = \int_0^{2\pi} f(s)\, ds$
- $I_1 = \int_0^{2\pi} K(2,s) f(s)\, ds$
- Uniformly-spaced quadrature points?!?

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
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256	2.056e-16	5.142e-15	1.322e-14	3.669e-14

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 $(f, g) \doteq \int_\Omega f\, \overline{g}\, dx$

Improving Computational Efficiency Via Conjugation

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

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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

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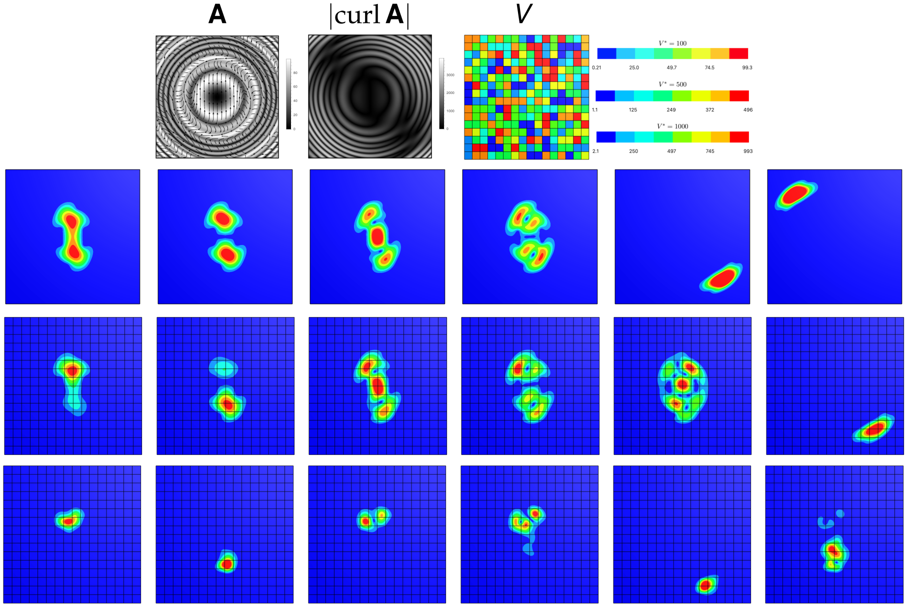
See reproducibility of computational results at end of the article.

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



Gauge Invariance, Conugation = “Preconditioning” ?

Lemma (Conjugation, Gauge Invariance)

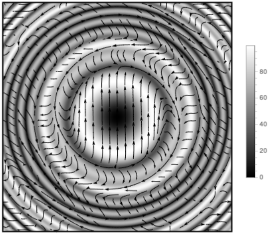
Suppose that $\mathbf{A} = \nabla a + \mathbf{F}$ *in* Ω *for some scalar field* a *and vector field* $\mathbf{F}$*. Then* $e^{-\mathrm{i}a} H(\mathbf{A}, V) e^{\mathrm{i}a} = H(\mathbf{F}, V)$*. Furthermore,* (λ, ψ) *is an eigenpair of* $H(\mathbf{A}, V)$ *if and only if* $(\lambda, e^{-\mathrm{i}a}\psi)$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

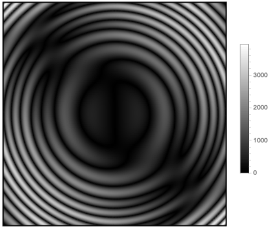
- Same eigevalues, remodulated eigenvectors:
  (λ, ψ) for $H(\mathbf{A}, V)$ iff (λ, ϕ) for $H(\mathbf{F}, V)$, $\phi = e^{-\mathrm{i}\,a}\psi$, $|\phi| = |\psi|$
- Physically irrelevant which eigenpairs we compute $H(\mathbf{A}, V)$ vs. $H(\mathbf{F}, V)$

Research Question (“Preconditioning”)

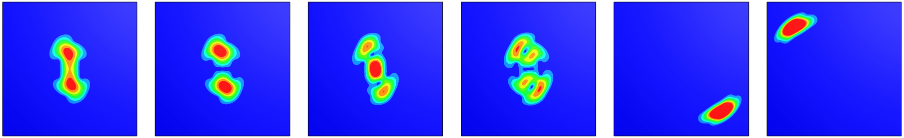
Given **A**, can we efficiently produce equivalent **F** for which computing eigenpairs of $H(\mathbf{F}, V)$ is **easier** than computing eigenpairs of $H(\mathbf{A}, V)$?

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





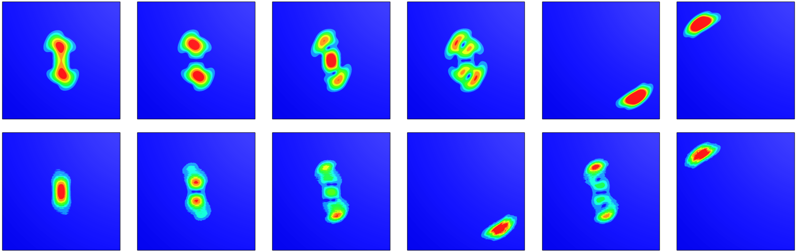
h	DOF
0.01	417451
0.03	46996
0.05	17017



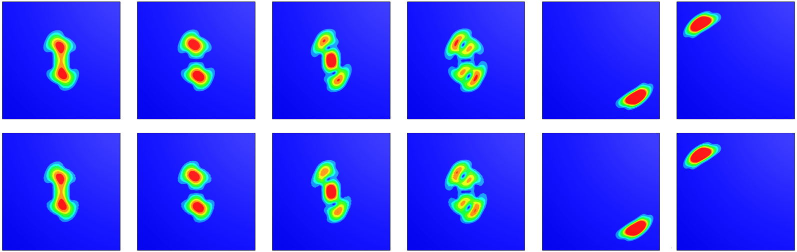
	h	Time	λ_1	λ_2	λ_3	λ_4	λ_5	λ_6
$H(\mathbf{A})$	0.01	310.55s	104.069	111.630	154.607	177.494	196.589	196.590
	0.03	77.08s	109.963	119.903	159.500	184.112	200.066	200.089
	0.05	25.93s	134.774	176.245	219.781	237.908	238.637	238.910
$H(\mathbf{F})$	0.01	354.08s	104.057	111.613	154.598	177.481	196.583	196.583
	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 $H(\mathbf{F})$

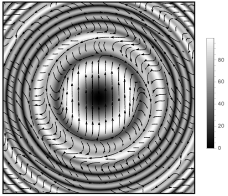
$H(\mathbf{A})$, $h = 0.01$ **(top) and** $h = 0.05$

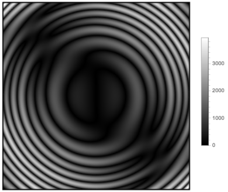


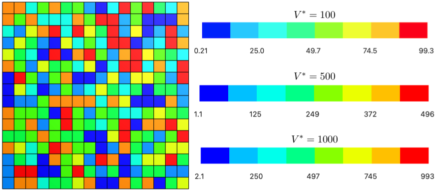
$H(\mathbf{F})$, $h = 0.01$ **(top) and** $h = 0.05$



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

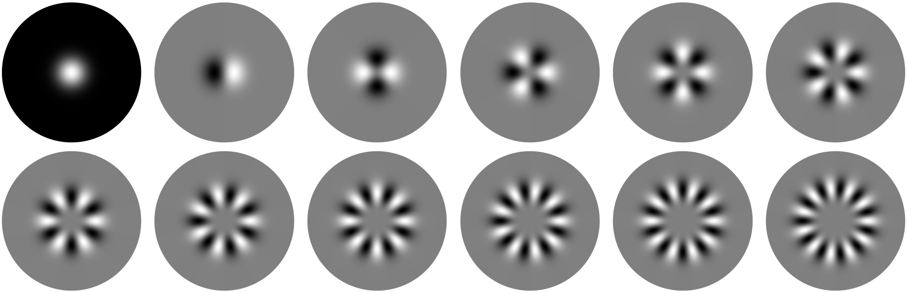
$\\|\nabla\psi_j\\|_{L^2(\Omega)}$	72.8499	73.1349	83.2860	64.7322	71.1297	52.4223
$\\|\mathbf{A}\psi_j\\|_{L^2(\Omega)}$	72.3454	72.6661	82.5599	63.8395	69.9942	51.8223
$\\|\nabla\phi_j\\|_{L^2(\Omega)}$	30.3262	39.2781	43.9434	34.4332	35.8518	18.3745
$\\|\mathbf{F}\phi_j\\|_{L^2(\Omega)}$	29.0915	38.3966	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	100.0000000000000000019	-6	1	100.0000000000358522353
-1	1	100.0000000000000000925	-7	1	100.0000000002499287314
-2	1	100.0000000000000022631	-8	1	100.0000000015234998522
-3	1	100.0000000000000368942	-9	1	100.0000000082493117125
-4	1	100.0000000000004508745	-10	1	100.0000000401715705360
-5	1	100.0000000000044055783	-11	1	100.0000001777011768016

Real parts of eigenvectors below



A High-Order BIE Technique (for a simpler problem)

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

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

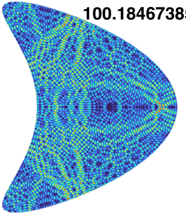
$$u(x) = \int_{\partial\Omega} G_\kappa(x,y)\phi(y)\, dS(y)\ ,\ x \in \Omega \rightsquigarrow -\Delta u = \kappa^2 u \text{ in } \Omega$$

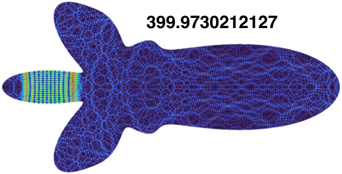
- Find $\kappa > 0$ such that

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

  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.

A Non-Linear Matrix Eigenvalue Problem

From (Non-Linear) Operator EVP to Matrix EVP

- Find $\mu > 0$, and non-trivial $\phi \in C(\partial\Omega)$ such that

$$\int_{\partial\Omega} G_\mu(x,y)\phi(y)\,dS(y) = 0 \text{ on } \partial\Omega \quad , \quad \int_0^{2\pi} \underbrace{K_\mu(t,s)}_{\text{naughty}} \overbrace{f(s)}^{\text{nice}}\,ds = 0 \text{ for } t \in [0,2\pi)$$

- naughty $=$ (naughty $-$ special naughty) $+$ special naughty $=$ nice $+$ special naughty

$$\int_0^{2\pi} K_\mu(t,s)f(s)\,ds = \int_0^{2\pi} \underbrace{[K_\mu(t,s) - L_\mu(t,s)]}_{M_\mu(t,s)} g(s)\,ds + \int_0^{2\pi} L_\mu(t,s)\,f(s)\,ds$$

- Nyström discretization

$$\frac{2\pi}{n}\sum_{j=0}^{n-1} M_\mu(t_i,t_j)\tilde{f}(t_j) + \sum_{j=0}^{n-1} \underbrace{w_j^{(\mu)}(t_i)}_{\omega_{|i-j|}^{(\mu)}}\,\tilde{f}(t_j) = 0 \text{ for } i \in \{0,1,\ldots,n-1\}$$

- Find μ such that $B(\mu)$ is singular, $[B(\mu)]_{ij} = \frac{2\pi}{n}\,M_\mu(t_i,t_j) + \omega_{|i-j|}^{(\mu)}$

Typical Examples of "Special Naughty"

Operator	Naughty	Special Naughty
Laplace	$-\frac{1}{2\pi}\ln r$	$-\frac{1}{4\pi}\ln\left(4\sin^2\left(\frac{s-t}{2}\right)\right)$
Helmholtz	$\frac{\mathrm{i}}{4}H_0^{(1)}(\kappa r)$	$-\frac{1}{4\pi}\ln\left(4\sin^2\left(\frac{s-t}{2}\right)\right)J_0(\kappa r)$

- $x:[0,2\pi)\to\partial\Omega$ a smooth parameterization
- $r=|x(t)-x(s)|$
- When $x(t)=(\cos t,\sin t)$, $r^2=4\sin^2\left(\frac{s-t}{2}\right)J_0(\kappa r)$
- For large κ, both $J_0(\kappa r)$ and the "nice term" are highly oscillatory, making high-order quadrature challenging

Special Case: Hankel Quadratures on Unit Disk

Lemma (Fourier Coefficients of Single- and Double-Layer Kernels)

Let $G_\kappa(x,y) = \frac{\mathrm{i}}{4} H_0^{(1)}(\kappa|x-y|)$, $x = (\cos t, \sin t)$ *and* $y = (\cos s, \sin s)$.
If $K(t,s) = G_\kappa(x,y)$, *then*

$$\int_0^{2\pi} K(t,s)\, e^{\mathrm{i}\, m\, s}\, ds = c_m\, e^{\mathrm{i}\, m\, t} \quad \text{where} \quad c_m = \frac{\mathrm{i}\pi}{2} J_{|m|}(\kappa)\, H_{|m|}^{(1)}(\kappa)$$

If $K(t,s) = \partial G_\kappa(x,y)/\partial n(y)$, *then*

$$\int_0^{2\pi} K(t,s)\, e^{\mathrm{i}\, m\, s}\, ds = c_m\, e^{\mathrm{i}\, m\, t} \quad \text{where} \quad c_m = \frac{\mathrm{i}\kappa\pi}{2} J'_{|m|}(\kappa)\, H_{|m|}^{(1)}(\kappa) - \frac{1}{2}$$

Special Case: Hankel Quadratures on Unit Disk

Martensen-Kussmaul Type Quadrature

$$\int_0^{2\pi} K(t,s)f(s)\,ds = \sum_{m\in\mathbb{Z}} \hat{f}(m)\, c_m\, e^{\mathrm{i}\,m\,t}$$
$$= \frac{c_0}{2\pi}\int_0^{2\pi} f(s)\,ds + \sum_{m\in\mathbb{N}} \frac{c_m}{\pi}\int_0^{2\pi} f(s)\cos(m(t-s))\,ds$$

- Truncate the infinite sum $n/2$ terms (n even)
- Replace each $\int_0^{2\pi} f(s)\cos(m(t-s))\,ds$ with n-point trapezoid rule approx.

$$\int_0^{2\pi} f(s)\cos(m(t-s))\,ds \approx \frac{2\pi}{n}\sum_{j=0}^{n-1} f(t_j)\cos(m(t-t_j))$$

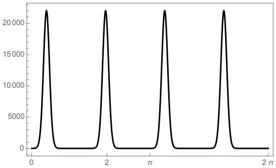
- Final quadrature approx.

$$\int_0^{2\pi} K(t,s)f(s)\,ds \approx \sum_{j=0}^{n-1} f(t_j)w_j(t) \quad , \quad w_j(t) = \frac{2}{n}\sum_{m=0}^{n/2}{}' c_m\cos(m(t-t_k))$$

Magic Quadrature for Hankel Kernel

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

$f(s) = e^{10 \sin(4s)}$



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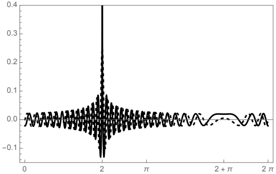

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