High-frequency cavity modes: fast methods and quantum chaos

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Dirichlet eigenvalue problem

bounded domain
\( \Omega \subset \mathbb{R}^2 \)

\[-\Delta \phi_j = E_j \phi_j \quad \text{in } \Omega \]

\( \phi_j = 0 \quad \text{on } \partial \Omega \)

‘frequency’ eigenvalues
\( E_1 < E_2 \leq E_3 \leq \cdots \infty \)
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- Modes of a ‘drum’: acoustics, optics, EM resonators, radar, quantum.
  
  Recall analytic solns only if \( \Delta \) separable (rectangle, ellipse…)

\( E_1 = 11.508 \quad E_2 = 25.550 \quad E_3 = 29.124 \quad E_4 = 43.050 \quad E_5 = 44.209 \quad E_6 = 53.053 \quad E_7 = 55.201 \quad E_8 = 66.423 \quad E_9 = 69.226 \quad E_{10} = 82.011 \quad E_{11} = 87.424 \quad E_{12} = 92.250 \)
Dirichlet eigenvalue problem

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- Modes of a ‘drum’: acoustics, optics, EM resonators, radar, quantum.
  Recall analytic solns only if \( \Delta \) separable (rectangle, ellipse…)
- Desires: fast numerical method for high frequency \( j \gg 1 \),
  rapid convergence, corners, multiply connected, \( \Omega \subset \mathbb{R}^3 \ldots ? \)
Motivation for high frequency modes

*leaky* resonant cavities

quantum-cascade laser

- 2D cavity confinement due to total internal reflection \((n = 3.3)\)
- high-power design: need many modes for many shapes (Tureci '03)
- wavelength \(\ll\) system size \((\text{wavenumber } k \gg 1)\): multiscale problem
Method of Particular Solutions

Given trial energy parameter $E > 0$:

- choose basis function set $\{\xi_i\}_{i=1}^N$ with $-\Delta \xi_i = E \xi_i$ in $\Omega$, $\forall i$
  
  global Helmholtz solutions, e.g. plane waves, Fourier-Bessel functions

then $u = \sum_{i=1}^N a_i \xi_i$ obeys $-\Delta u = E u$ in $\Omega$
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- if can find coeff vector $a \in \mathbb{R}^N$ giving $u|_{\partial \Omega} = 0$, but $u \neq 0$ in $\Omega$
  … then $u$ is a mode $\phi_j$ and $E$ is its eigenvalue $E_j$
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‘boundary tension’ $t(E) := \min_{u \in \text{Span}\{\xi_i\}} \frac{\|u\|_{L^2(\partial \Omega)}}{\|u\|_{L^2(\Omega)}}$  
Rayleigh quotient
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`boundary tension` $t(E) := \min_{u \in \text{Span}\{\xi_i\}} \frac{\|u\|_{L^2(\partial\Omega)}}{\|u\|_{L^2(\Omega)}}$  \hspace{2cm} \text{Rayleigh quotient}

\[\phi_j^2: \Omega = \text{peanut}, j \approx 700\]

- Locate $\{E_j\}$ as minima of $t(E)$
Computing boundary tension

\[ t(E) = \min_{\substack{u \neq 0 \\ u \in \text{Span}\{\xi_i\}}} \frac{\|u\|_{L^2(\partial\Omega)}}{\|u\|_{L^2(\Omega)}} = \min_{a \neq 0} \sqrt{\frac{a^T Fa}{a^T Ga}} = \sqrt{\lambda_1} \quad \text{→ lowest generalized eigenvalue of} \quad Fa = \lambda Ga \]

with matrix elements \( F_{ij}(E) = \int_{\partial\Omega} \xi_i \xi_j, \quad G_{ij}(E) = \int_{\Omega} \xi_i \xi_j \)
Computing boundary tension

\[ t(E) = \min_{u \neq 0, u \in \text{Span}\{\xi_i\}} \frac{\|u\|_{L^2(\partial \Omega)}}{\|u\|_{L^2(\Omega)}} = \min_{a \neq 0} \sqrt{\frac{a^T F a}{a^T G a}} = \sqrt{\lambda_1} \quad \text{lowest generalized eigenvalue of } F a = \lambda G a \]

with matrix elements \( F_{ij}(E) = \int_{\partial \Omega} \xi_i \xi_j, \quad G_{ij}(E) = \int_{\Omega} \xi_i \xi_j \)

In practise: as \( N \) grows, find \( \exists a, |a| = 1, \sum_{i=1}^{N} a_i \xi_i = O(e^{-cN}) \) in \( \Omega \)

- caused normalization problem in original MPS (Fox-Henrici-Moler ’67)
- our \( t(E) \) choice fixes it; but \( F, G \) have common numerical nullspace: Cholesky, QZ, \( \text{eig}(F, G) \) fail...

need regularized (\( \epsilon_{\text{mach}} \)-truncated) inverse of \( G \) (B ’00)
Bifurcated genealogy

**NUMERICAL ANALYSIS: high accuracy**

- Vekua ('60s)
- MPS (Fox–Henrici–Moler ’67)
- Complex approximation theory
  - Schryer, Eisenstat ('70s)
  - Still ('80s)
  - Trefethen
- Fundamental solns (MFS)
  - (Karageorghis ’00)
- GSVD (Betcke–Trefethen ’05)
- Driscoll
- Barnett ('00, ’06)

**QUANTUM PHYSICS: high freq**

- Plane wave method
  - (Heller ’80s)
- Scaling method
  - (Vergini–Saraceno ’94)

- Recent cross-pollination of ideas
Compare MPS to standard methods

Direct discretization (mesh)
finite differencing
finite element method

- local basis representation
- basis satisfies BCs
- find basis coeffs to solve PDE

Boundary methods (meshless)
integral equation methods
method of particular solutions (MPS)

- global basis representation
- basis satisfies PDE
- find basis coeffs to match BCs

\[ N = O(k^2) \]
\[ k \approx \text{wavenumber} \]
\[ N = O(k) \]

Huge gain at high freq

Algebraic convergence

MPS: exponential convergence

Possible in many shapes
Compare MPS to standard methods

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algebraic convergence

**Boundary methods (meshless)**
- integral equation methods
- method of particular solutions (MPS)

- **global basis representation**
- basis satisfies PDE
- find basis coeffs to match BCs

\[ N = O(k) \quad \text{huge gain at high freq} \]

**MPS**: exponential convergence possible in many shapes
Basis functions
Each basis func $\xi_i(x)$ is a global Helmholtz soln at freq param $E \ldots$
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\begin{cases}
\text{Plane waves} & \sin(kn_i \cdot x), \quad k^2 = E \\
\text{Fourier-Bessel} & J_l(kr) \sin(l\theta)
\end{cases}
\]

Thm: $\Omega$ smooth $\Rightarrow$ exponential convergence *(Eisenstat ’74)*
Practice: *fail for nonconvex* $\Omega$ (coeff sizes $|a| \gg 10^{16}$)
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Fundamental solutions (MFS)
$Y_0(k|x - y_i|)$ with \{y_i\} on outer boundary

Practice: excellent, also w/ non-reentrant corners (B ’06)
Ongoing analysis of coeff sizes (w/ Timo Betcke)
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Corner-adapted Fourier-Bessel:

singular corners $\theta \neq \frac{\pi}{n}$
Practice: exp. conv. for multiple corners (Betcke ’05)
Scaling method

Recall $Fa = \lambda Ga$  
$F, G$ basis reps. of Rayleigh quotient $\|u\|_{L^2(\partial \Omega)}^2/\|u\|_{L^2(\Omega)}^2$

Minimizing $\lambda_1(E)$ slow; nearby minima easily missed—can do better?
Scaling method

Recall $F a = \lambda G a$  

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Minimizing $\lambda_1(E)$ slow; nearby minima easily missed—can do better?

Plot higher generalized eigenvalues…

- Clue: spectrum at single $E$ has info about many nearby $\hat{\lambda}_1$ minima  

- p. 9
Scaling method

(Vergini-Saraceno ’94; B ’00, ’06)

New Rayleigh quotient: \[ \frac{\int_{\partial \Omega} (\mathbf{x} \cdot \mathbf{n})^{-1} |\mathbf{u}|^2}{\int_{\partial \Omega} (\mathbf{x} \cdot \mathbf{n})^{-1} \mathbf{u} \cdot \nabla \mathbf{u}} \]
Scaling method

New Rayleigh quotient: \( \int_{\partial \Omega} (\mathbf{x} \cdot \mathbf{n})^{-1} |u|^2 / \int_{\partial \Omega} (\mathbf{x} \cdot \mathbf{n})^{-1} u \mathbf{x} \cdot \nabla u \)

Generalized eigenvalues \( \lambda_l(E) \) linear in \( E - E_j \) (for \( \Omega \) star-shaped):

- solving \( F \mathbf{a} = \lambda G \mathbf{a} \) at single \( E \) value gives all nearest \( O(k) \) modes
- no root search, no missing levels, speed gain \( O(k) \) over MPS
- eigenvectors \( \mathbf{a}_l \) give dilated (rescaled) approximations to modes \( \phi_j \)
- errors grow like \( t \sim |E_j - E|^3 \) (3rd-order convergence with effort)
Application: Quantum ergodicity

**Q:** If ray dynamics completely *chaotic* in $\Omega$... 
... how fast do the modes $\{\phi_j\}$ become spatially uniform?
Application: Quantum ergodicity

**Q:** If ray dynamics completely *chaotic* in $\Omega$... 
...how fast do the modes $\{\phi_j\}$ become spatially uniform?

*compute $3 \times 10^4$ modes up to $j \sim 10^6$: a few laptop-CPU-days*

**A:** deviations from uniformity die asymptotically as $O(E_j^{-1/4})$

(B, Comm Pure App. Math, ’06)
Application: Mushroom cavity

(joint w/ T. Betcke)

Ray dynamics has two phase space regions: regular & chaotic

- verified conjecture (Percival ’73): modes localize to one region
- discovered new ‘migrating scar’ effect: MOVIE

$k = 100, j \approx 2000$
Conclusion

Dirichlet eigenvalues: paradigm linear wave resonance problem

Global basis approximation methods excel at high frequency $k \gg 1$:
- scaling method $O(k)$ (typ. $10^3$) faster than any known method

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