High-frequency cavity modes: fast methods and quantum chaos

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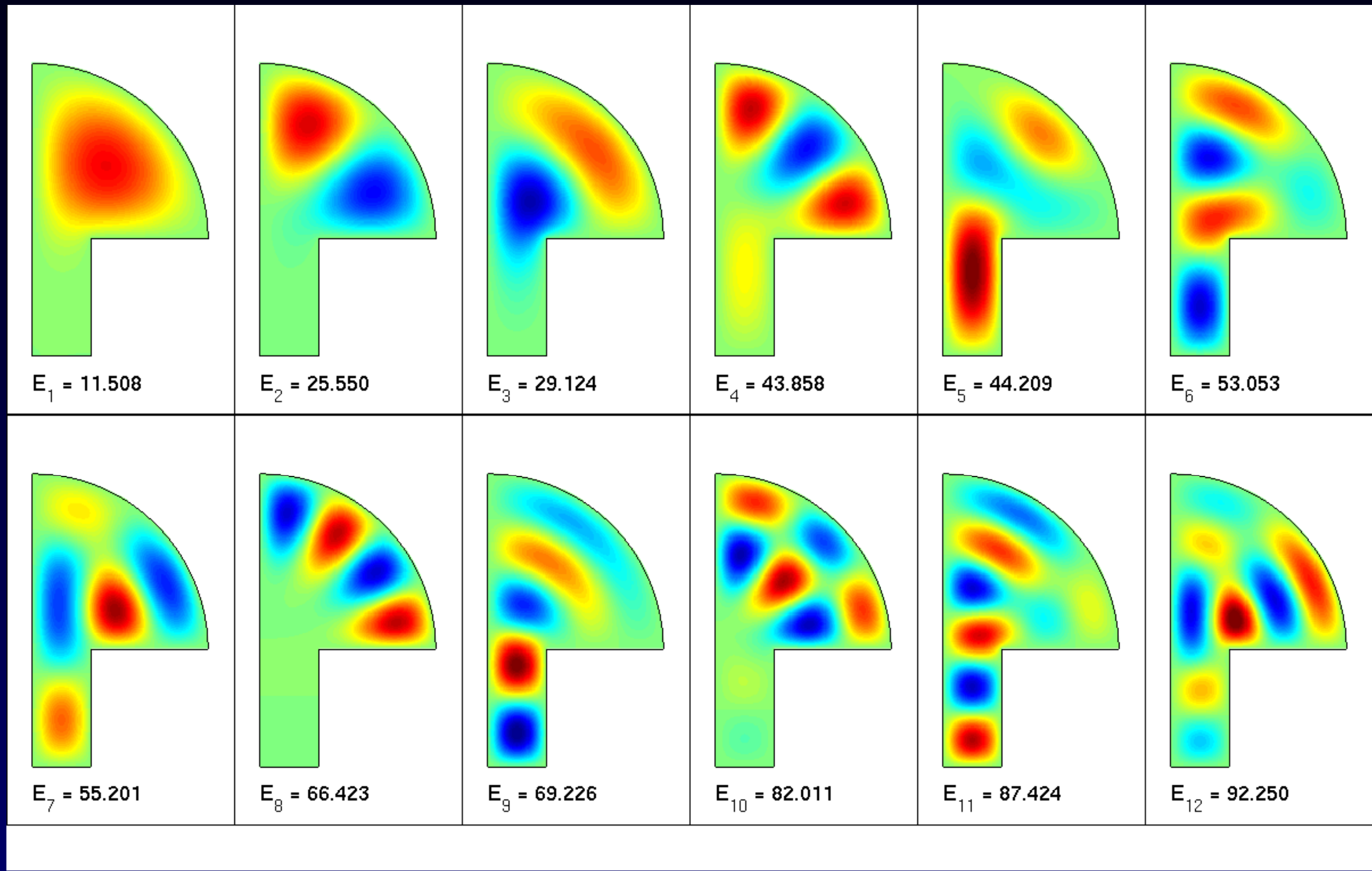
Dirichlet eigenvalue problem

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
$E_1 < E_2 \le E_3 \le \cdots \infty$



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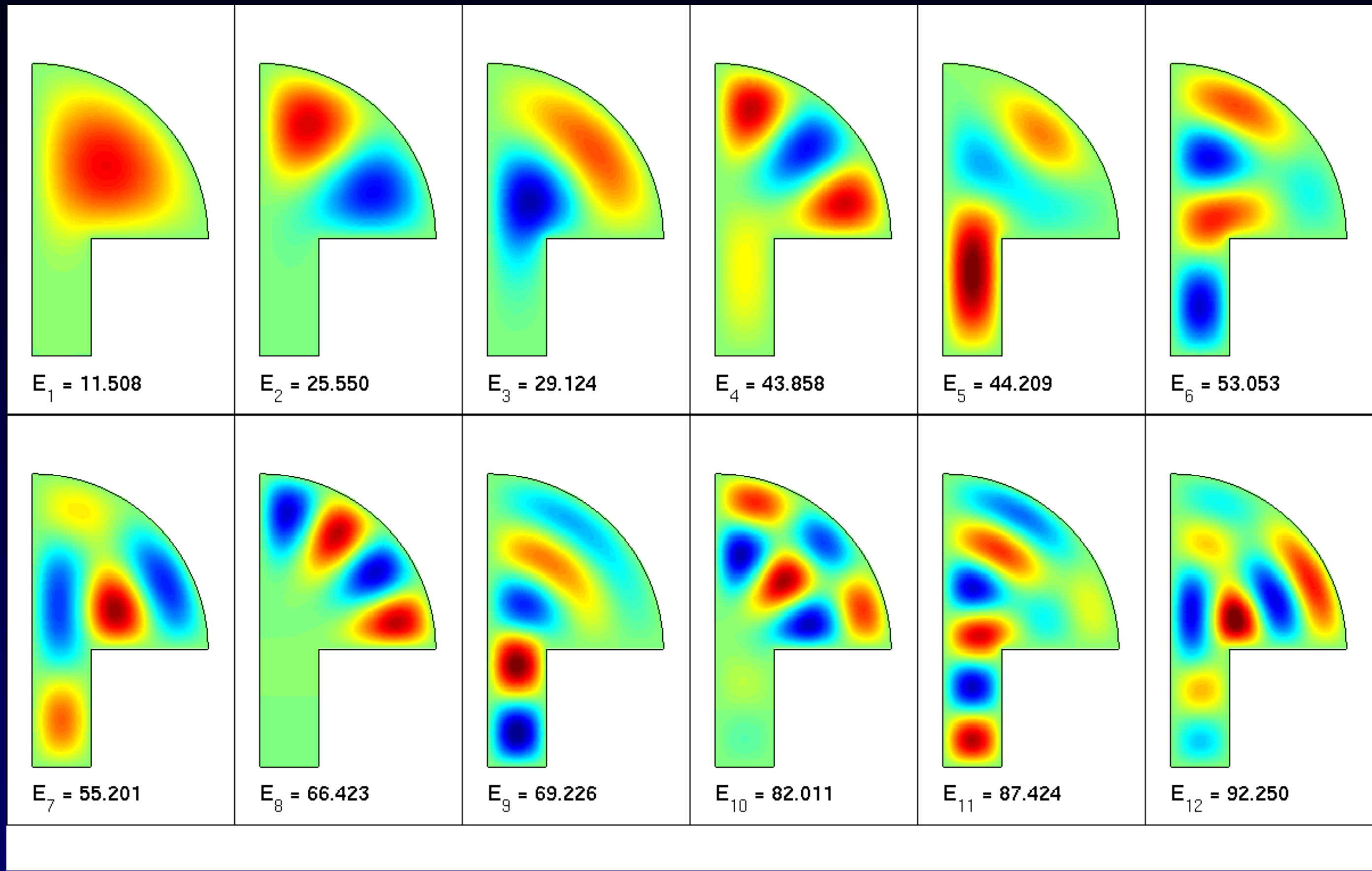

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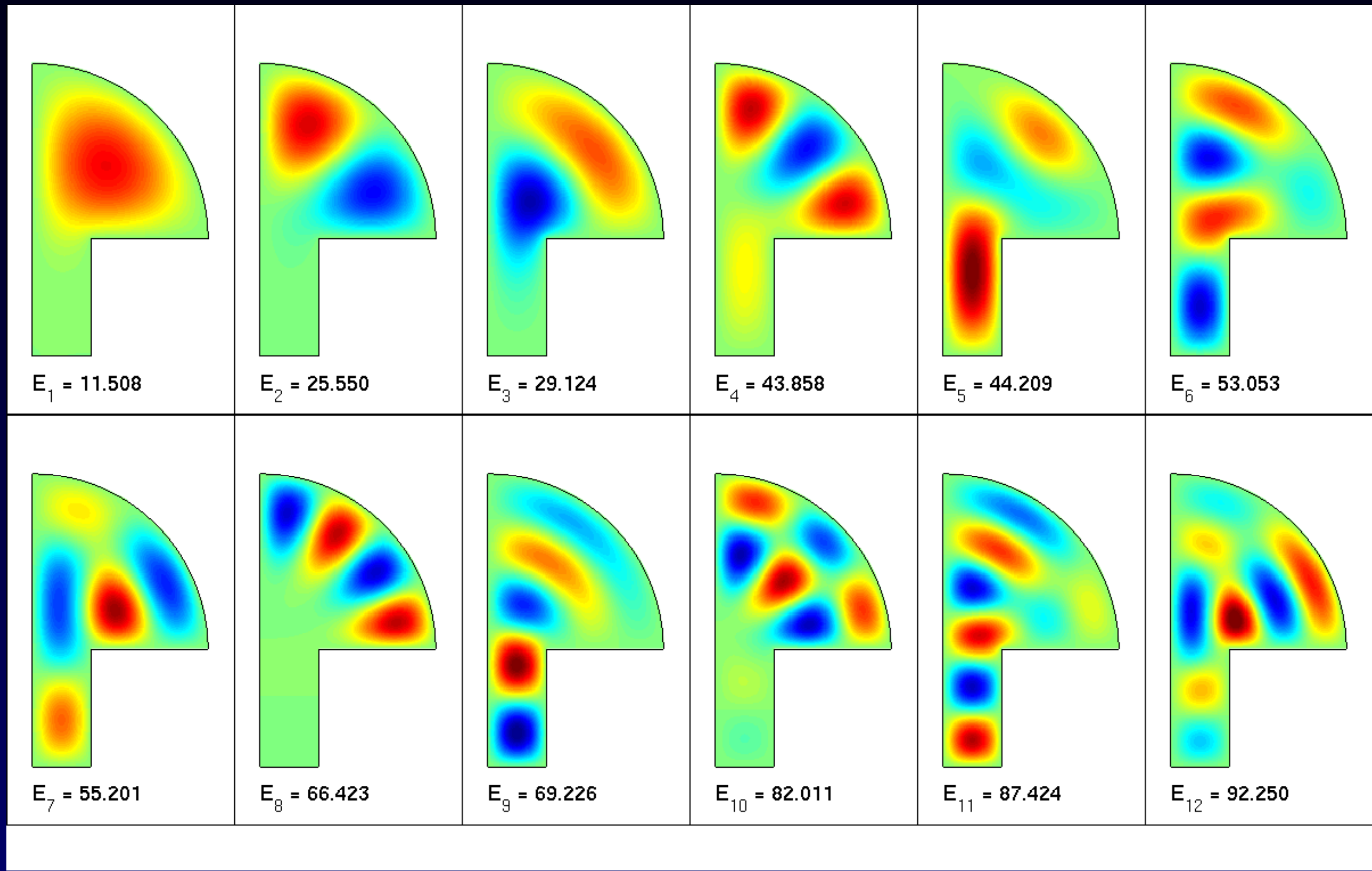

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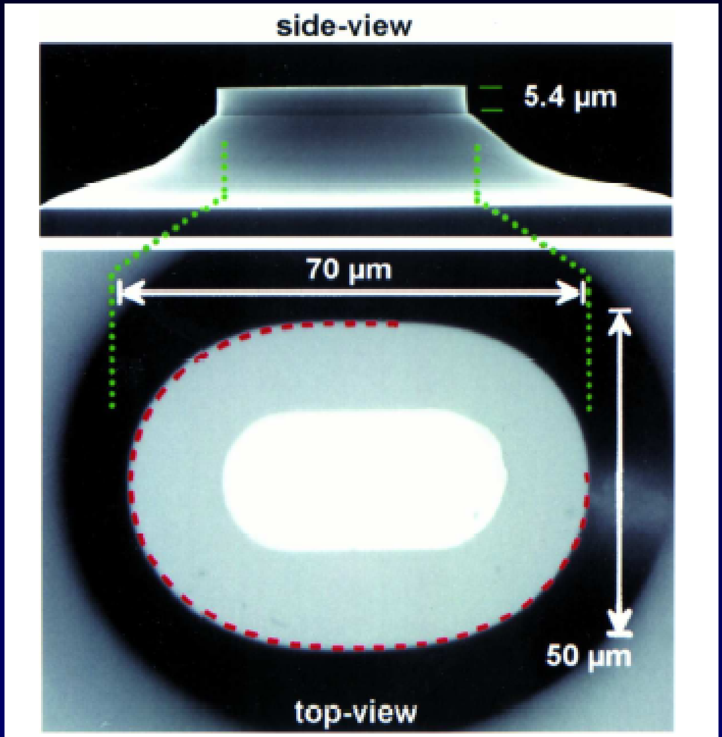
  Recall analytic solns only if Δ separable (rectangle, ellipse…)
- Desires: fast numerical method for high frequency $j \gg 1$,
  rapid convergence, corners, multiply connected, $\Omega \subset \mathbb{R}^3$…?

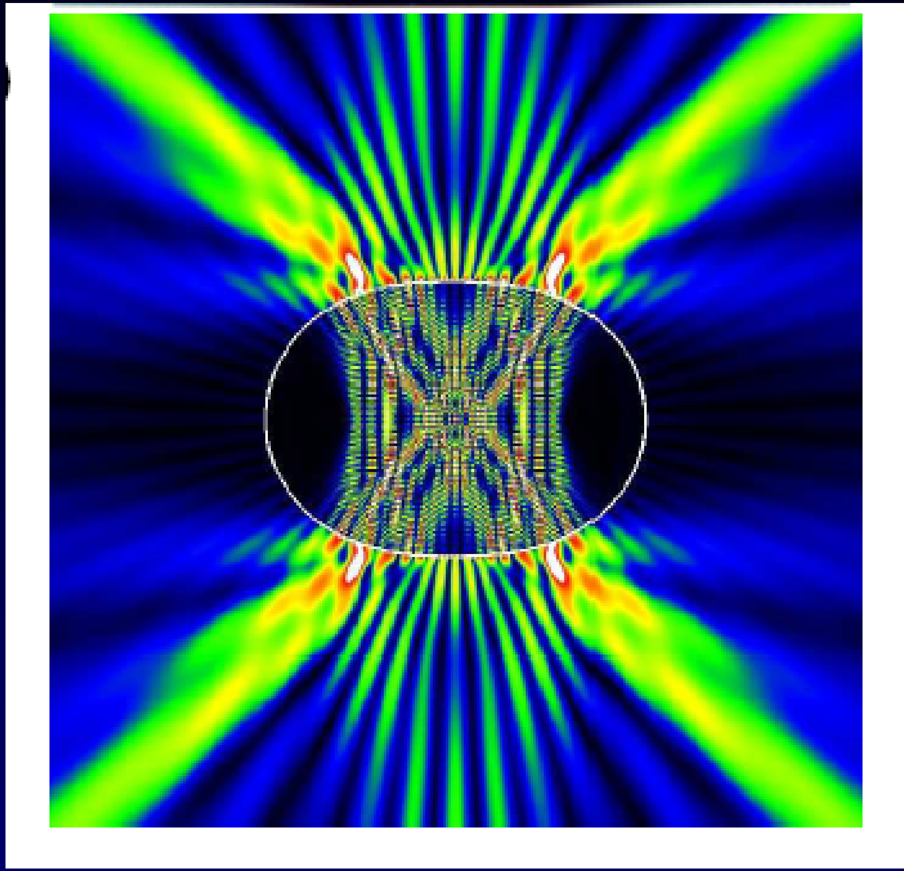
Motivation for high frequency modes

leaky resonant cavities

quantum-cascade laser



mode and emission pattern



- 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 (wavenumber $k \gg 1$): multiscale problem

Method of Particular Solutions

Given trial energy parameter $E > 0$:

- choose basis function set $\{\xi_i\}_{i=1\dots N}$ with $-\Delta\xi_i = E\xi_i$ in Ω, $\forall i$

  global Helmholtz solutions, *e.g.* plane waves, Fourier-Bessel functions

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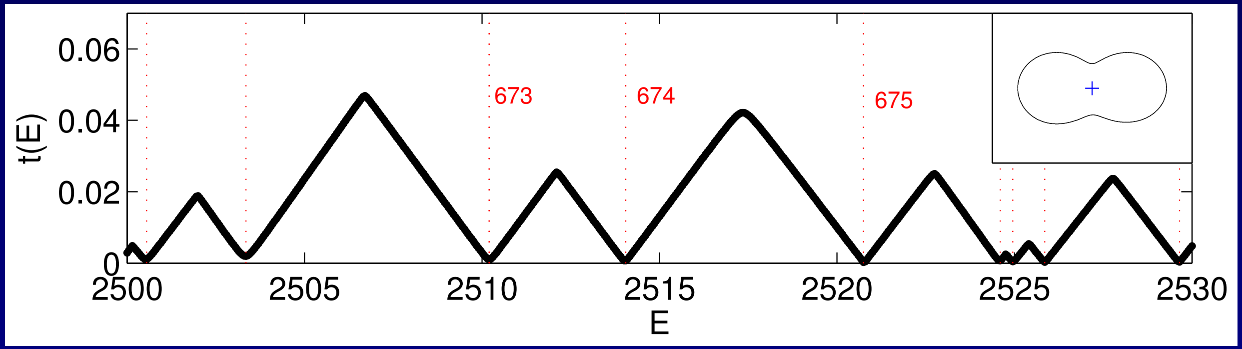
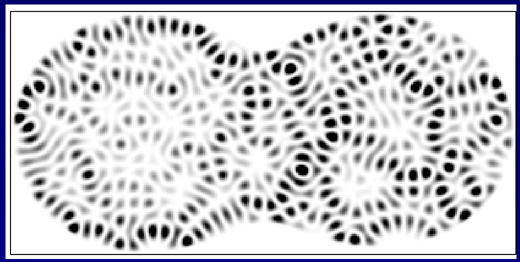


ϕ_j^2: $\Omega =$ peanut, $j \approx 700$



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

Computing boundary tension

$$t(E) = \min_{\substack{u \neq 0 \\ u \in \mathrm{Span}\{\xi_i\}}} \frac{\|u\|_{L^2(\partial\Omega)}}{\|u\|_{L^2(\Omega)}} = \min_{\mathbf{a}\neq\mathbf{0}} \sqrt{\frac{\mathbf{a}^T F \mathbf{a}}{\mathbf{a}^T G \mathbf{a}}} = \sqrt{\lambda_1} \quad \leftarrow$$

lowest generalized eigenvalue of $F\mathbf{a} = \lambda G \mathbf{a}$

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

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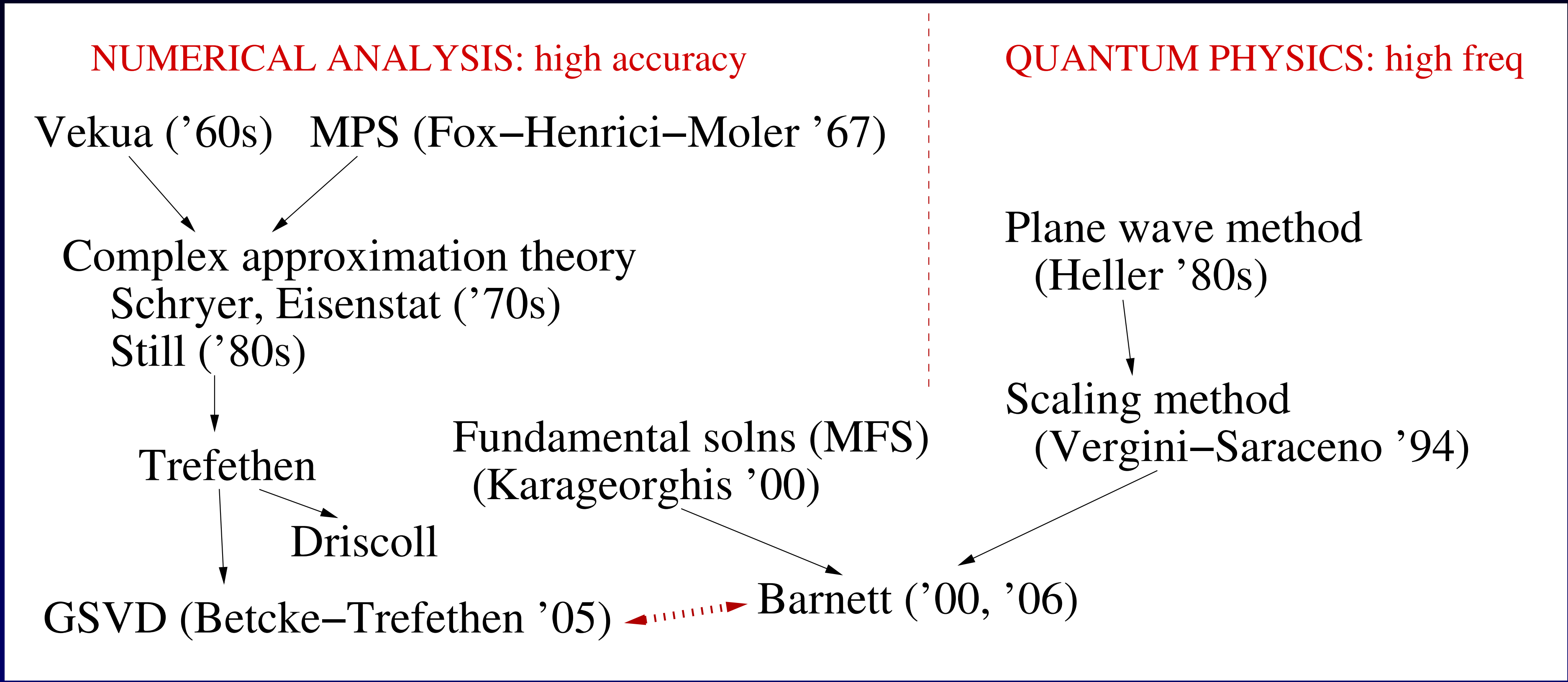
In practise: as N grows, find $\exists\mathbf{a}$, $|\mathbf{a}| = 1$, $\sum_{i=1}^N a_i\xi_i = O(e^{-cN})$ in $\overline{\Omega}$

- 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, `eig(F,G)` fail. . .
  need regularized (ϵ_{mach}-truncated) inverse of G (B '00)

Bifurcated genealogy



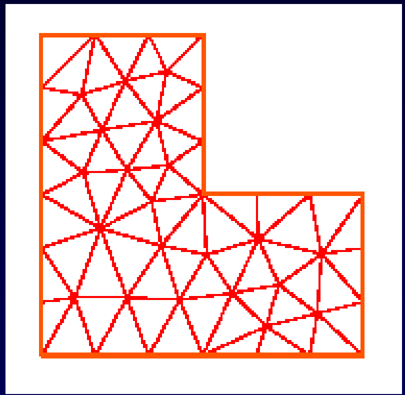
- Recent cross-pollination of ideas

Compare MPS to standard methods

Direct discretization (mesh)

finite differencing

finite element method



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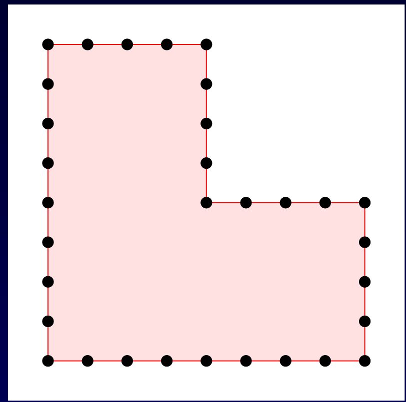
- basis satisfies BCs
- find basis coeffs to solve PDE

Boundary methods (meshless)

integral equation methods

method of particular solutions (MPS)



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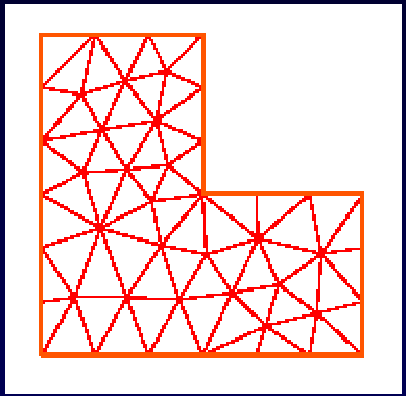

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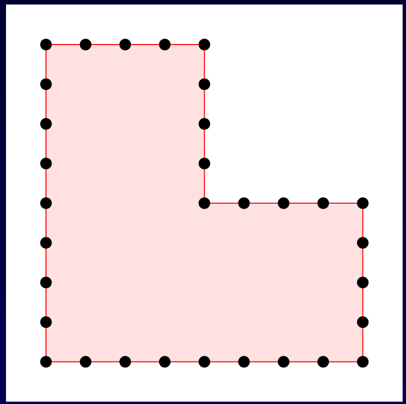

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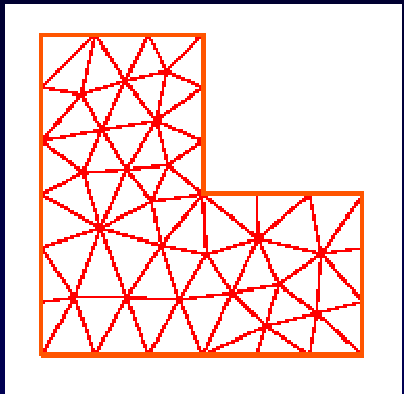

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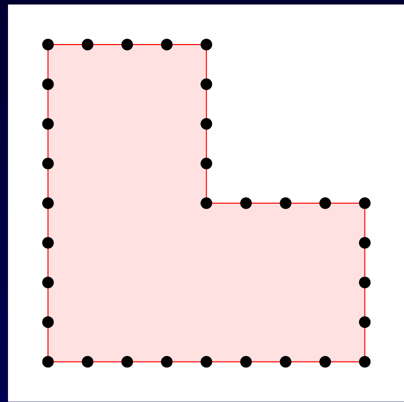

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MPS: exponential convergence
possible in many shapes

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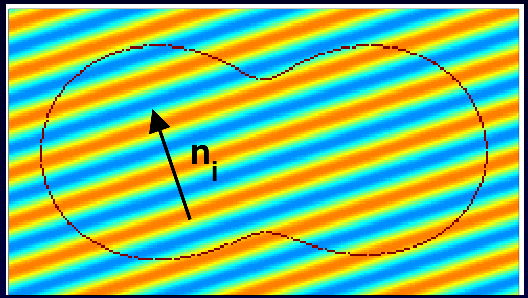

$$\begin{cases} \text{Plane waves} & \sin(k\mathbf{n}_i \cdot \mathbf{x}), \qquad k^2 = E \\ \text{Fourier-Bessel} & J_l(kr)\sin(l\theta) \end{cases}$$

Thm: Ω smooth $\Rightarrow$ exponential convergence (Eisenstat '74)

Practice: fail for nonconvex Ω (coeff sizes $|\mathbf{a}| \gg 10^{16}$)

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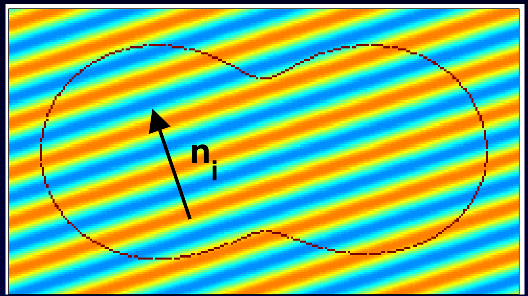

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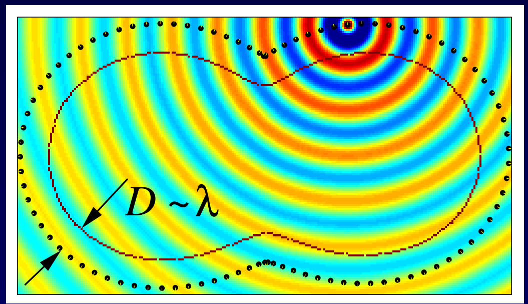

Fundamental solutions (MFS)

$Y_0(k|\mathbf{x} - \mathbf{y}_i|)$ 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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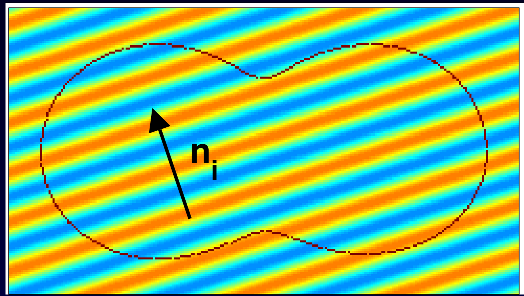

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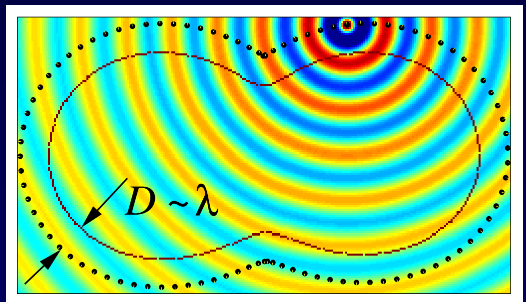

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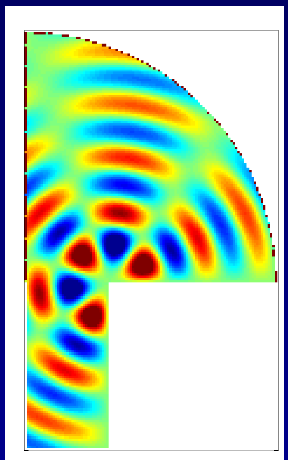

Corner-adapted Fourier-Bessel:

$$\text{singular corners } \theta \neq \frac{\pi}{n}$$

Practice: exp. conv. for multiple corners (Betcke '05)

Scaling method

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

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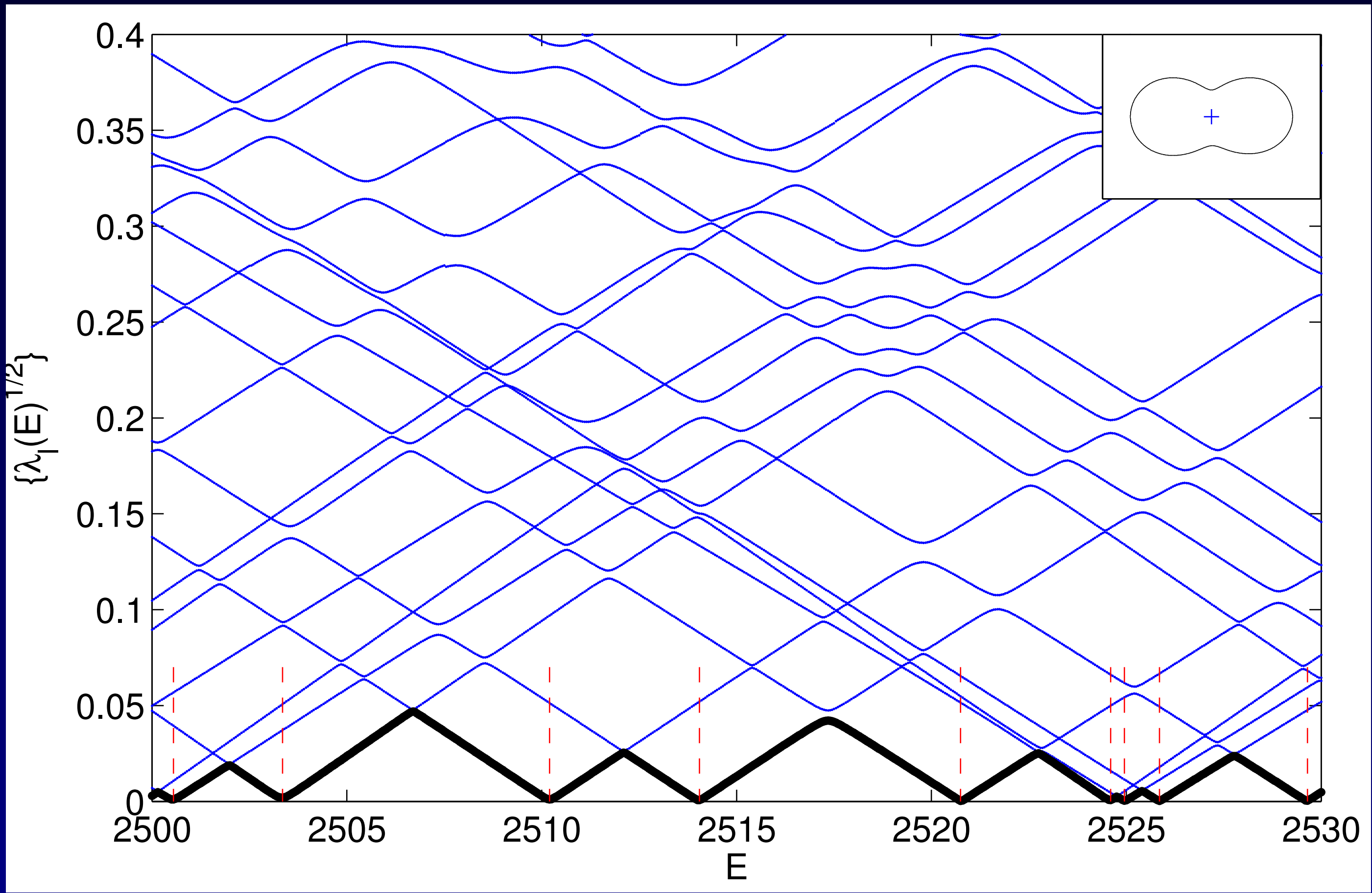
Plot higher generalized eigenvalues…



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

Scaling method

(Vergini-Saraceno '94; B '00, '06)

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

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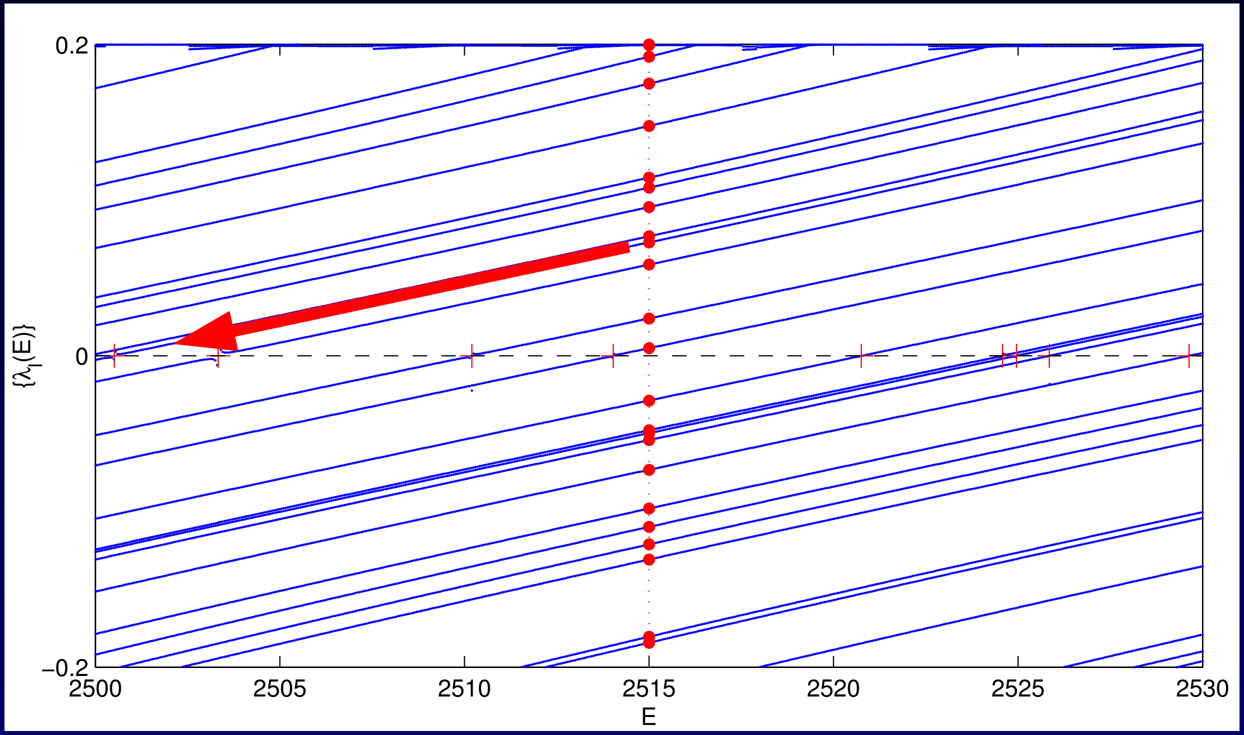
Generalized eigenvalues $\lambda_l(E)$ linear in $E - E_j$ (for Ω star-shaped):



- 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 ϕ_j
- errors grow like $t \sim |E_j - E|^3$ (3^{rd}-order convergence with effort)

Application: Quantum ergodicity

Q: If ray dynamics completely *chaotic* in Ω…
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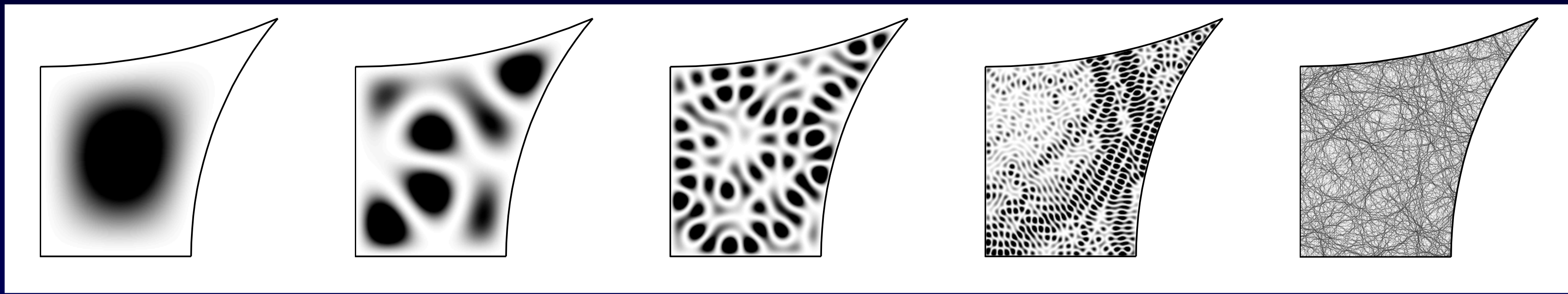


$j = 1$ $\quad$ $j = 10$ $\quad$ $j = 10^2$ $\quad$ $j = 10^3$ $\quad$ $j \approx 5 \times 10^4$

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

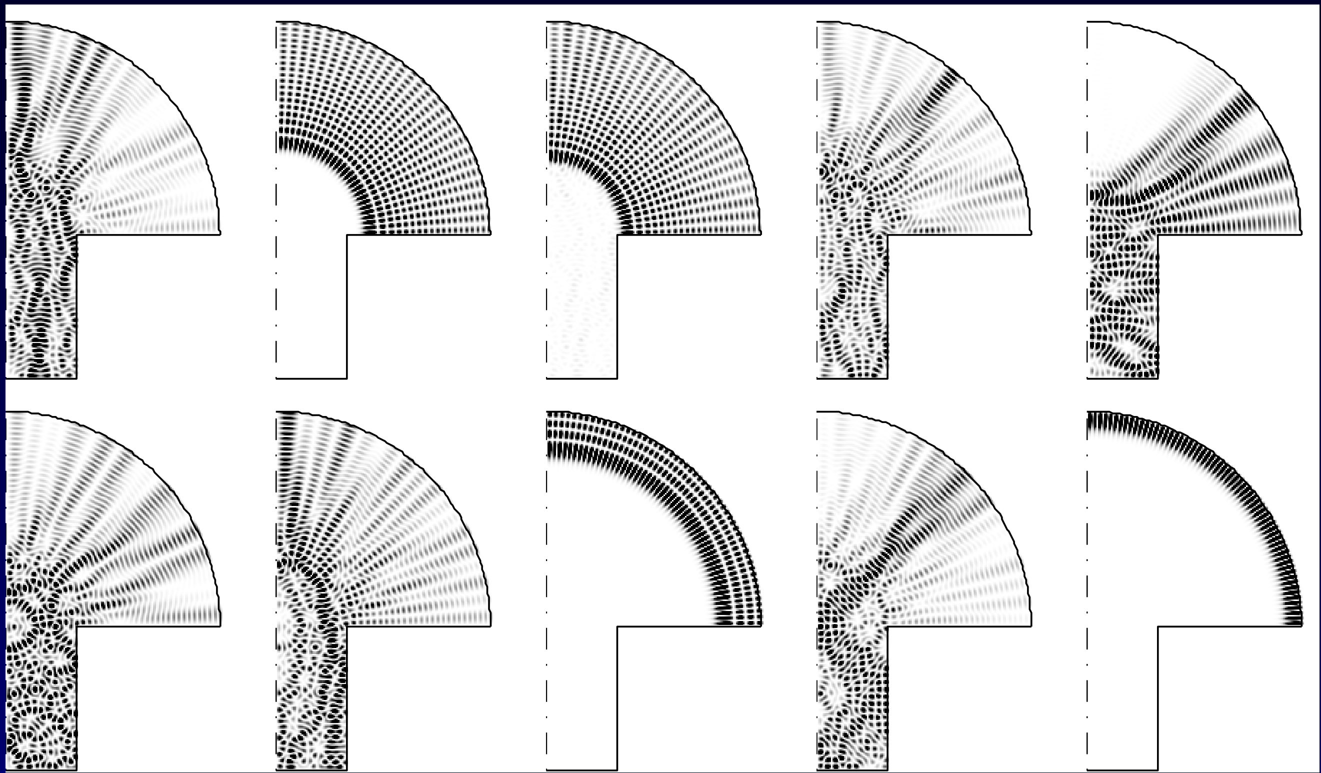
A: deviations from uniformity die asymptotically as $O(E_j^{-1/4})$

(B, Comm Pure App. Math, '06)

Application: Mushroom cavity

(joint w/ T. Betcke)

Ray dynamics has two phase space regions: *regular* & *chaotic*



$k = 100, j \approx 2000$

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

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
- Apps: quantum chaos. Broad engineering applications await …

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