Eigenmodes and quantum chaos: Lost on the frequency axis? Check your Dirichlet-to-Neumann map!

McGill-CRM, Mar 11, 2008

Alex Barnett — Mathematics, Dartmouth College, USA

some work joint w/ T. Betcke, Manchester, UK

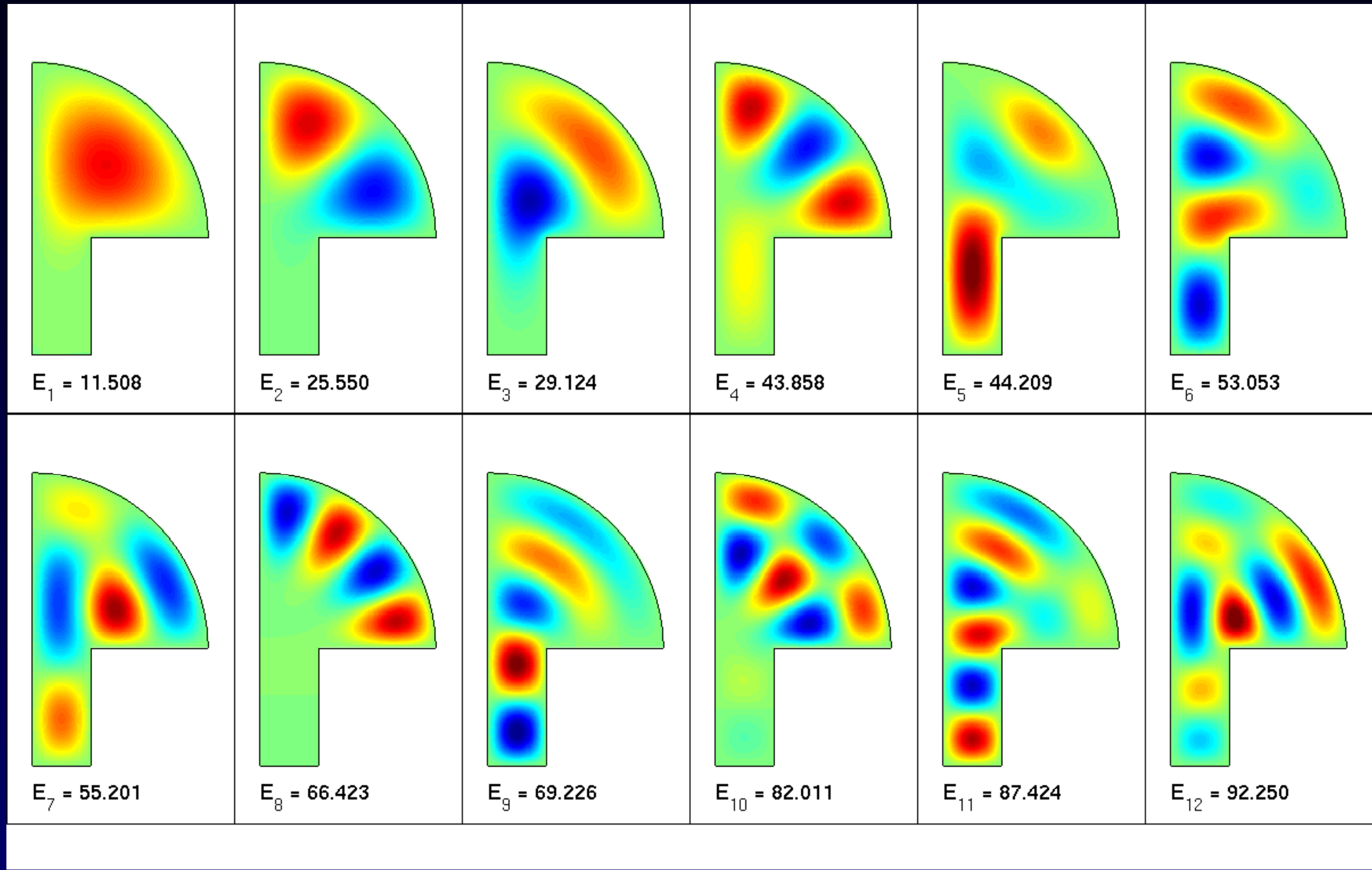
Planar Dirichlet eigenvalue problem

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

$\{E_j\} := \sigma_D$



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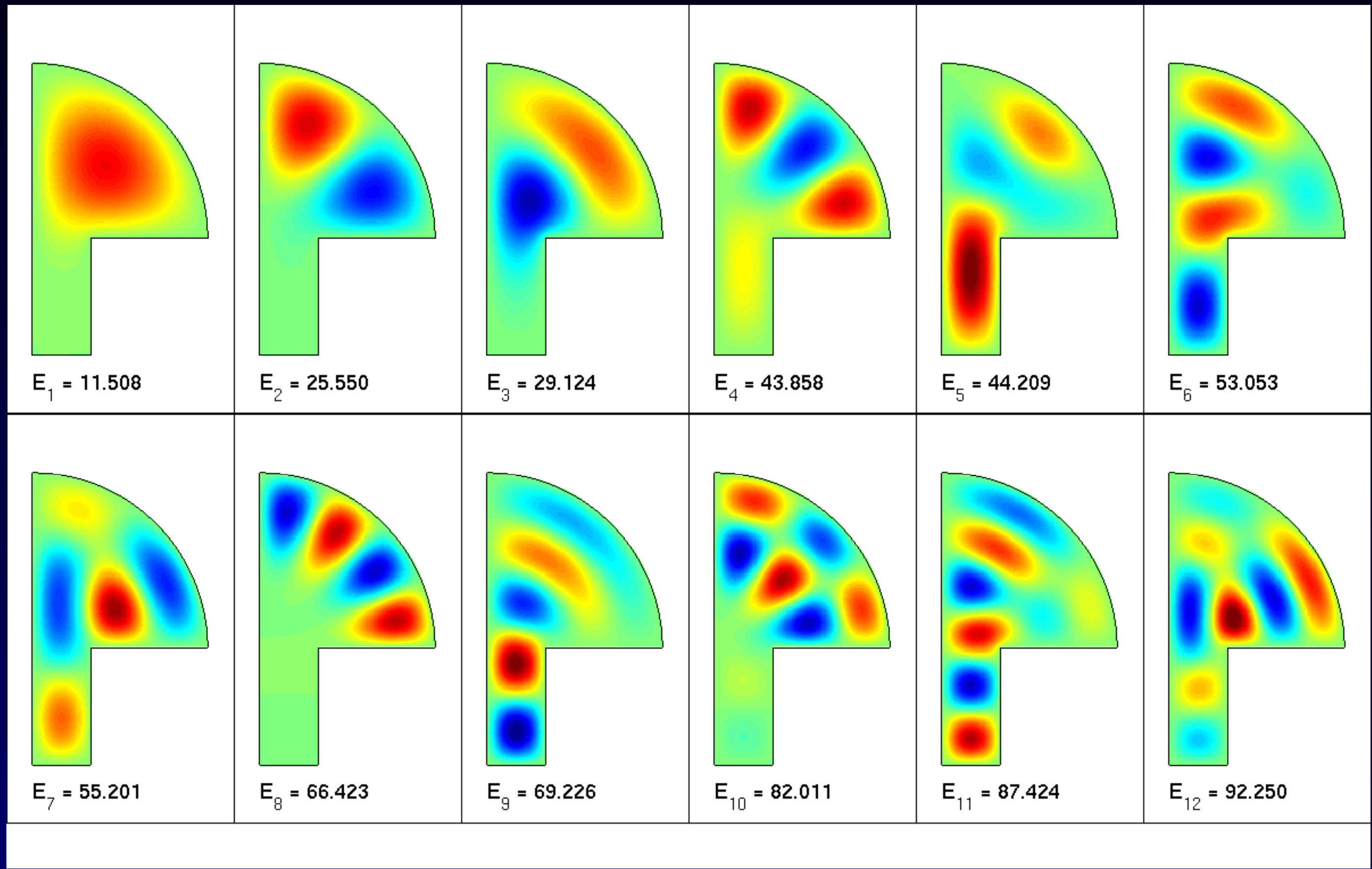

- Modes of a 'drum': acoustics, optics, EM resonators, quantum
  paradigm for harder problems: general BCs, resonances, Maxwell…

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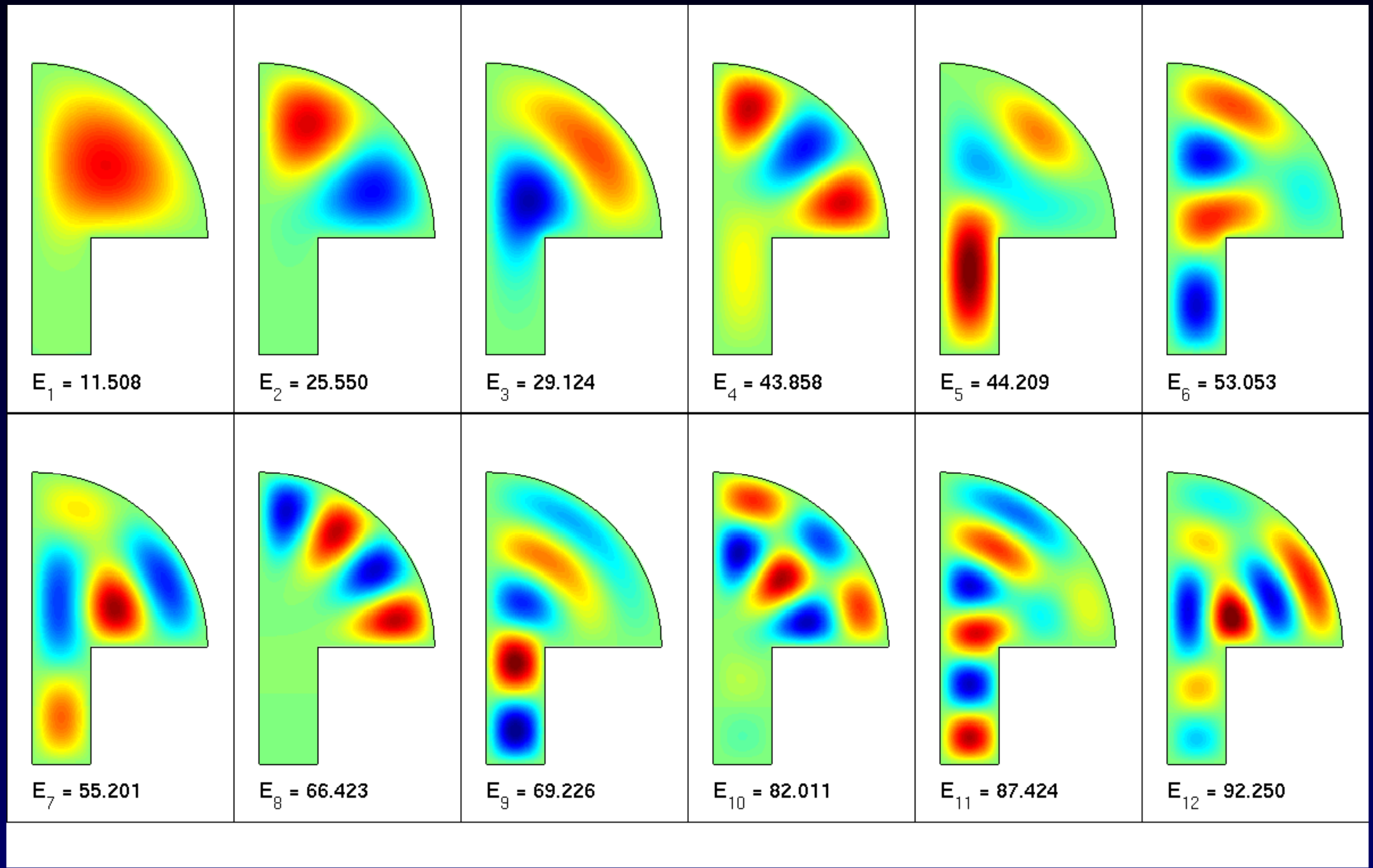


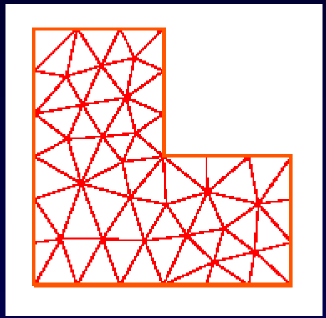
- Modes of a 'drum': acoustics, optics, EM resonators, quantum
  paradigm for harder problems: general BCs, resonances, Maxwell…
- Care about high-frequency regime: wavenumber $k_j := \sqrt{E_j} \gg 1$
  then E_j, ϕ_j expensive to compute by standard methods

Two classes of methods for eigenmodes

Direct discretization (mesh)

finite differencing

finite element methods



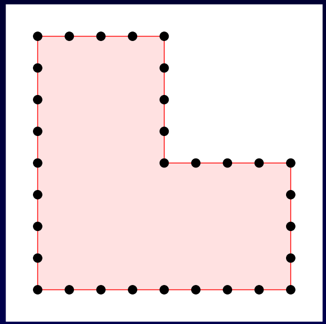
- local basis representation

  e.g. polynomials in elements
- basis satisfies BCs, not the PDE
- solve: sparse matrix eigenvalue

Boundary methods (meshless)

boundary integral equations

method of particular solutions (MPS)



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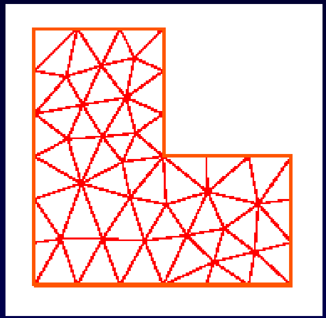

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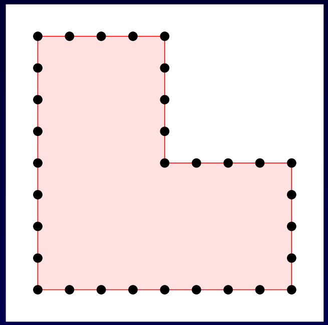

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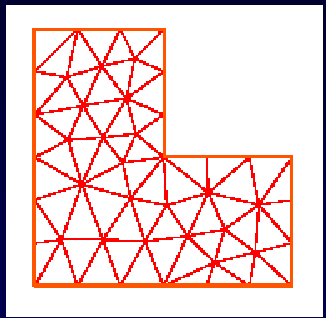

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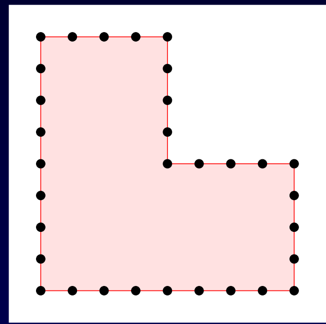

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$N = O(k)$ huge gain at high freq

$k \gg 1$: boundary methods excel. Bottleneck: basis depends on freq E

$\Rightarrow$ must locate each E_j one-by-one as minima of some func $t(E)$

Outline

1. Method of Particular Solutions
   searching on the frequency axis for each eigenvalue

2. Scaling method
   using Dirichlet-to-Neumann map to break the bottleneck

3. Quantum Chaos
   high-freq asymptotics and statistics of eigenmodes

   (a) rate of quantum ergodicity

   (b) mixed dynamics: mushroom cavity

Method of Particular Solutions

Given trial freq parameter $E > 0$:

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

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

  then $u = \sum_{i=1}^{N} \alpha_i \xi_i$ obeys $-\Delta u = Eu$ in Ω

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- if can find coeff vector $\boldsymbol{\alpha} \in \mathbb{R}^N$ giving $u|_{\partial\Omega} = 0$, but $u \neq 0$ in Ω

  $\ldots$ then u is a mode ϕ_j and E is its eigenvalue E_j

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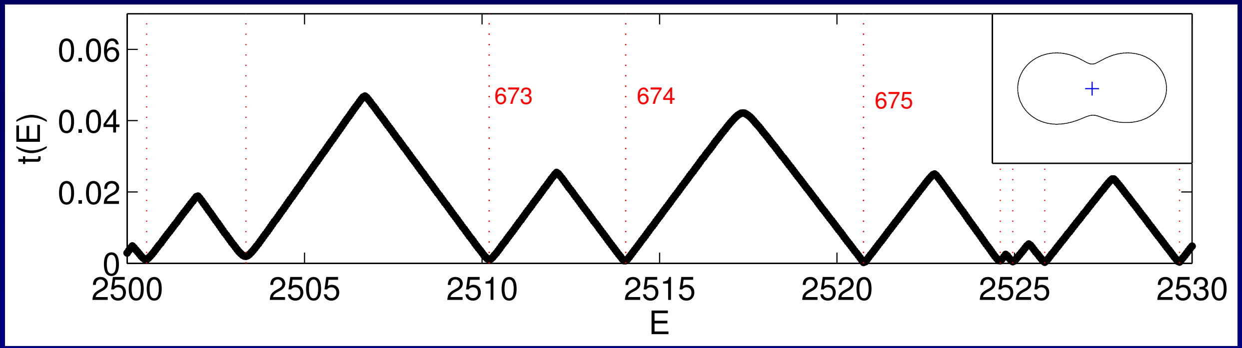
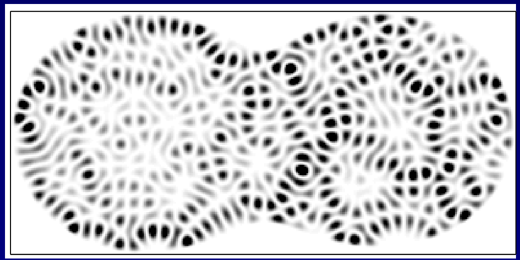


$\Omega =$ peanut, $j \approx 700$



- Locate each approximate eigenvalue as one minimum of $t(E)$

Boundary tension given by linear algebra

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

lowest generalized eigenvalue of $F\boldsymbol{\alpha} = \lambda G \boldsymbol{\alpha}$

matrix elements $F_{ij}(E) = \int_{\partial\Omega} \xi_i \xi_j ds, \quad G_{ij}(E) = \int_\Omega \xi_i \xi_j d\mathbf{x}$ $\leftarrow$ use identities to push to $\partial\Omega$

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- Dividing by $\|u\|_{L^2(\Omega)}$ cures normalization problem of original MPS
  (Fox-Henrici-Moler '67, Betcke-Trefethen '05)
- In practice, increase N for accuracy: F, G numerically singular
  ... QZ fails; must regularize G^{-1} (B '00) ... or GSVD approach (Betcke '07)

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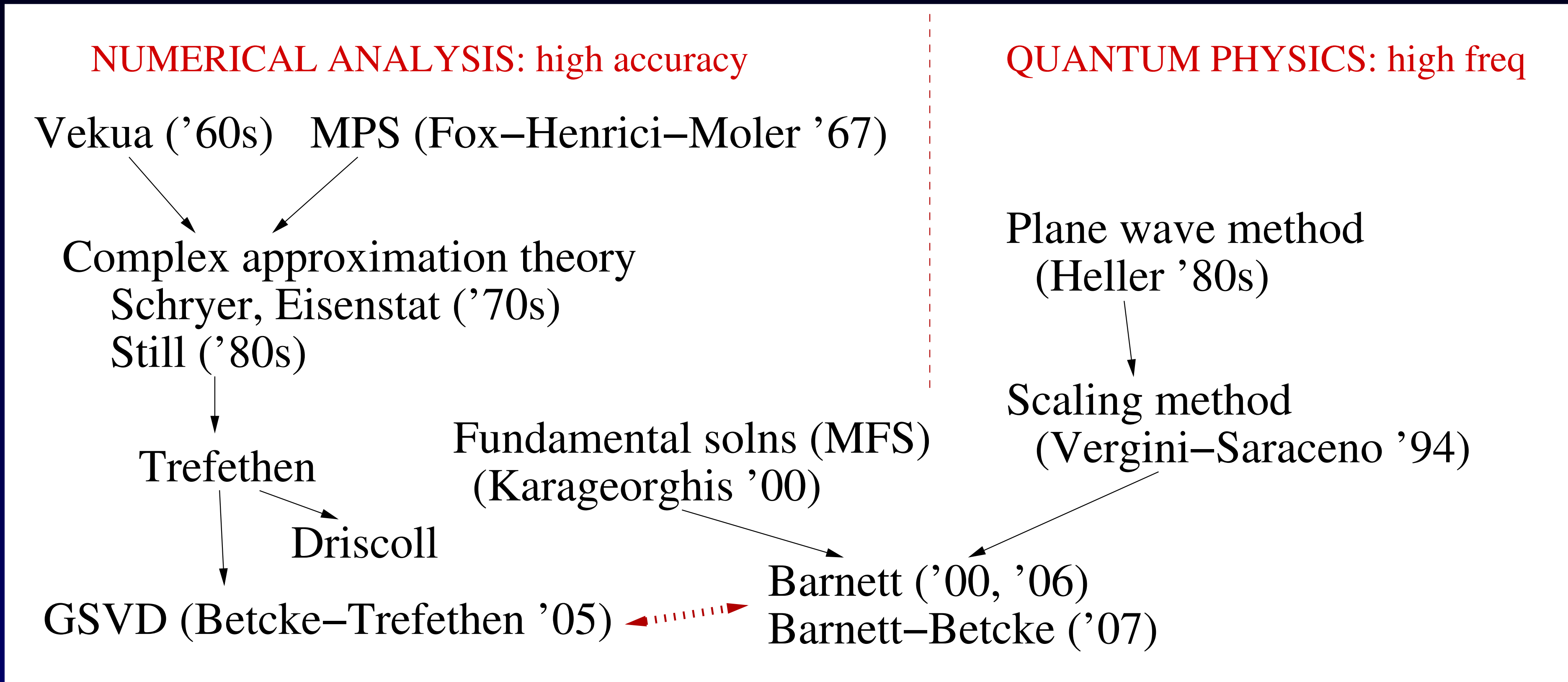
Relative eigenvalue error bounded: $\frac{|E-E_j|}{E_j} \leq C_\Omega t(E)$ (Moler-Payne ’68)

- Thm (via perturbation): bound improved by factor $O(E^{1/2})$ (B, preprint)

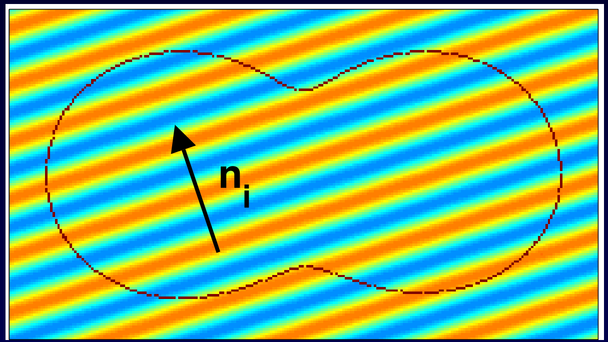
Bifurcated genealogy



- Early on, MPS faired poorly due to normalization/cond-# problems
- Recent cross-pollination of ideas addresses these issues

Given Ω, how choose basis functions?

- Each basis func $\xi_i(\mathbf{x})$ is a *global* Helmholtz soln at freq param E
- Want a set $\{\xi_i(\mathbf{x})\}$ giving small t error



A natural choice is plane waves

$$\sin(k\mathbf{n}_i \cdot \mathbf{x}), \qquad k^2 = E$$

equivalent to Fourier-Bessel (Jacobi-Anger exp)

$$J_l(kr)\exp(il\theta), \quad l \in \mathbb{Z}$$

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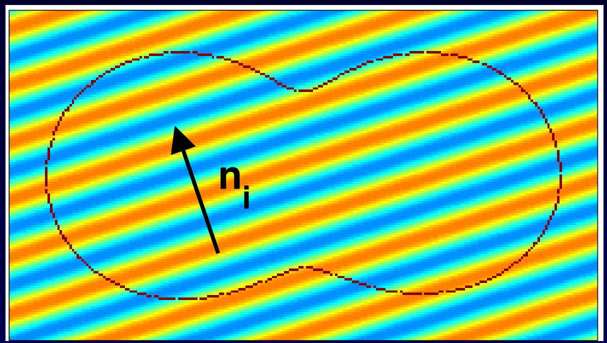

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$\partial\Omega$ analytic: exponential convergence, rate controlled by…

Conformal distance to nearest singularity in analytic continuation of ϕ_j

Vekua $\leftrightarrow$ approximation in $\mathbb{C}$ by polynomials (Betcke '05)

However in practice often useless: *e.g.* t no lower than 10^{-2}

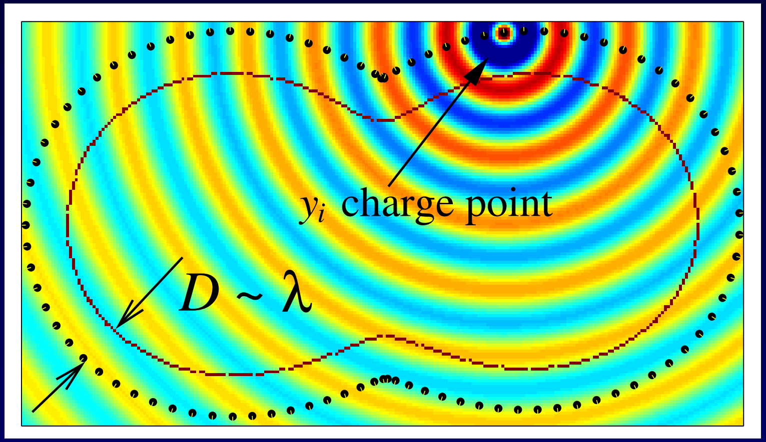
(PWs analysed on unit disc: Perrey-Debain '06)

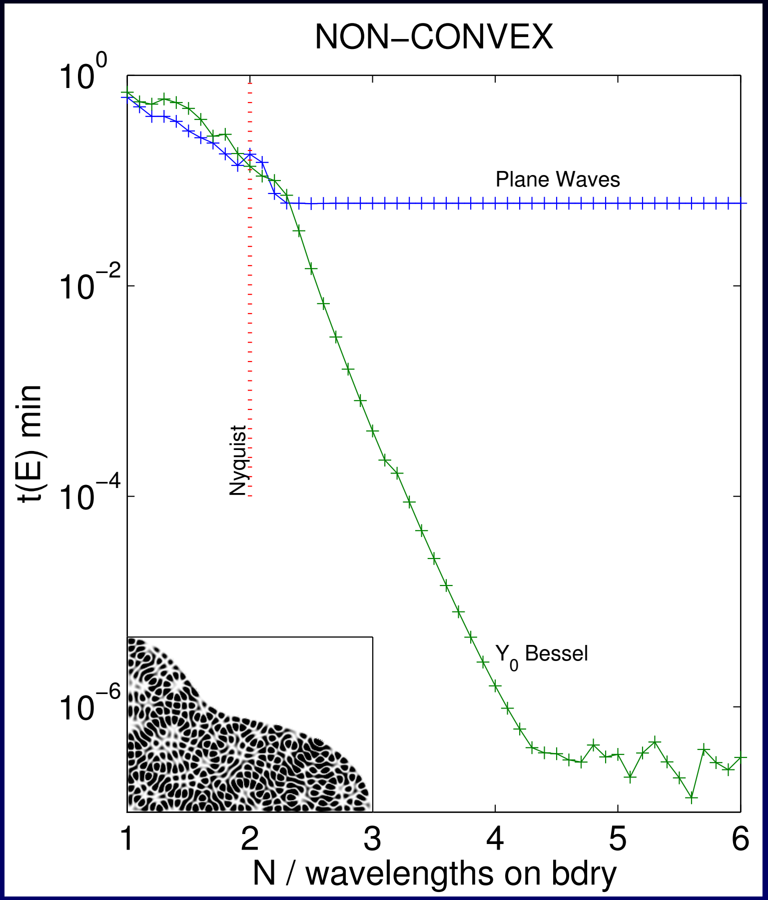
Fundamental solutions basis (MFS)

$H_0^{(1)}(k|x - y_i|)$
charge points $\{y_i\}$ outside Ω

Observe: much lower achievable t

(Karageorghis '00, B '06, B-Betcke '07)





However best t error still $\gg \epsilon_{\text{mach}} \approx 10^{-16}\ldots$

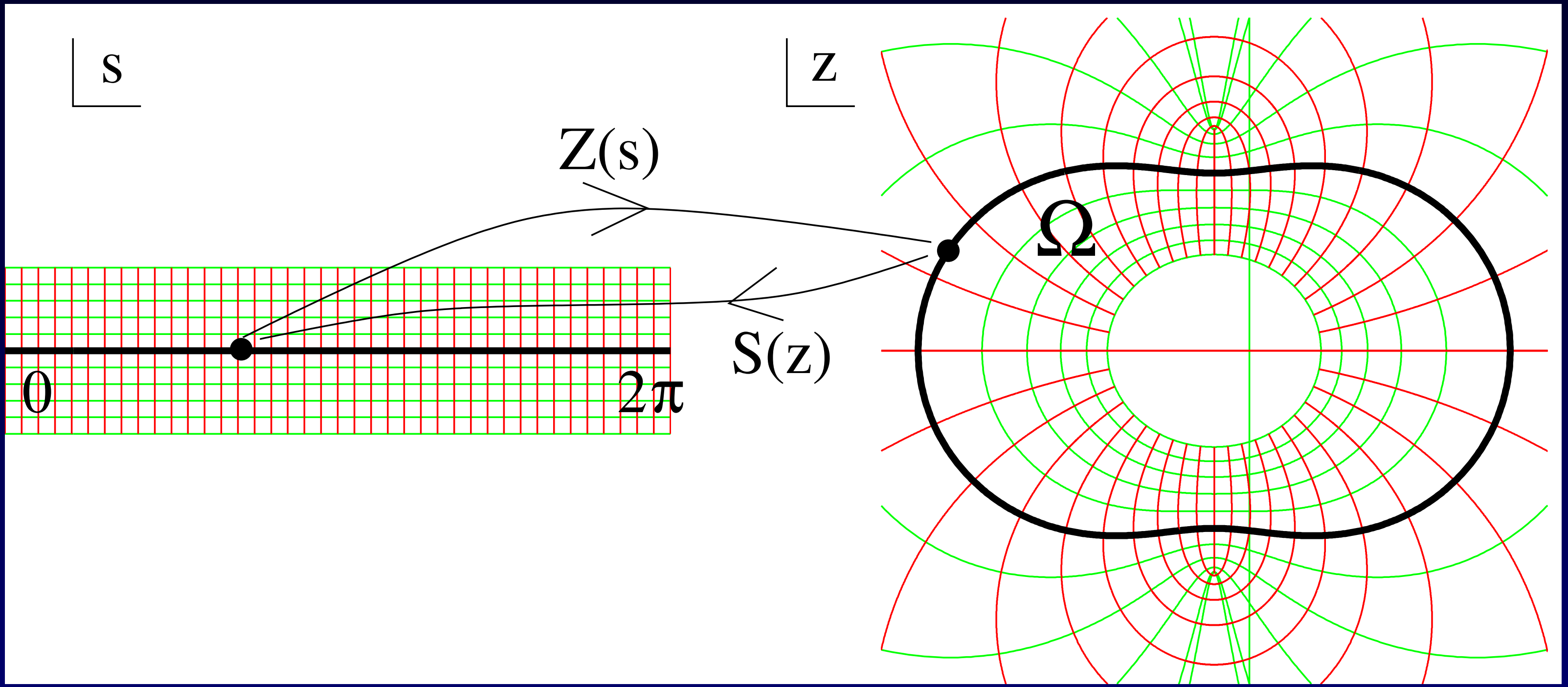
What controls $\left\{ \begin{array}{l} \text{convergence rate ?} \\ \text{when convergence halts?} \end{array} \right.$

(joint work with Timo Betcke, Manchester, UK)

Singularities in continuation of eigenmodes

analytically continue mode ϕ_j : where are nearest singularities?

Define analytic curve $\partial\Omega$ by image of $[0, 2\pi]$ in map $Z(s)$



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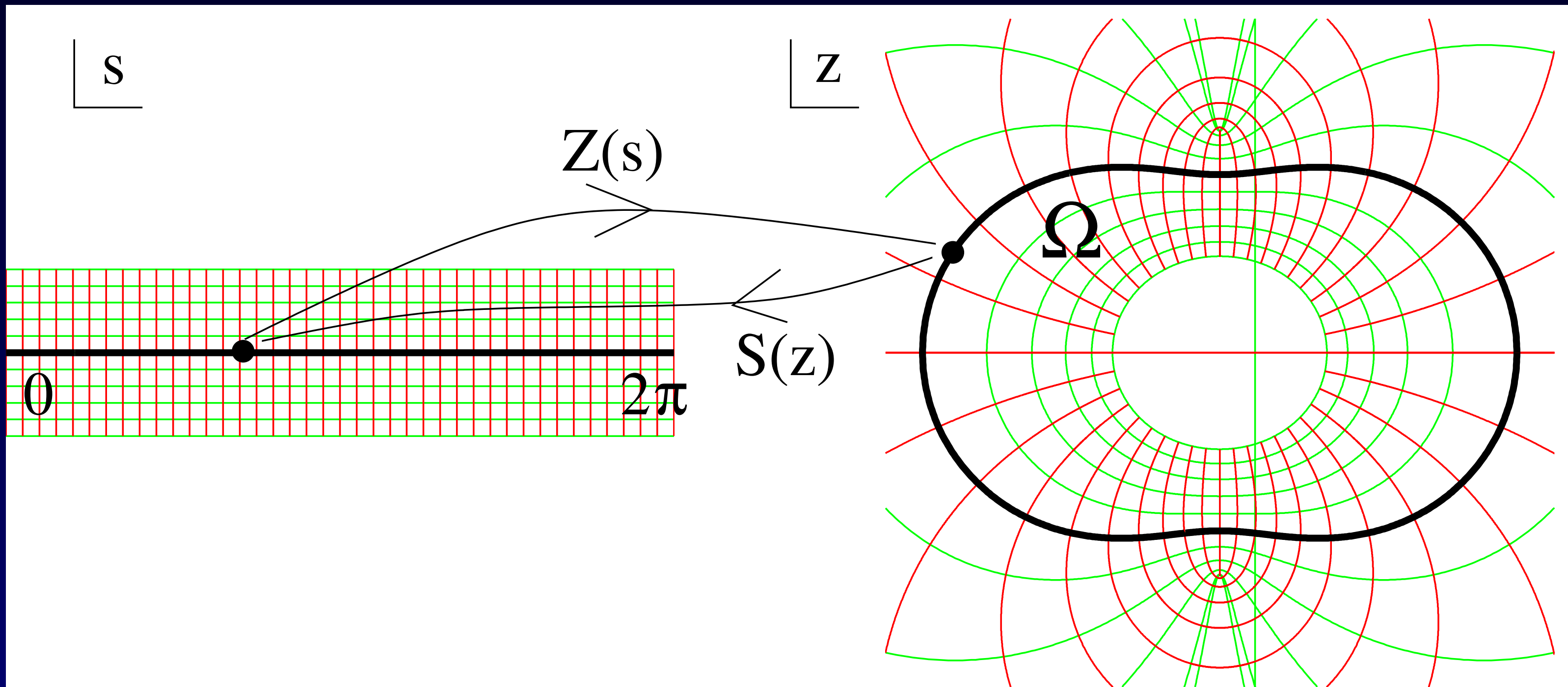
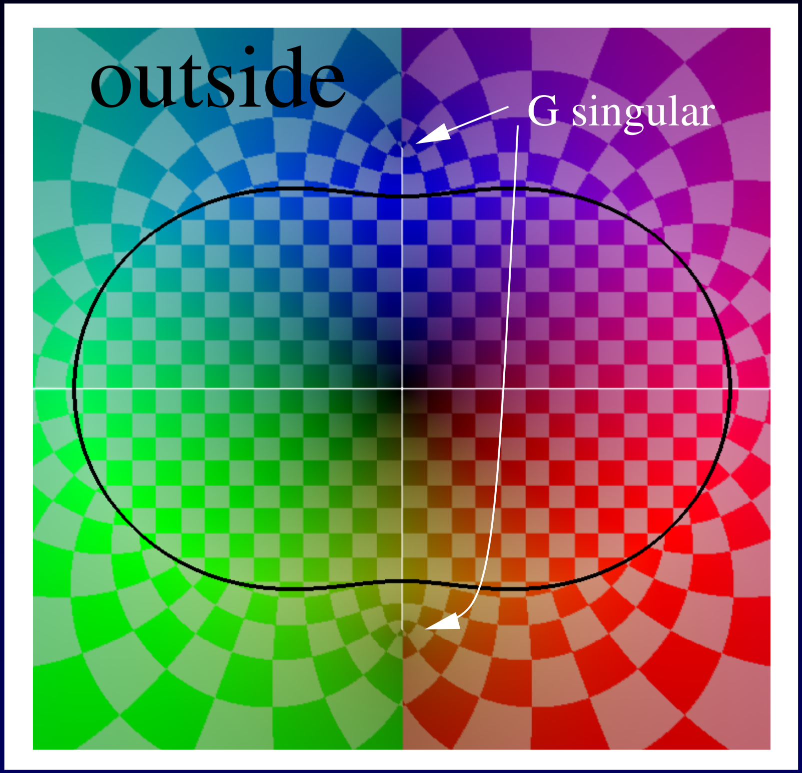
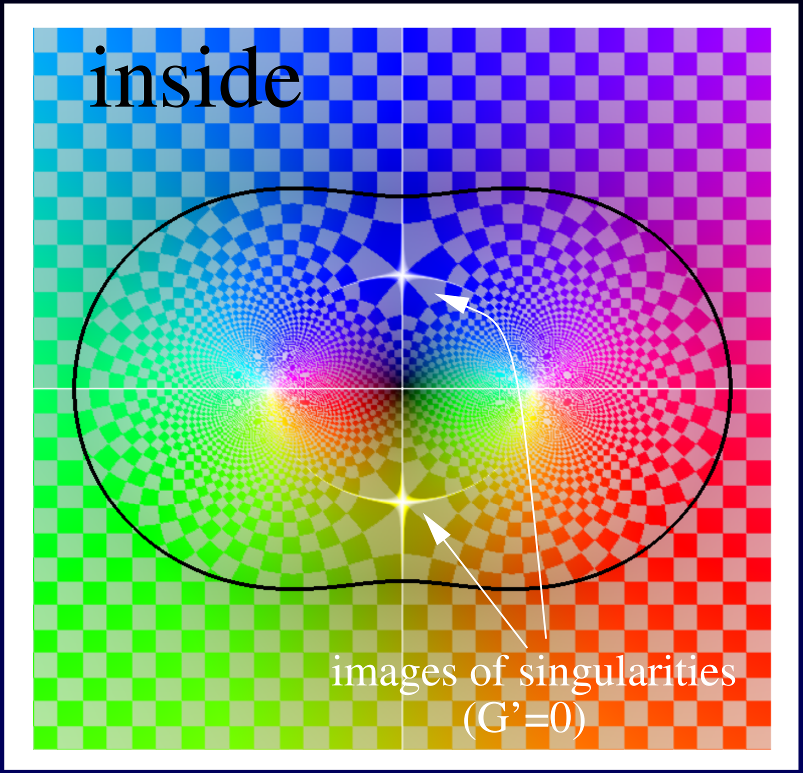


Singularities connected to reflection across an analytic arc:

- Domain has unique Schwarz func $G(z) := \overline{Z(\overline{S(z)})}$ (Davis '74)
- $\overline{G(z)}$ is then reflection of z in arc $\partial\Omega$ (inside↔outside)

Singularities in Schwarz reflection map





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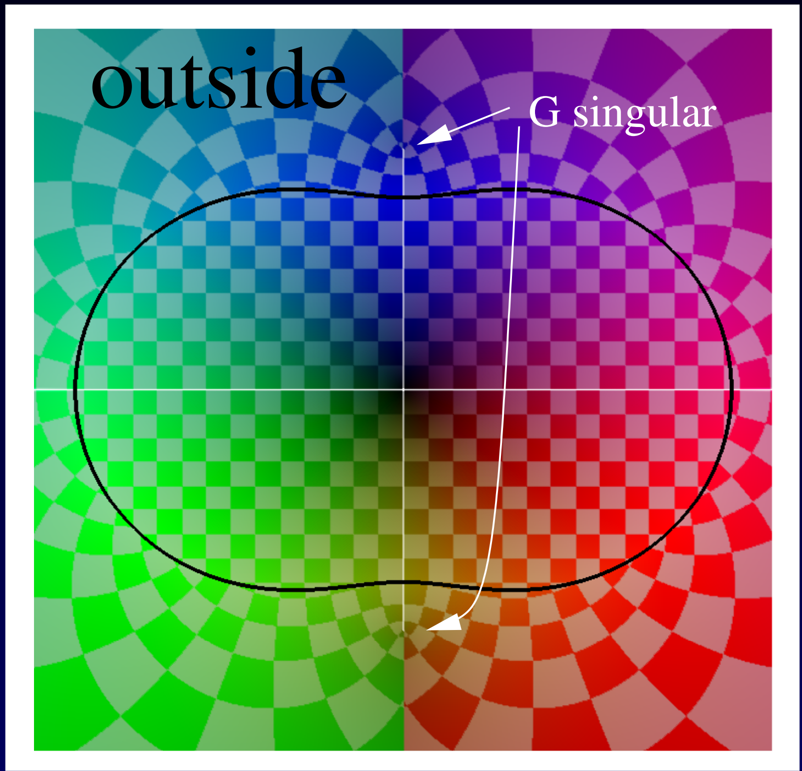

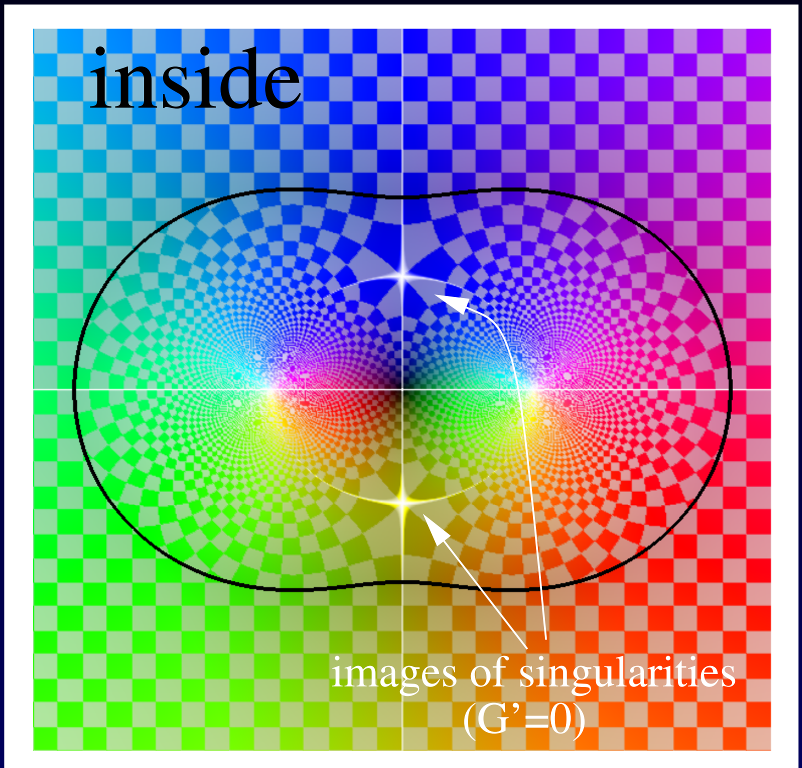

Result: (Millar '86) (Bergman-Vekua integral operator, complexified coords)

If $(\Delta + E)u = 0$, with data $u \equiv v$ on $\partial\Omega$, candidates for singularities in u are: singularities in G and/or in the analytic continuation of data v

- eigenmodes have $v \equiv 0$ so their singularities due to G alone

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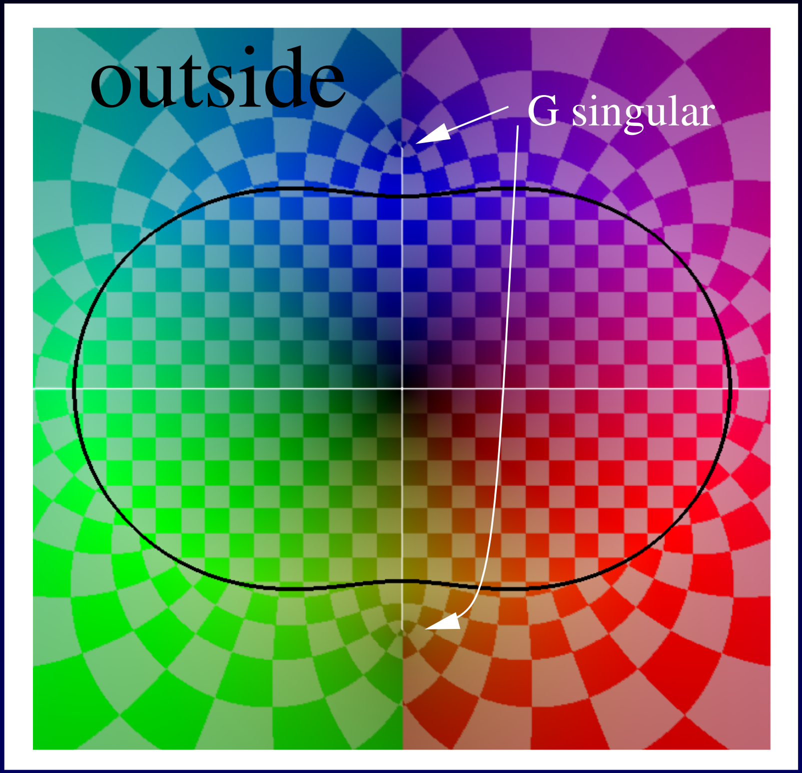

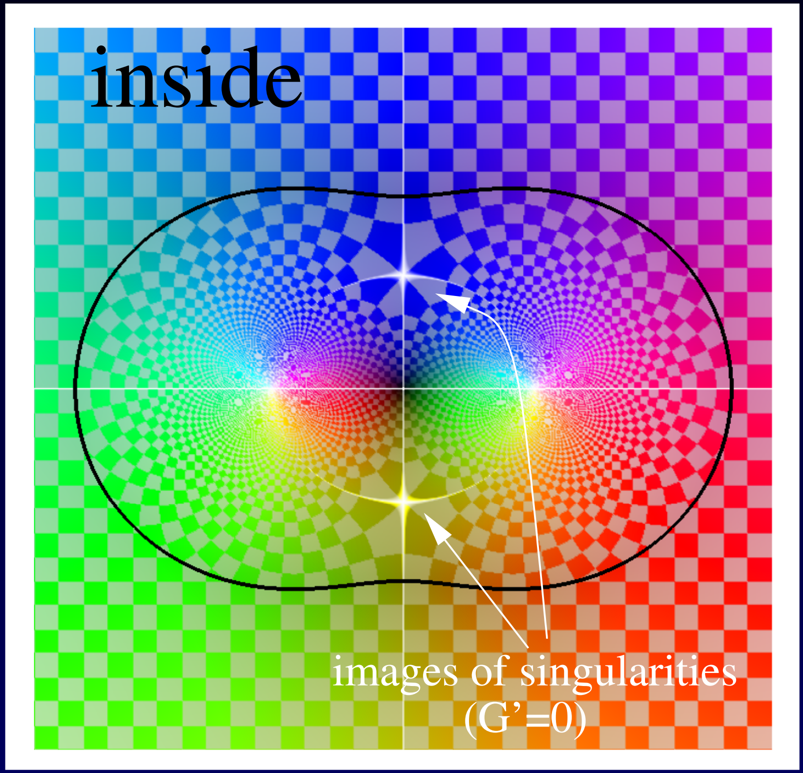

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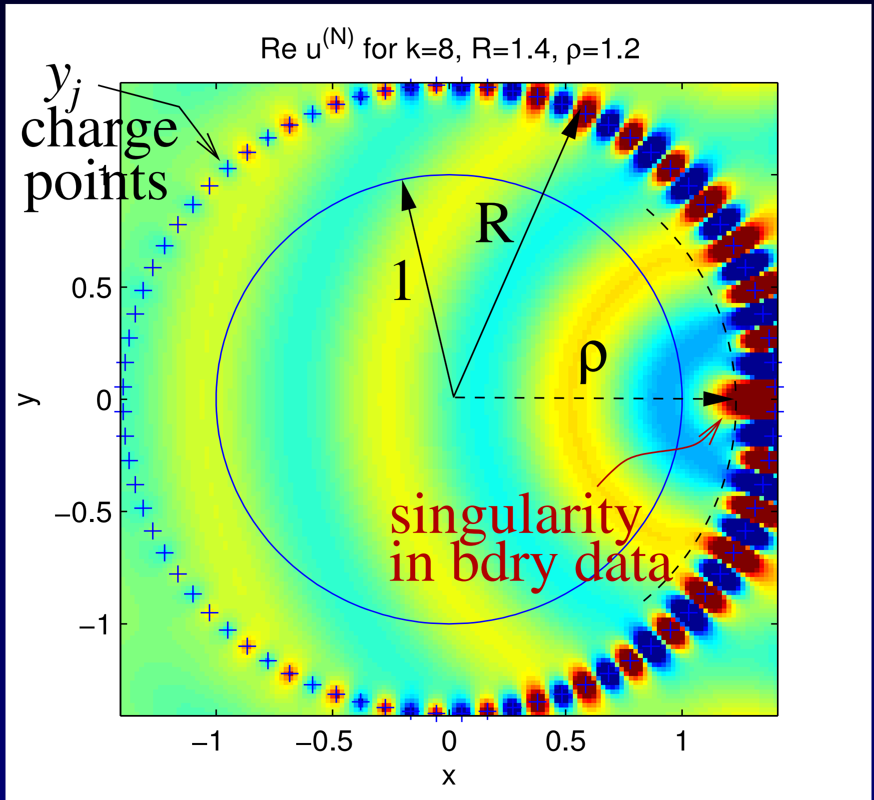
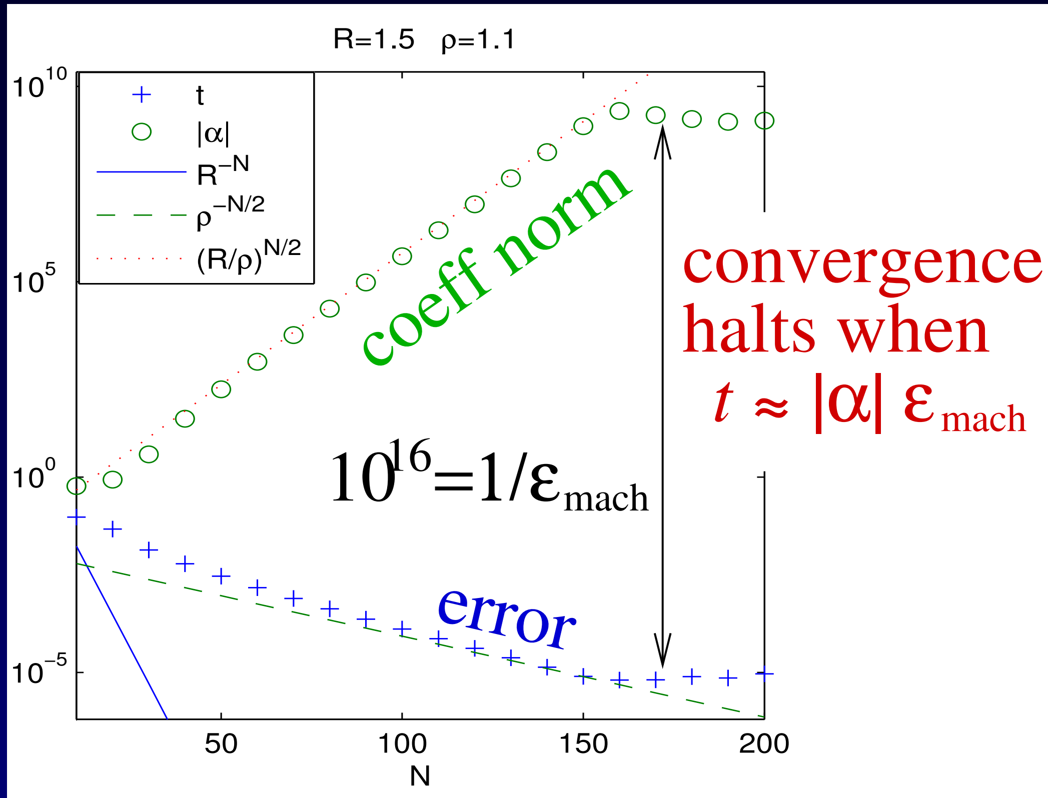
We now study BVP (MPS finds modes using BVP with data $v \equiv 0$)

Helmholtz BVP for Ω = disc

$$(\Delta + E)u = 0 \quad \text{in } \Omega, \qquad u = v \quad \text{on } \partial\Omega$$

Fundamental solns basis, with nearby v singularity: (via Fourier analysis)





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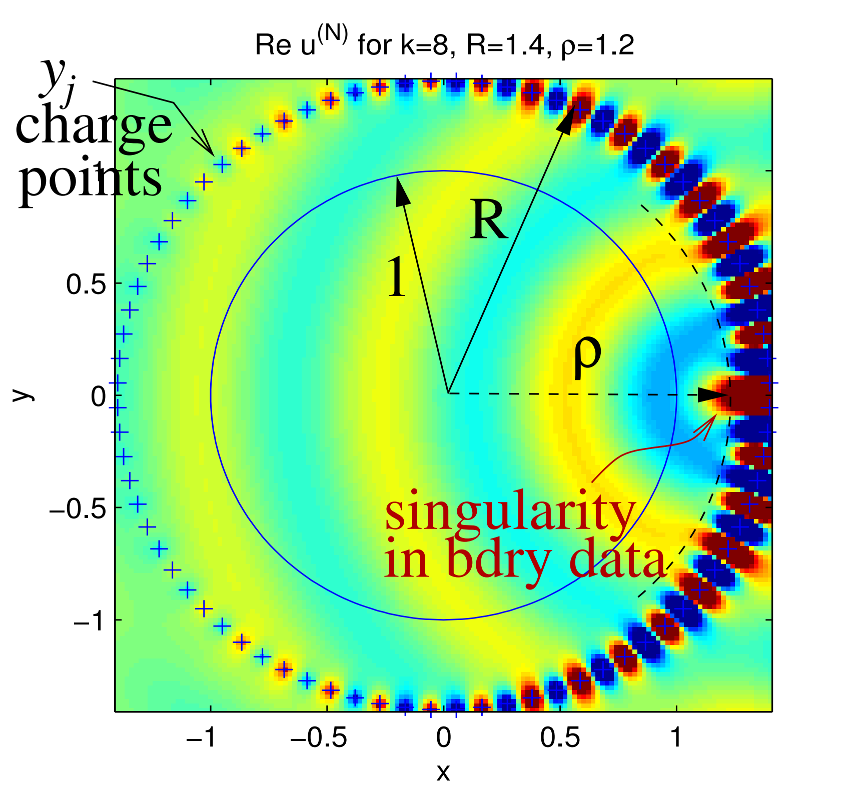
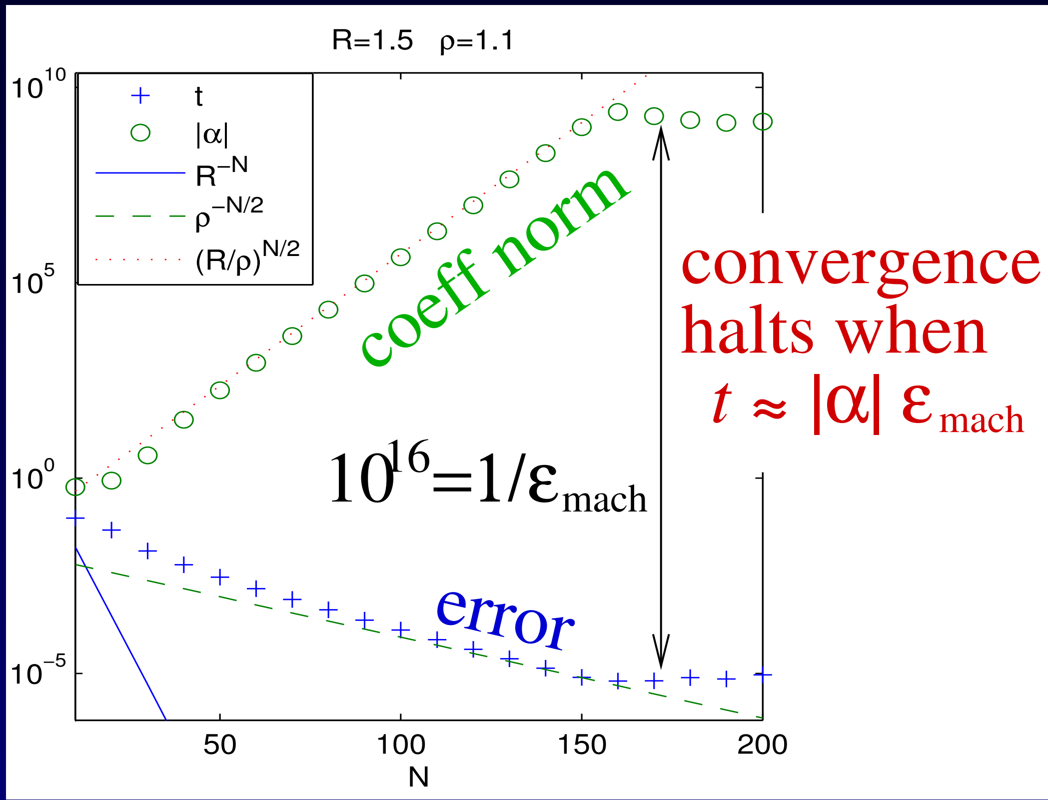


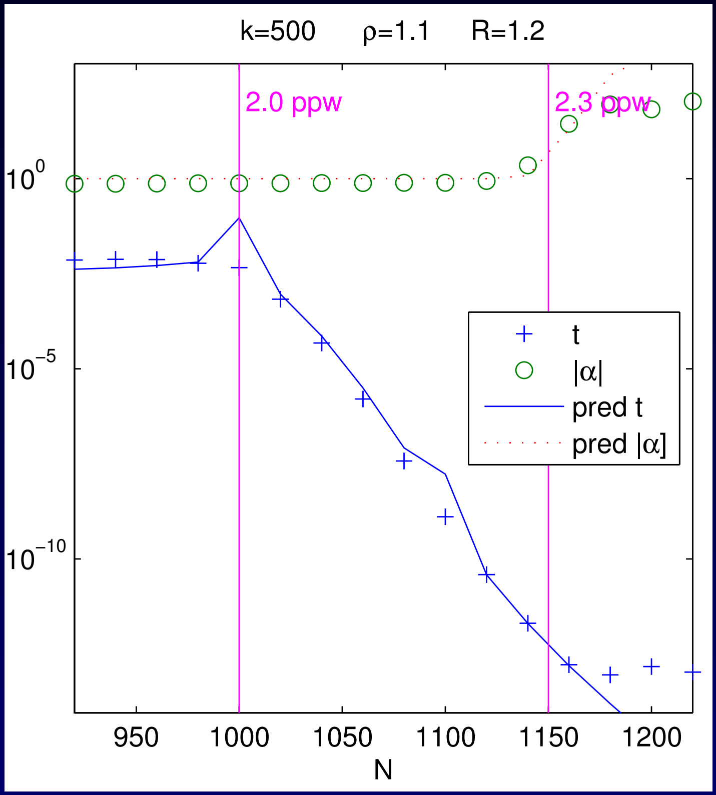


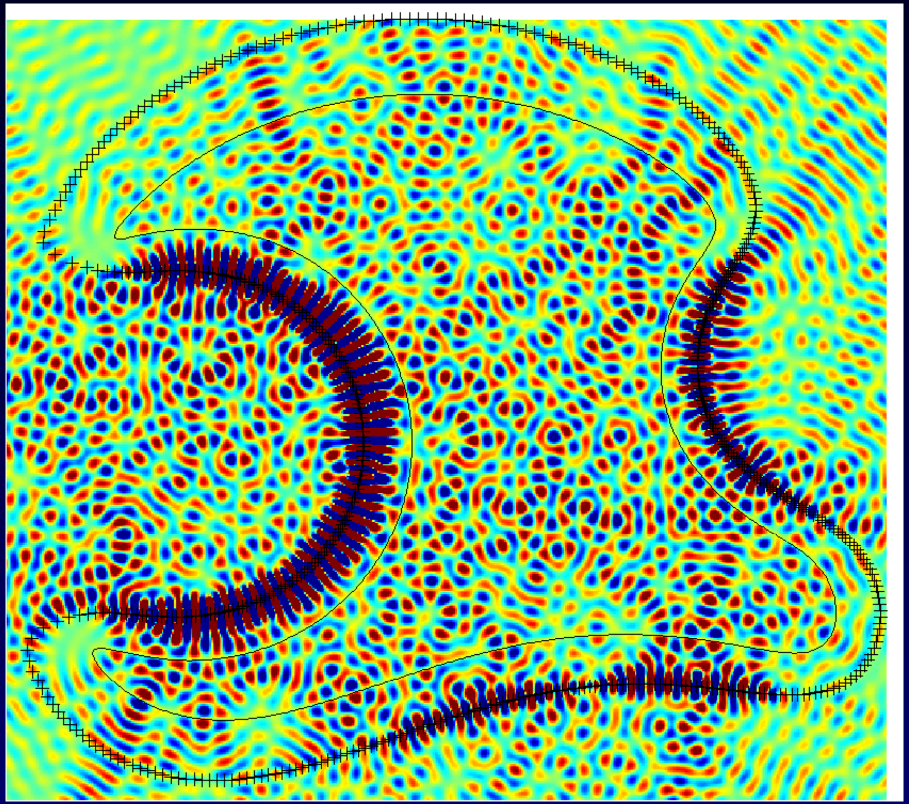
Thm: for $\rho < R$, coefficients grow as $|\boldsymbol{\alpha}| \geq C \left(\frac{R}{\rho}\right)^{N/2}$ …best if $R = \rho$

Other shapes: find $|\boldsymbol{\alpha}|$ grows iff charge curve encloses sing. in G or v

High wavenumbers $k \gg 1$, analytic Ω

Disc analysis: asymptotic $N \to 2$ charge points per wavelength on $\partial\Omega$

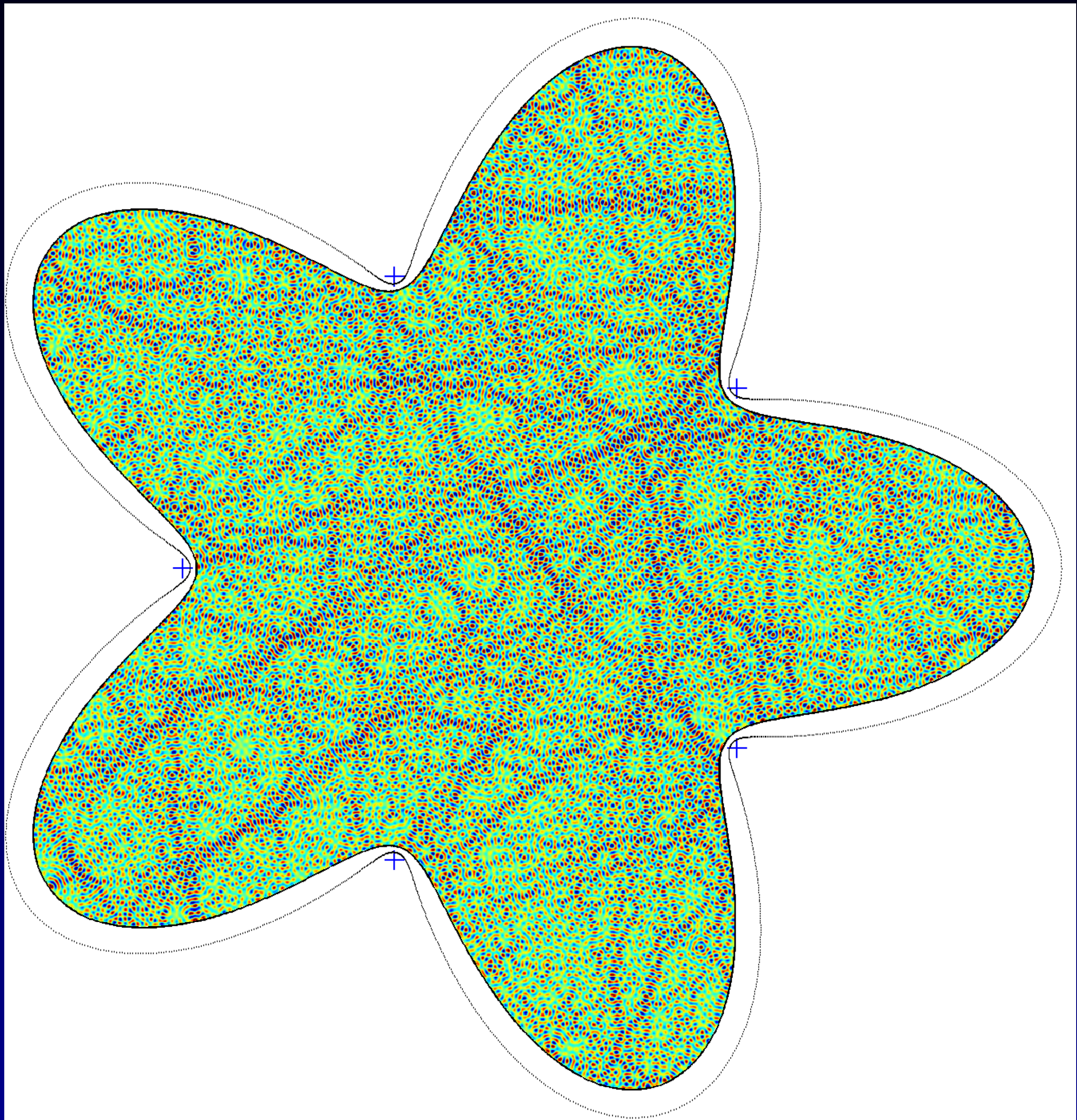




Singularity-adapted algorithm to choose charge points (N typ 3 ppw)

- # quadrature points on $\partial\Omega$ can be similar (*e.g.* 3 ppw if smooth)
- Compare 2 ppw to integral eqns (typ 10 ppw, or 5 for high-order)

High wavenumber Helmholtz interior BVP



165 wavelengths across
3.5 ppw
$\|u - f\|_{L^2(\partial\Omega)} = 10^{-11}$
26 sec (to get α)

B-Betcke, *in review*
J. Comput. Phys. '07

Back to eigenmodes: The Bottleneck

Reminder: to locate Dirichlet eigenvalues E_j with MPS...

- 'tension' $t(E) := \min_{u \in \mathrm{Span}\{\xi_i\}} \dfrac{\|u\|_{L^2(\partial\Omega)}}{\|u\|_{L^2(\Omega)}}$
- must search on frequency axis E for each minimum of $t(E)$
- if neighbours lie close one or more can be missed

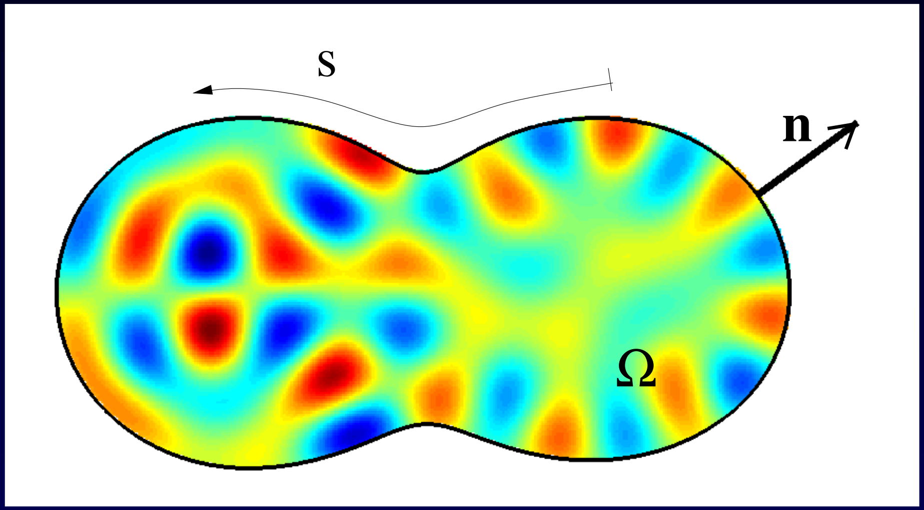
With the MPS you are 'lost on the frequency axis'

But you can bypass this search and vastly accelerate the method...

How to do better: the Dirichlet-to-Neumann map

Consider interior Dirichlet BVP for Helmholtz eqn:

$$\begin{aligned}(\Delta + E)u &= 0 \quad \text{in } \Omega \\ u &= U \quad \text{on } \partial\Omega\end{aligned}$$



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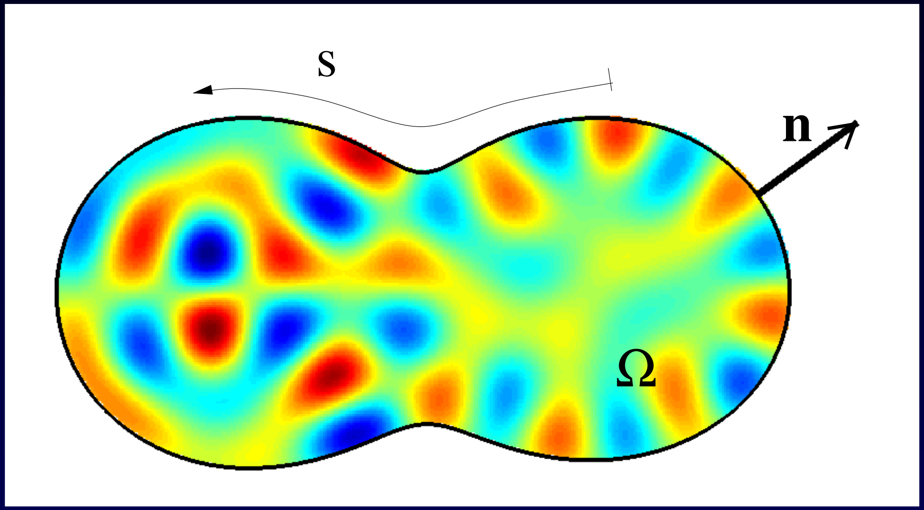

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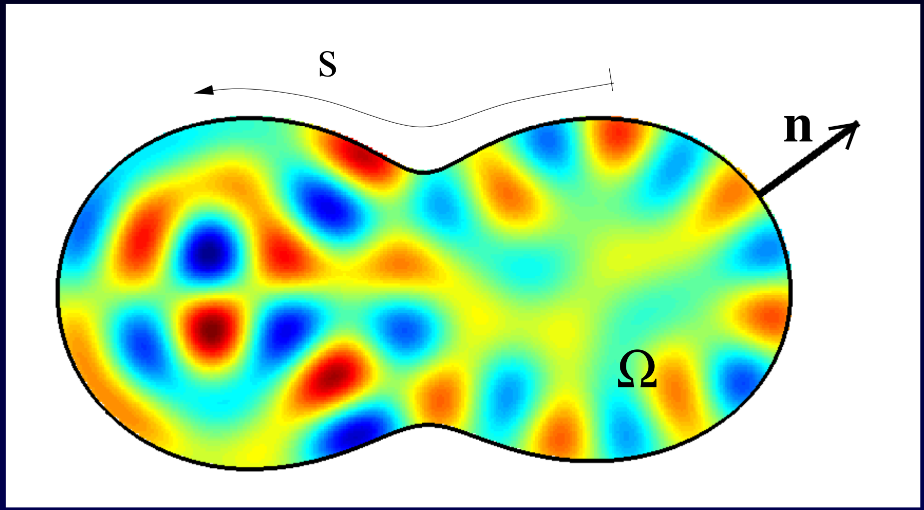
DtN operator $R = R(E)$ takes boundary data to normal derivative:

$$\boxed{\mathbf{n} \cdot \nabla u|_{\partial\Omega} =: \partial_n u = R\, u|_{\partial\Omega}}$$

Note R unbounded in L^2, for smooth domain $R : L^2(\partial\Omega) \to H^{-1}(\partial\Omega)$ bounded

How to do better: the Dirichlet-to-Neumann map

Consider interior Dirichlet BVP for Helmholtz eqn:



$$\begin{aligned}(\Delta + E)u &= 0 \quad \text{in } \Omega \\ u &= U \quad \text{on } \partial\Omega\end{aligned}$$

If $f \in L^2(\partial\Omega)$, and $E \notin \sigma_D$, unique solution u

DtN operator $R = R(E)$ takes boundary data to normal derivative:

$$\boxed{\mathbf{n} \cdot \nabla u|_{\partial\Omega} =: \partial_n u = R\,u|_{\partial\Omega}}$$

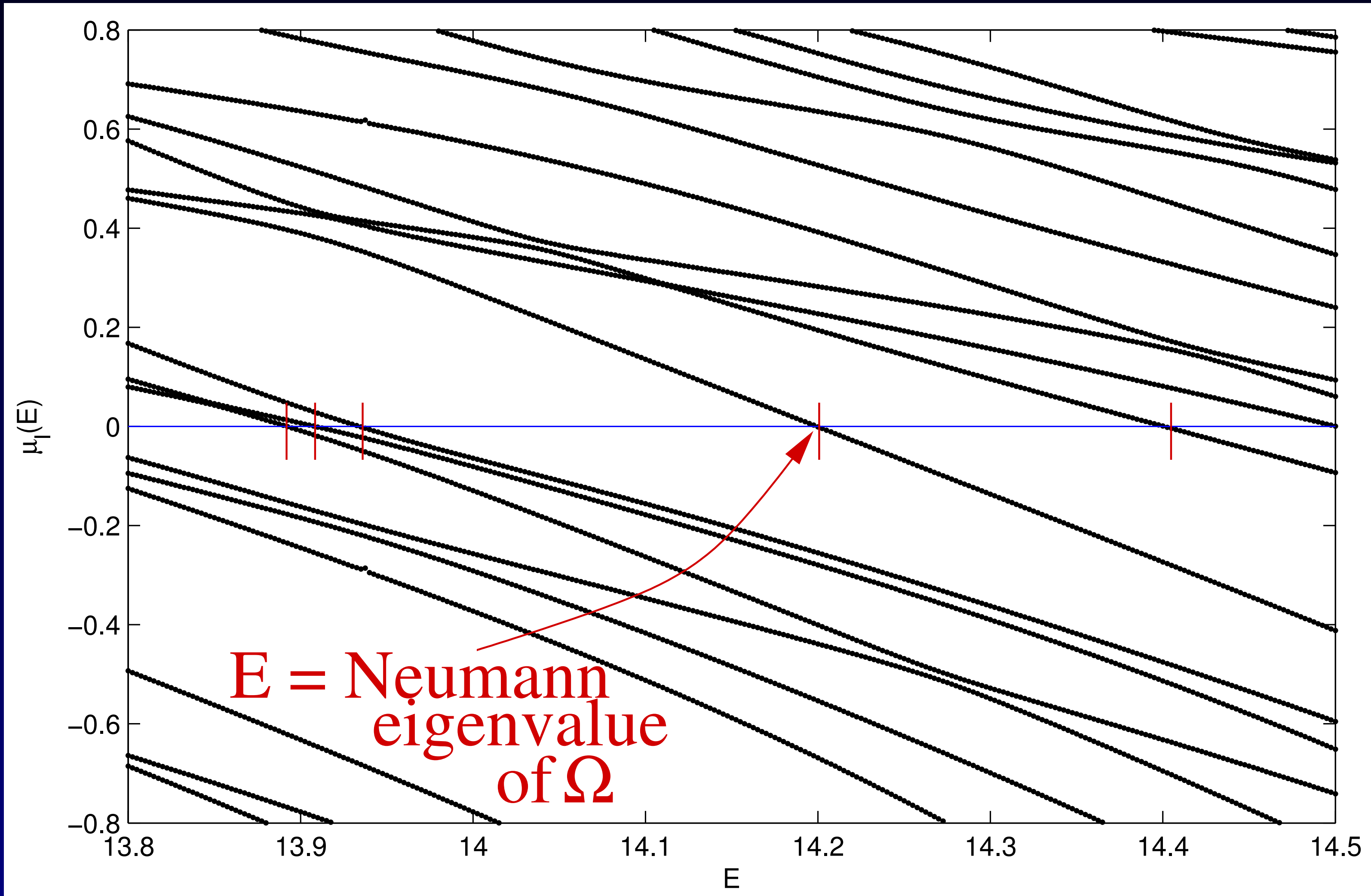
Note R unbounded in L^2, for smooth domain $R : L^2(\partial\Omega) \to H^{-1}(\partial\Omega)$ bounded

Let's take a visual tour of spectrum of operator R . . .

(numerical results done using MFS basis for interior BVP problem)

Eigenvalues of DtN map $R(E)$

$Rv = \mu v$ defines spectrum of R, depends on freq parameter E:

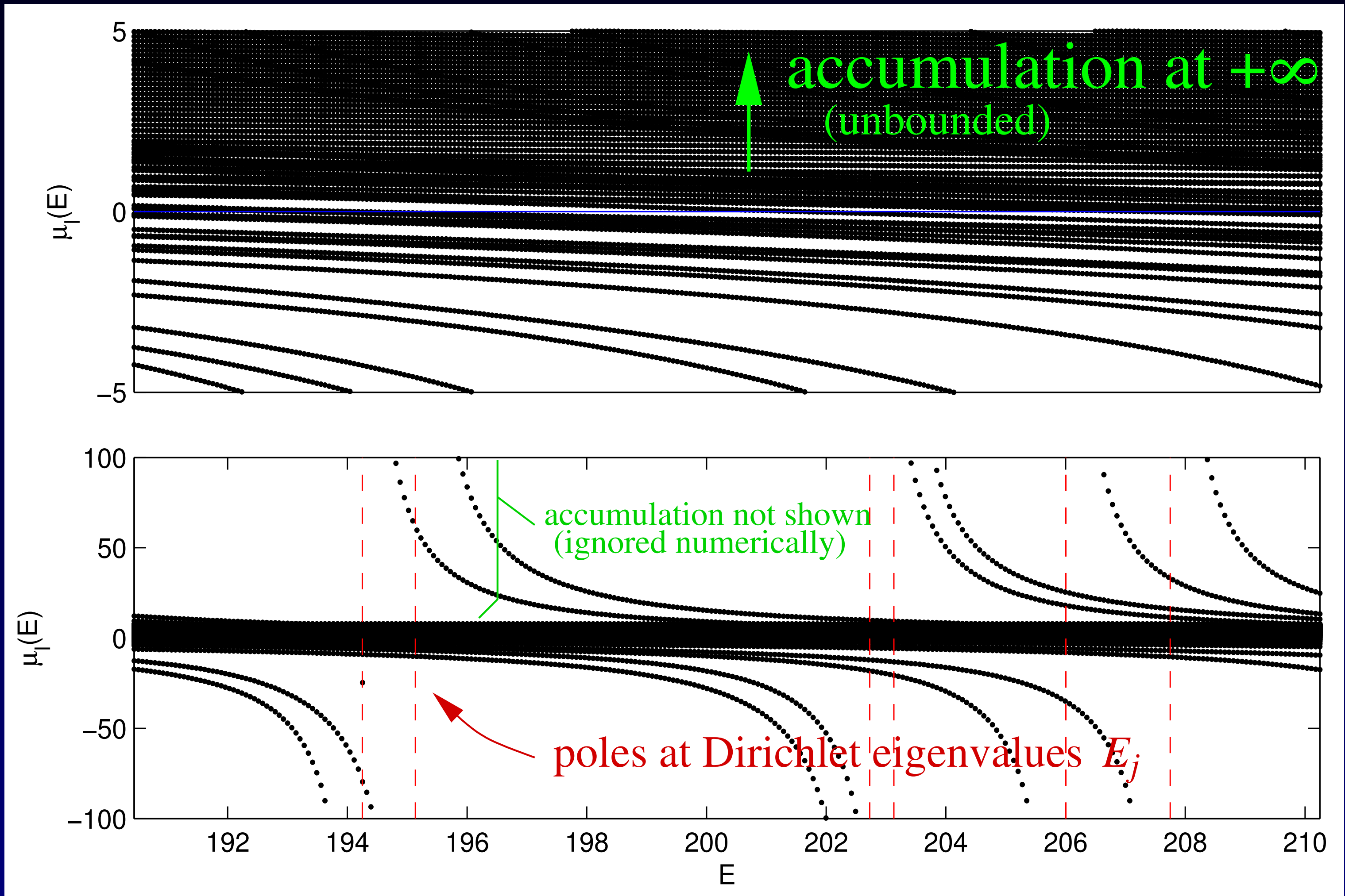


Why? At Neumann eigenvalue $\exists\ u|_{\partial\Omega}$ not identically zero but $\partial_n u \equiv 0$

Now zoom out to look at larger eigenvalues…

Larger eigenvalues of DtN map

R is semi-bounded from below (finite # of negative μ's) (Friedlander '91)

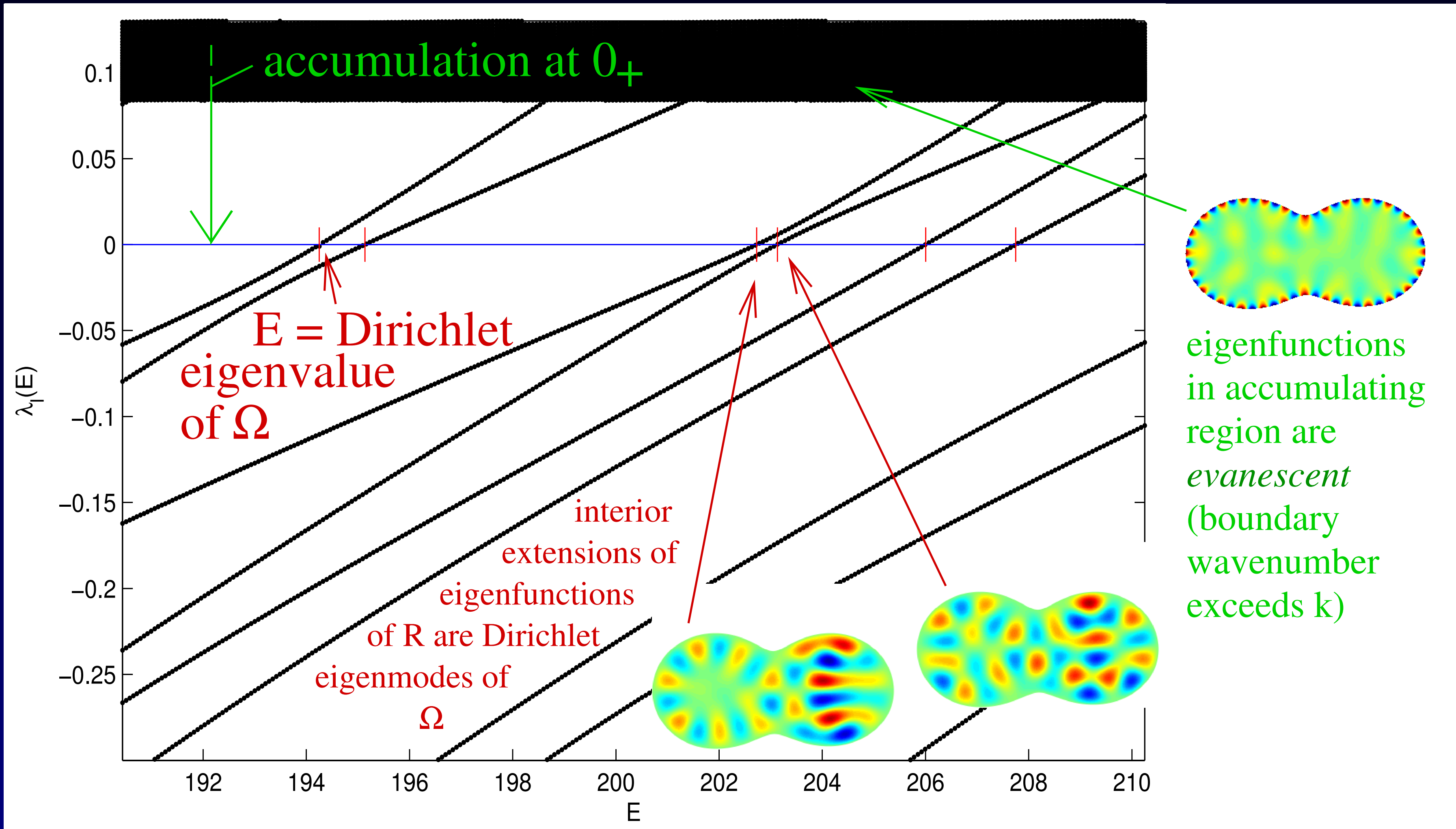


Why? At Dirichlet eigenvalue $\exists\ \partial_n u$ not identically zero but $u|_{\partial\Omega} \equiv 0$

($E = E_j$ gives nonunique BVP soln) Invert and look at $\lambda = 1/\mu \ldots$

Inverse eigenvalues λ of DtN map

$\lambda R(E)v = v$: Dirichlet eigenvalues E_j found where $\lambda(E) \to 0$:



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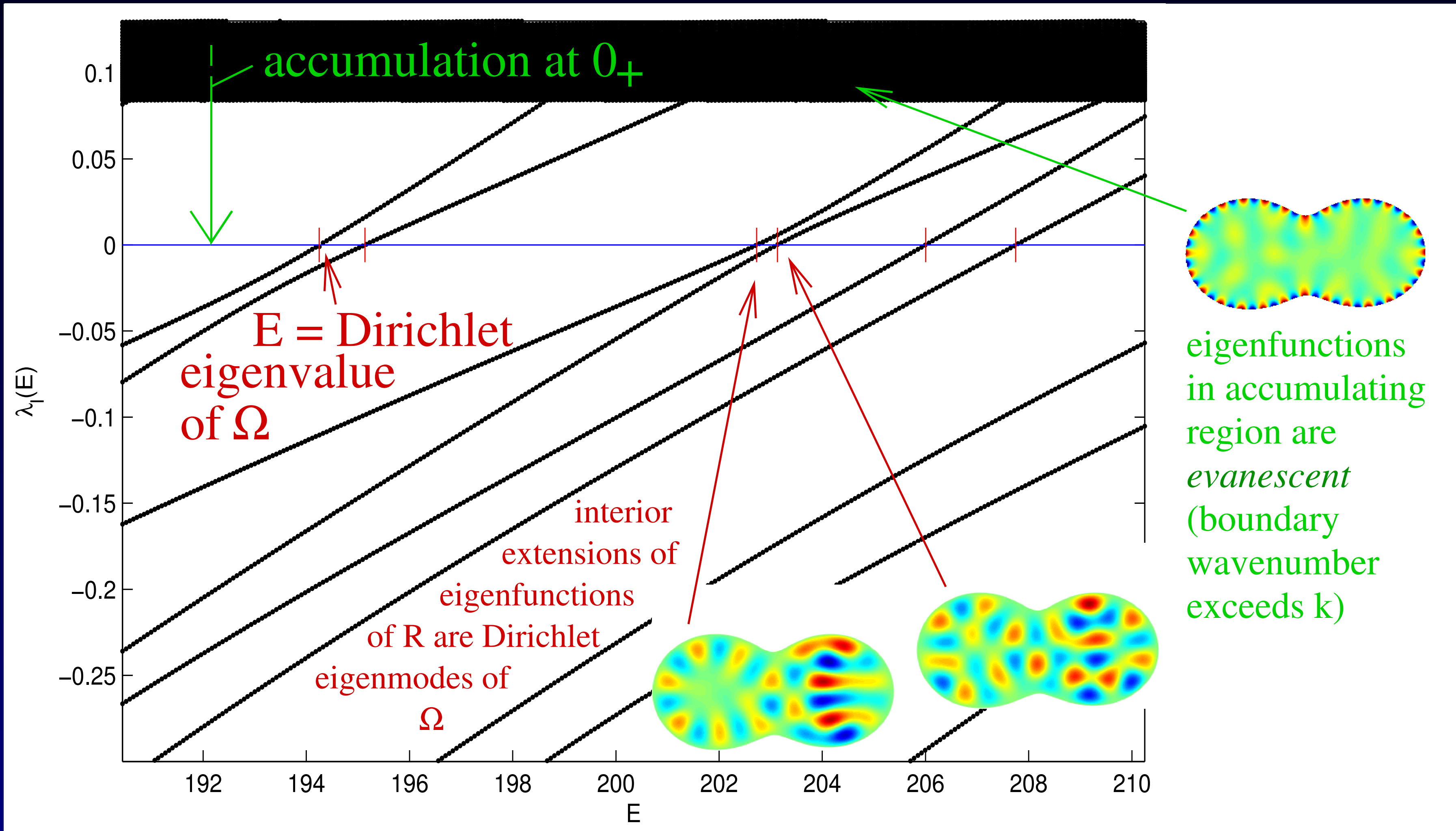
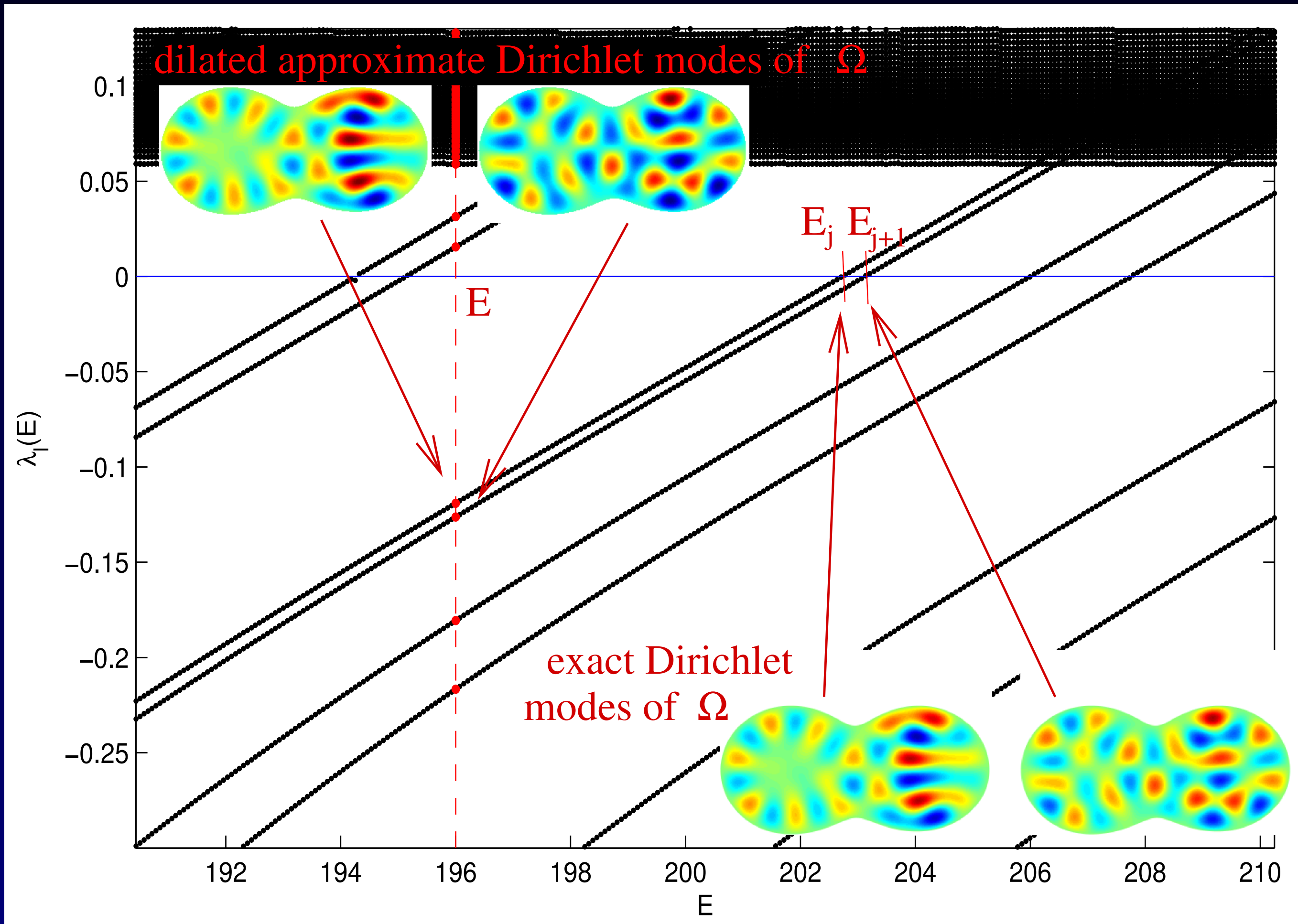


Linearize? But slopes vary with mode number j, $\lambda(E)$ strongly curved

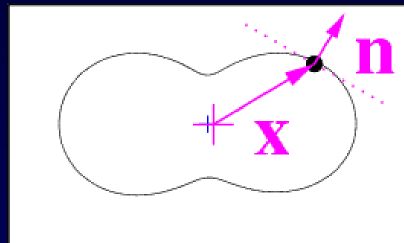
Wouldn't it be nice if all the slopes were known a priori?

Weighted DtN map: inverse eigenvalues λ

Premultiply R by weight function $\frac{1}{w}$, $\quad 0 < w \in L^1(\partial\Omega)$, boundary weight



$$\boxed{\lambda \frac{1}{w} R(E) v = v}$$



The weight

$$w = \frac{1}{\mathbf{x} \cdot \mathbf{n}}$$

is special!

Remarkably, slope when λ hits zero is: $\frac{d\lambda}{dE} = 1/2E_j, \quad \forall j$ *i.e.* predictable

As $E - E_j$ grows, extensions of eigenfuncs of R $\approx$ dilations of ϕ_j

Why is weight $w = (\mathbf{x} \cdot \mathbf{n})^{-1}$ special?

Helmholtz BVP solved by Poisson kernel $u(\mathbf{x}) = \int_{\partial\Omega} \partial_{n(s)} G(\mathbf{x}, s) u(s) ds$

$G(\mathbf{x}, \mathbf{y})$ is Green's func for Helmholtz eqn w/ Dirichlet BCs on $\partial\Omega$

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- mode expansion $G(\mathbf{x}, \mathbf{y}) = \sum_{j=1}^{\infty} \frac{\phi_j(\mathbf{x})\phi_j(\mathbf{y})}{E - E_j}$

Define weighted mode normal derivatives $\psi_j(s) := \frac{1}{w(s)} \partial_n \phi_j(s)$, then

$$\frac{1}{w} R(E) = \sum_{j=1}^{\infty} \frac{\psi_j \langle \psi_j, \cdot \rangle}{E - E_j}$$

sum of rank-1 operators, each with pole in E

w-weighted inner prod $\langle U, V \rangle := \int_{\partial\Omega} wUV\, ds$, norm $\|U\|_w^2 := \langle U, U \rangle$

(unweighted version appeared in Nachmann-Sylvester-Uhlmann '88)

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- Lemma: let $w = (\mathbf{x}\cdot\mathbf{n})^{-1}$, then $\|\psi_m\|_w^2 = 2E_m$ (Rellich '40)

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More subtle reason: perturbation theory in $\varepsilon := E - E_m$ gives

$$\left.\frac{dv}{d\varepsilon}\right|_{\varepsilon=0} = \sum_{j\neq m} \frac{Q_{mj}}{E_m - E_j} \psi_j + \big(\text{higher order}\big)$$

with 'mode coupling' $Q_{ij} := \langle \psi_i, \psi_j \rangle$

Q_{ij}: quasi-orthogonality on $\partial\Omega$

(B, math-ph/0601006)

Exact orthogonality in interior $\int_\Omega \phi_i \phi_j d\mathbf{x} = \delta_{ij}$

But, approx orthogonality on boundary! $Q_{ij} := \int_{\partial\Omega} \mathbf{x}\cdot\mathbf{n}\, \partial_n\phi_i\, \partial_n\phi_j\, ds$

Rellich gives $Q_{ij} = 2\delta_{ij}E_j + q_{ij}$ with $q_{jj} = 0$

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- assumption (Vergini '94): off-diag terms grow $|q_{ij}| \sim |E_i - E_j|$
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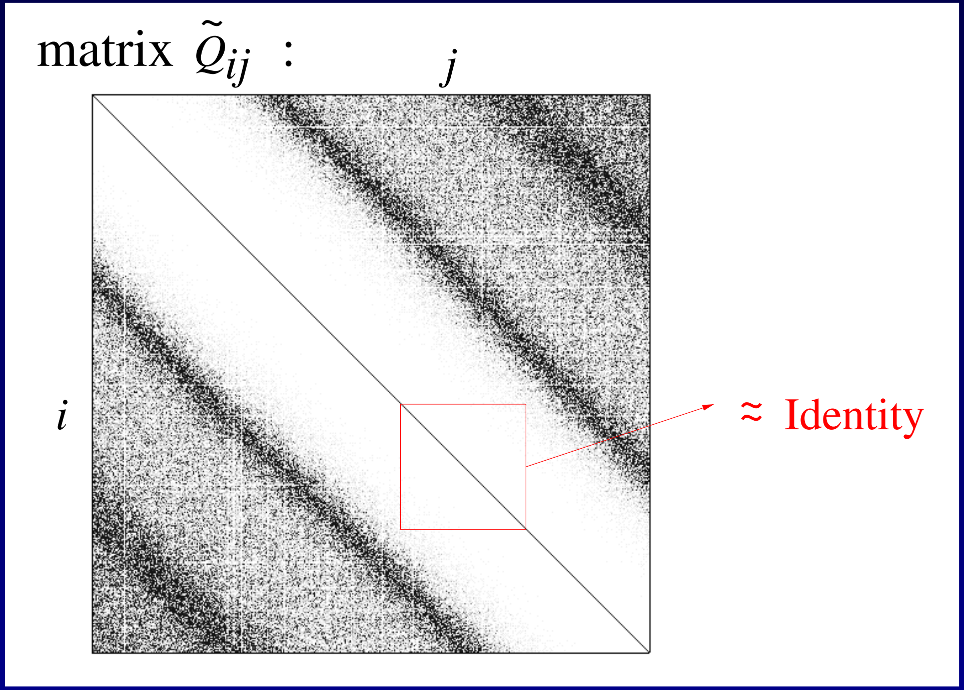
- Thm : (B) for *all* bounded piecewise-smooth Ω, $|q_{ij}| \leq C_\Omega (E_i - E_j)^2$



very small size of Q_{ij} close to the diagonal responsible for small perturbations in DtN eigenfunctions

Scaling method

fix an origin, $w = \frac{1}{\mathbf{x}\cdot\mathbf{n}}$; Ω star-shaped

Pick freq E, choose good Helmholtz basis set $\{\xi_i\}$ ... as with MPS

Inverse eigenvals. λ of $\frac{1}{w}R$ are extrema of $\dfrac{\|U\|_w^2}{\langle U, \frac{1}{w}RU\rangle}$ Rayleigh quotient

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quotient becomes $\frac{\boldsymbol{\alpha}^T F \boldsymbol{\alpha}}{\boldsymbol{\alpha}^T G \boldsymbol{\alpha}}$, extremized via gen. eig. prob. $F\boldsymbol{\alpha} = \lambda G \boldsymbol{\alpha}$

matrix elements $F_{ij}(E) = \int_{\partial\Omega} w \xi_i \xi_j ds$, $G_{ij}(E) = \int_{\partial\Omega} \xi_i \partial_n \xi_j ds +$ transpose

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Once GEP solved at a given freq E ...

Each small gen. eigval. λ_l gives a Dirichlet eigval. $E_j \approx E(1 - \lambda_l)$

Eigenvec. $\boldsymbol{\alpha}^{(l)}$ gives basis rep. of eigenmode $\phi_j \approx \sum_{i=1}^N \alpha_i^{(l)} \xi_i(E_j)$

- all modes in $O(1)$ k-window found (*e.g.* $k_j \in [99.9, 100.1]$) via single GEP

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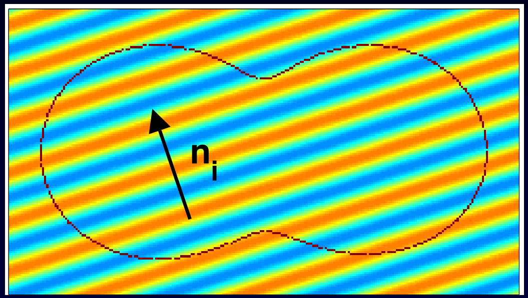
- all modes in $O(1)$ k-window found (*e.g.* $k_j \in [99.9, 100.1]$) via single GEP
- observe errors in E_j grow as $O(E-E_j)^3$ rigorous analysis ongoing
- variant of little-known method from quantum physics (Vergini-Saraceno '94)

Global basis functions (as in MPS)



Plane waves

Practice: fail to capture the field singularities outside Ω (coeff sizes $|\boldsymbol{\alpha}| \gg 10^{16}$)

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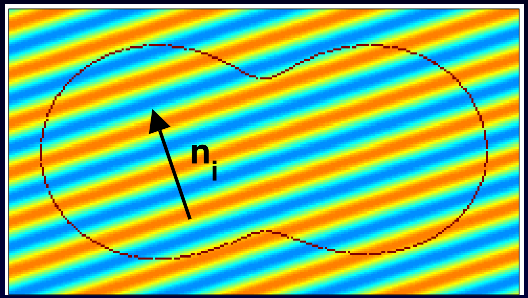

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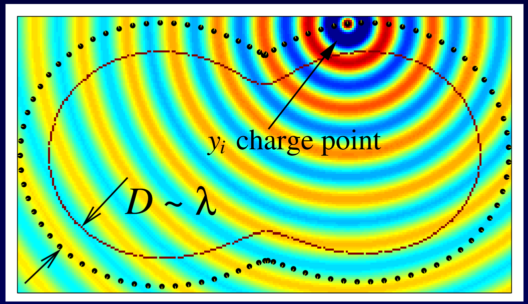

Fundamental solutions (MFS)

Practice: excellent apart from re-entrant corners

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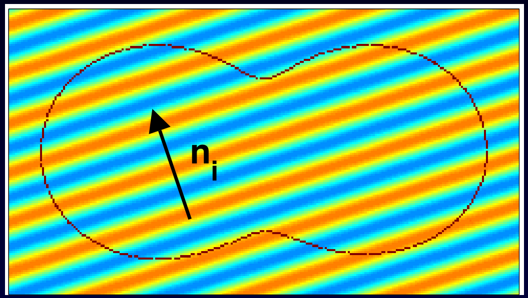

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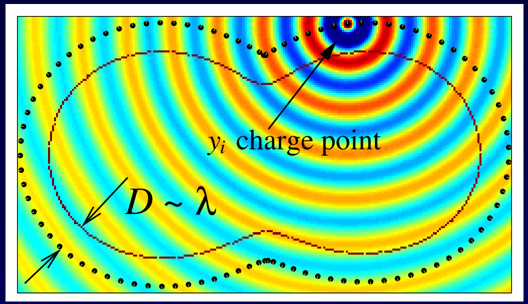

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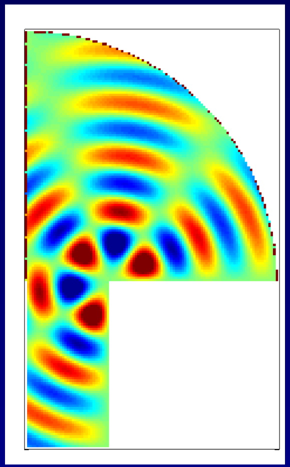


Corner-adapted Fourier-Bessel $J_{\beta l}(kr)\sin(\beta l\theta)$

for singular corner $\theta = \pi/\beta$, $\beta \notin \mathbb{Z}$

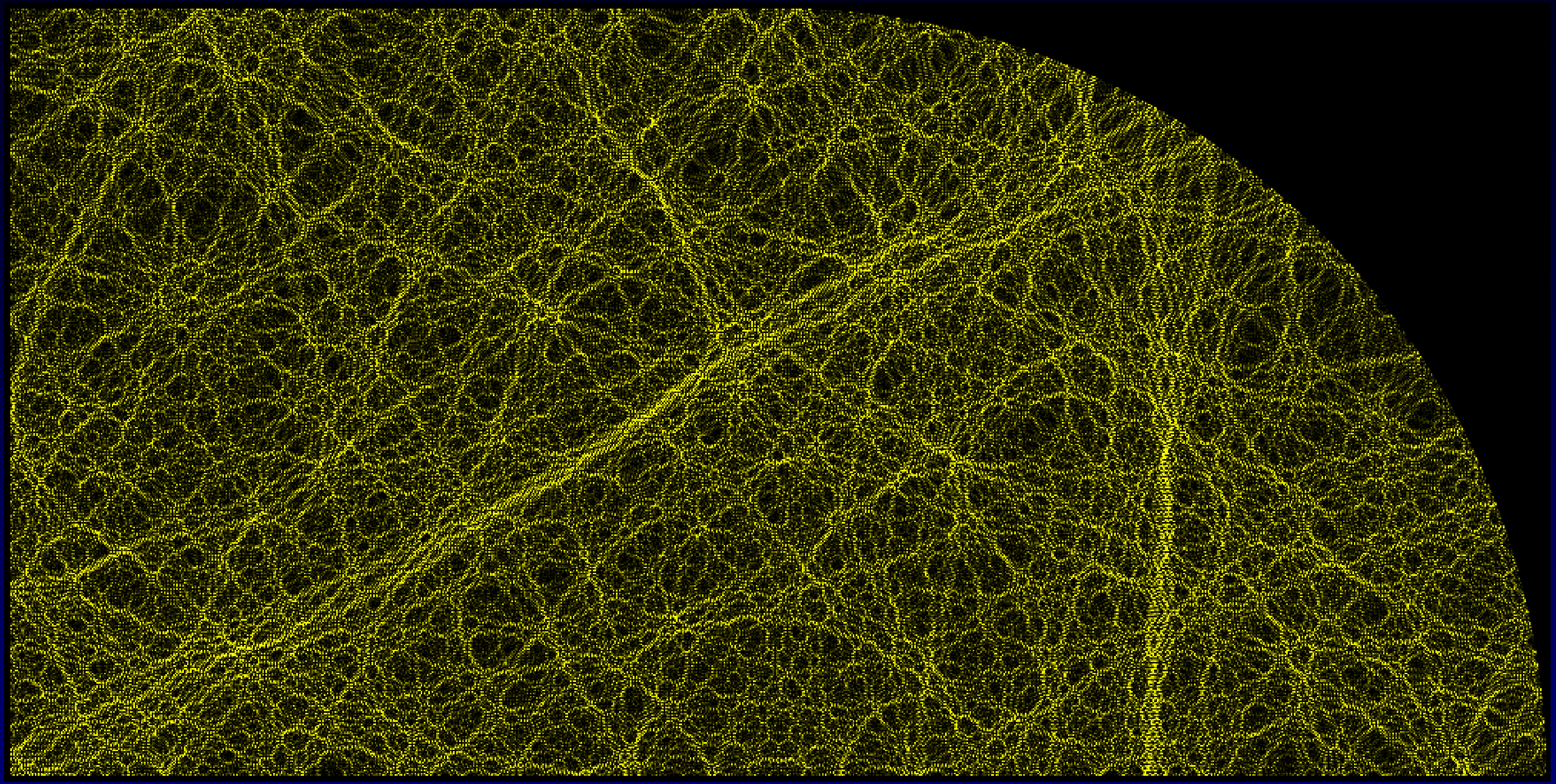
Scaling currently cannot handle > 1 singular corner

(dilated modes must be well approximated)

Note: basis size $N \approx 2$ per wavelength ($k \gg 1$)

High wavenumber example

convex (quarter stadium; plane-wave basis)



- $k = 10^3$, size 300λ, 1 sec laptop CPU time per mode, error $t \approx 10^{-4}$
- speedup vs MPS is 10^3 if only bdry values needed

Applications: Quantum ergodicity

Q: If ray dynamics completely *chaotic* (hyperbolic) in Ω…
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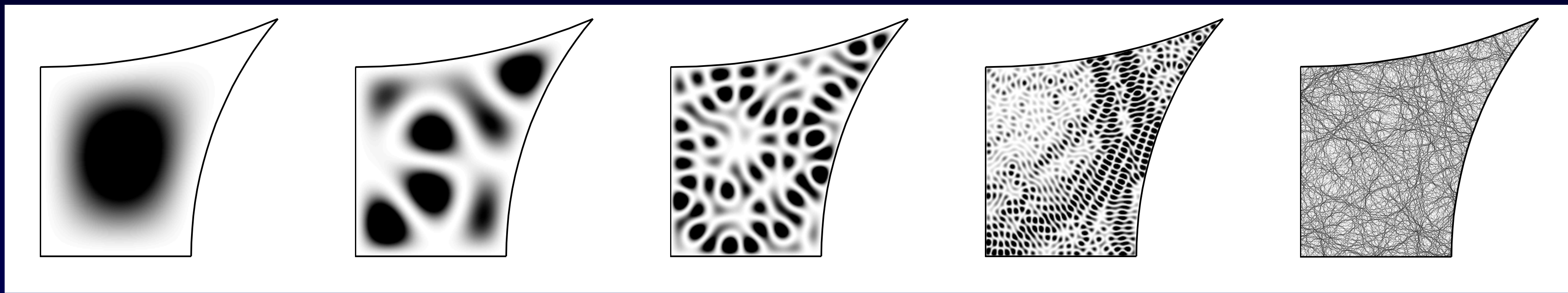


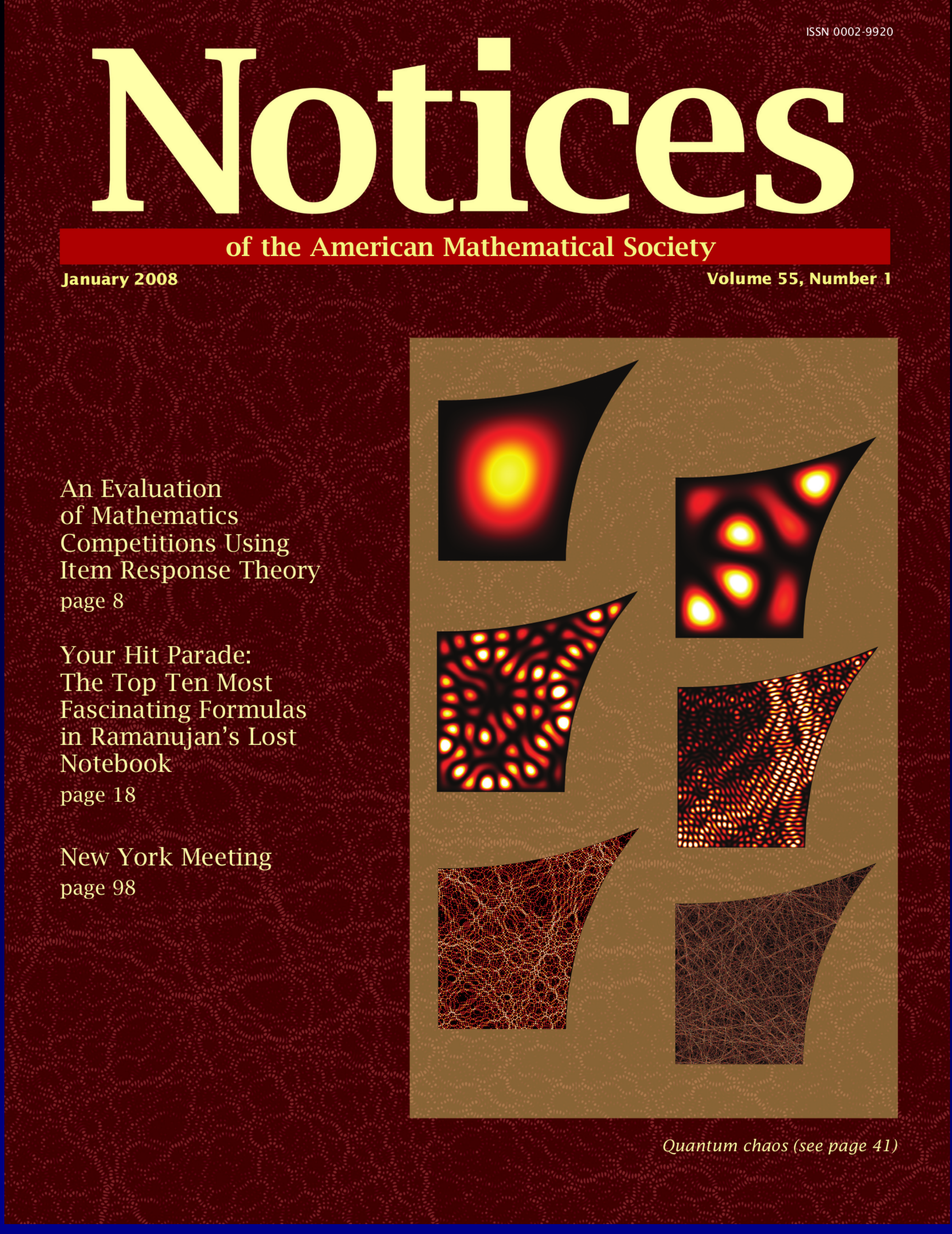
$j = 1$ $\quad$ $j = 10$ $\quad$ $j = 10^2$ $\quad$ $j = 10^3$ $\quad$ $j \approx 5 \times 10^4$

- compute 3×10^4 modes up to $j \sim 10^6$: a few CPU-days
- fundamental solns basis, asymptotically 3 ppw, use 4-fold symmetry

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

…also no exceptional modes 'scarred' (condensing) on periodic orbits

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



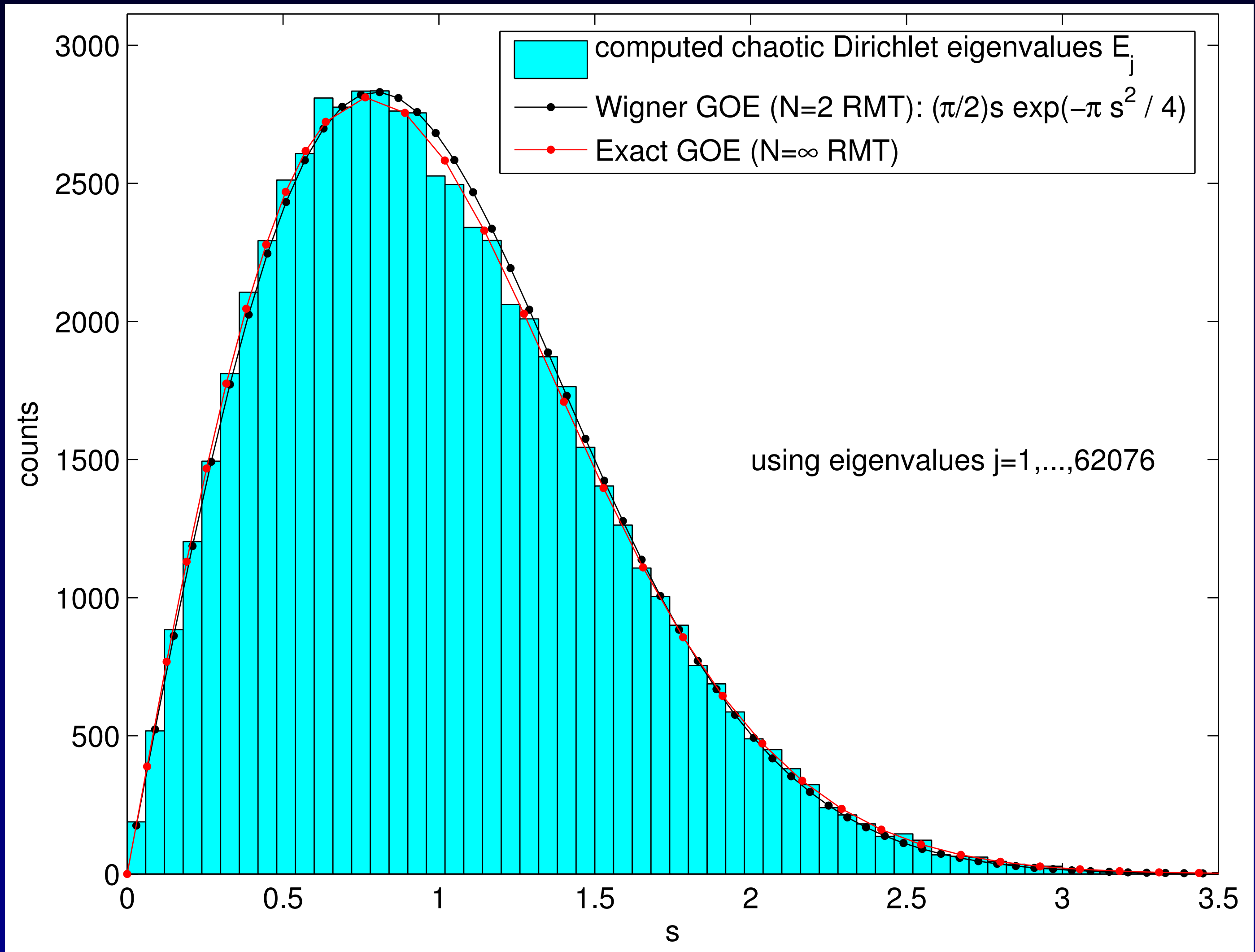
mode numbers $j = 1, 10, 10^2, 10^3, 10^4, 10^5$

background: random plane waves

Ergodic eigenvalues and random matrices

nearest-neighbor spacings $s_j := E_{j+1} - E_j$

Conjectured (unproven): has same pdf as in random matrices (RMT)



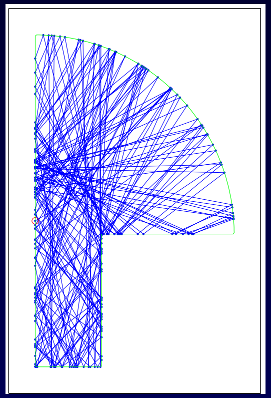
well-known, not well tested before in ergodic cavity

(*About the Cover*, Notices AMS, Jan '08)

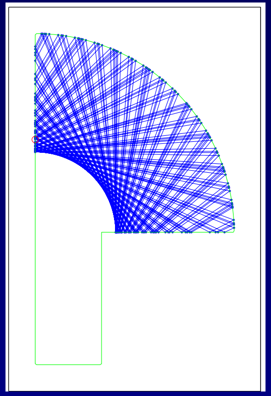
Application: Mushroom

(B-Betcke, CHAOS, Dec '07)

Unusually simple
divided phase space
(Bunimovich '01)



ergodic rays



regular rays

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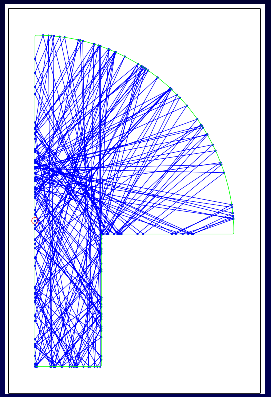

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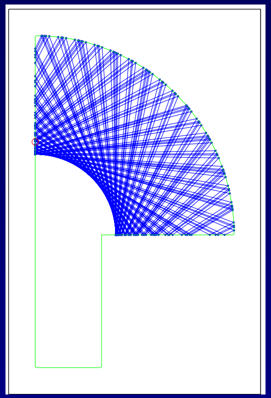
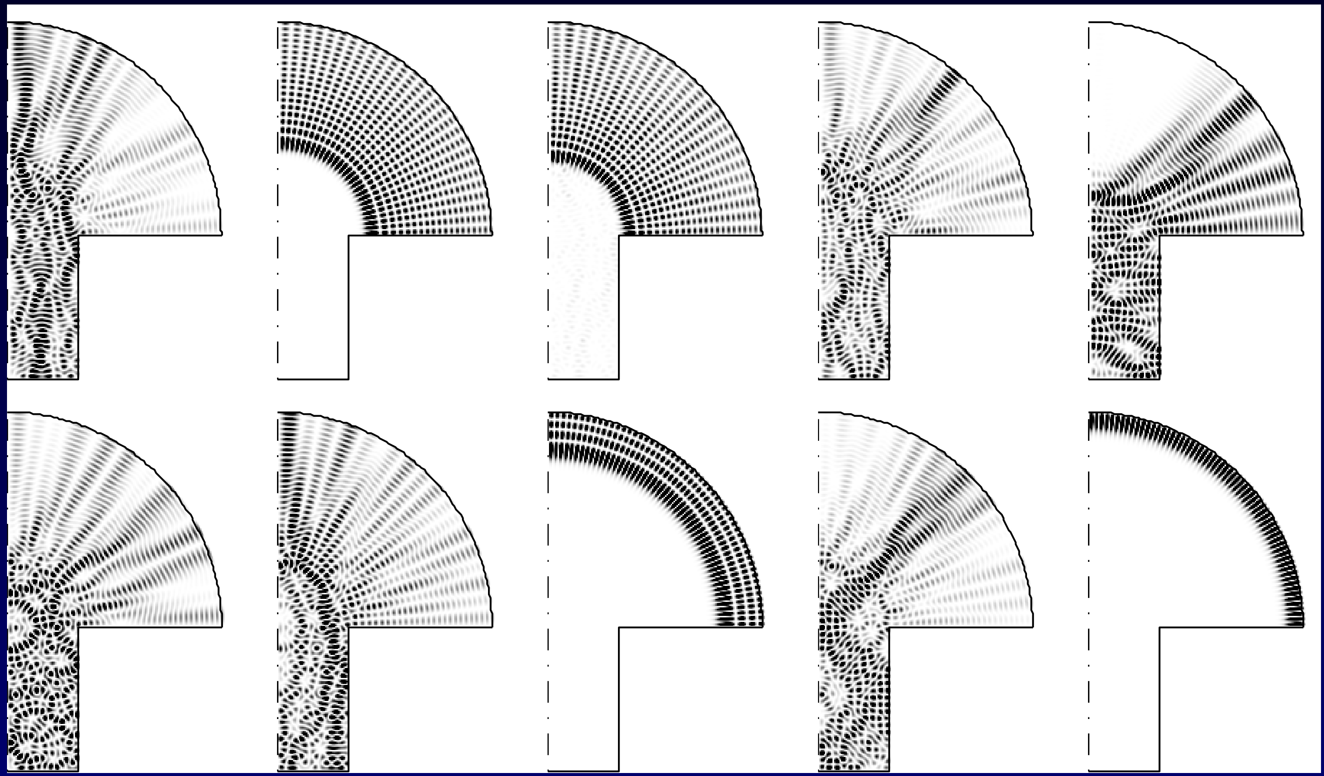


regular rays

First calculation of high-freq modes: $j = 1, \ldots, 16061$



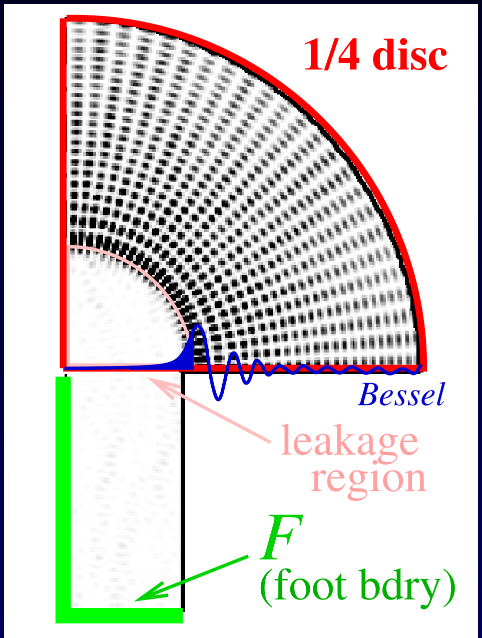
- Conjecture verified (Percival '73):

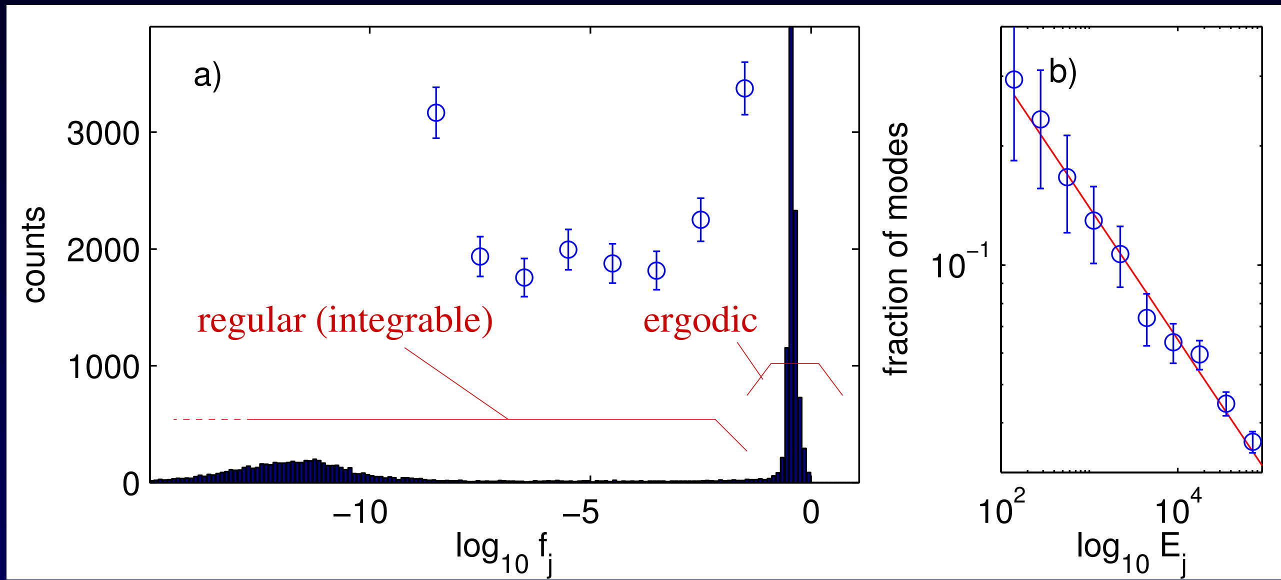
  modes localize to either regular or chaotic region

  44% are regular (cf regular phase space frac 45%)

Dynamical tunneling in the mushroom

All ‘regular’ modes have (exponentially) small ergodic component…





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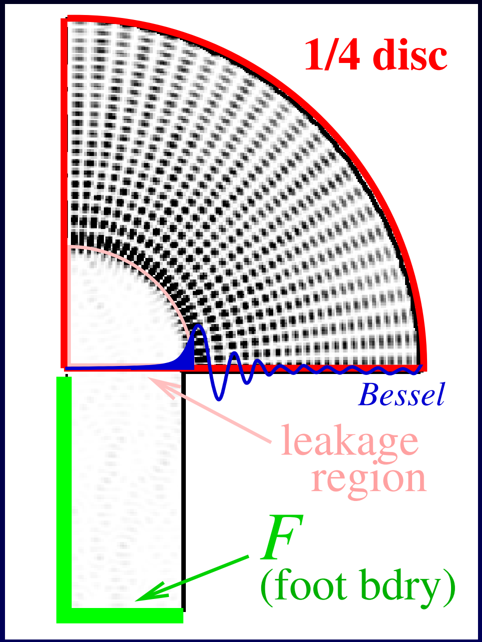

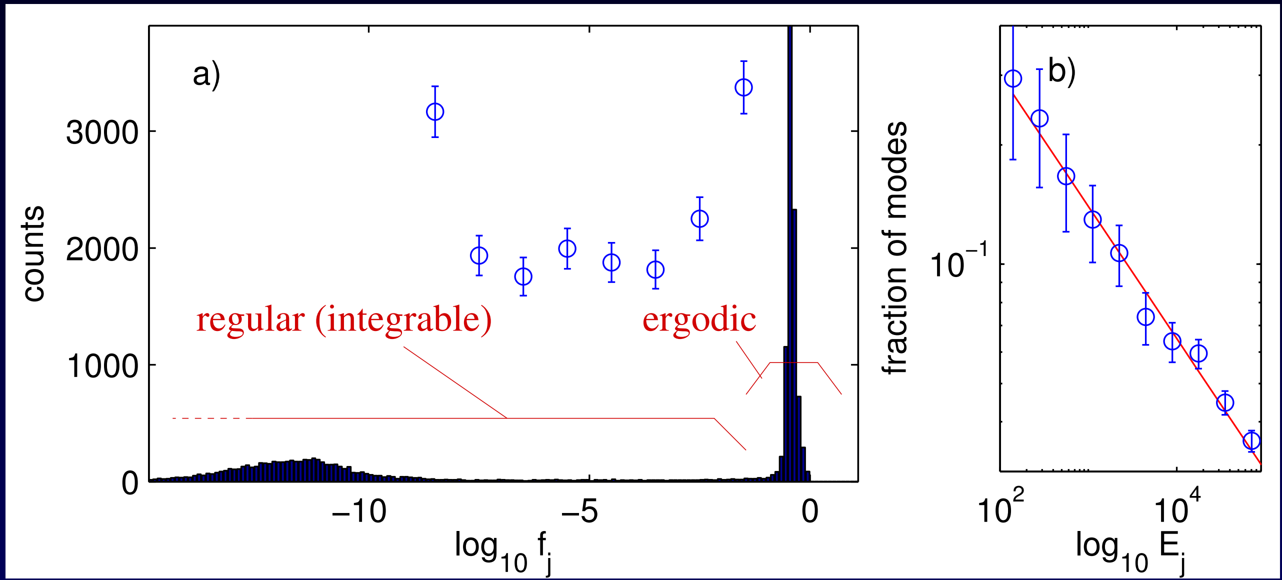

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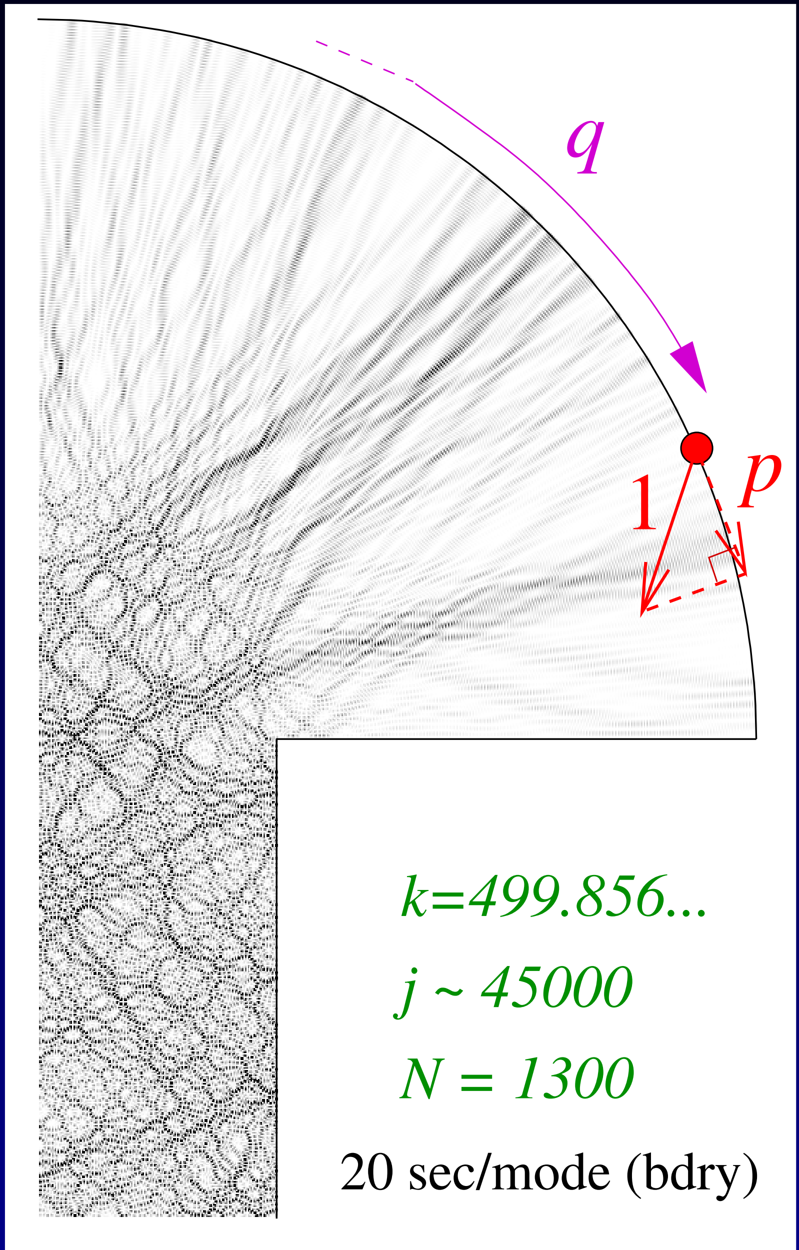
Find numerically: occurrence of f_j in given interval dies $\sim E_j^{-1/3}$

- predicted by Bessel asymptotics and heuristic leakage model
- (Bäcker et al. '08) improved fictitious system model (w/ our numerics)

High-lying ergodic mode & boundary coords



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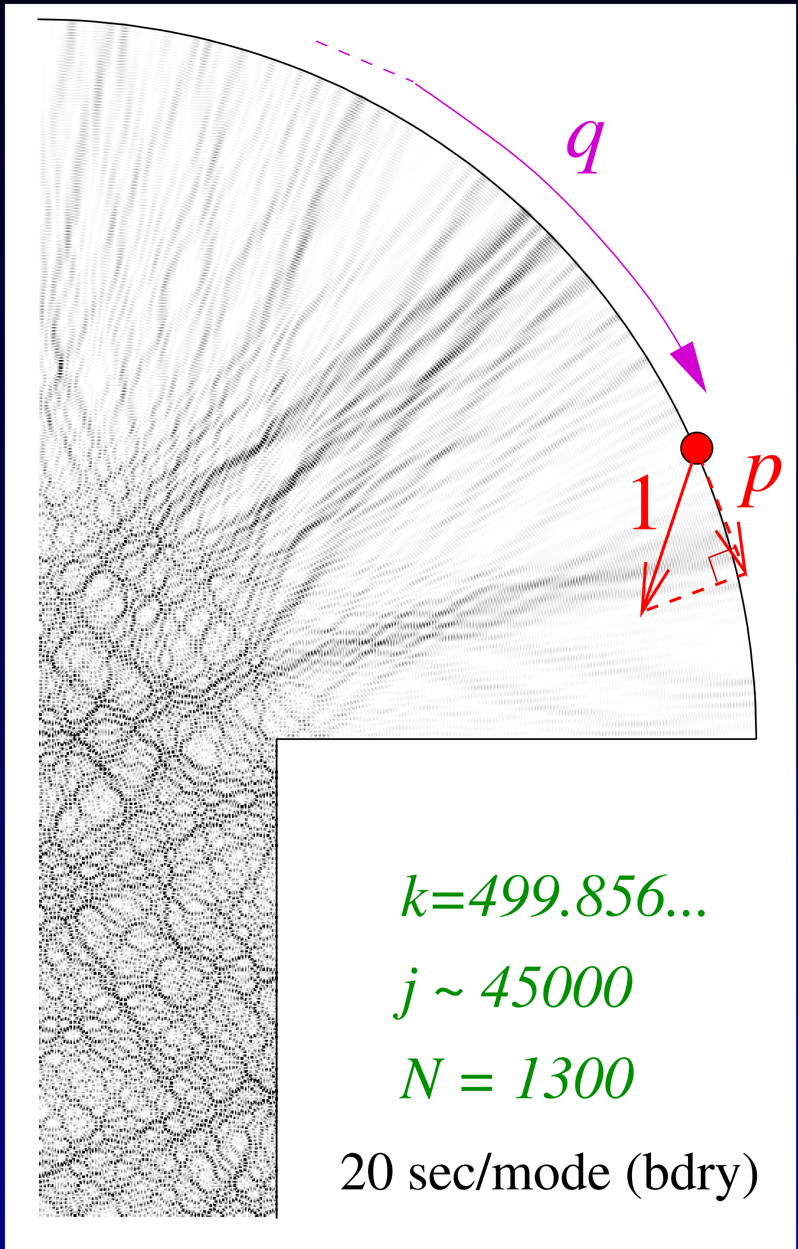
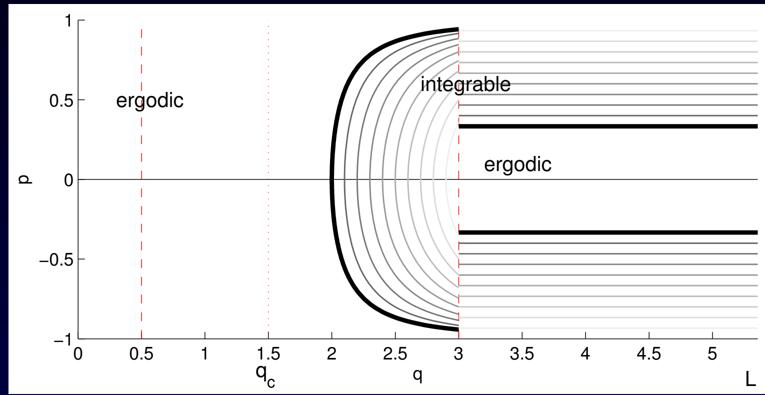
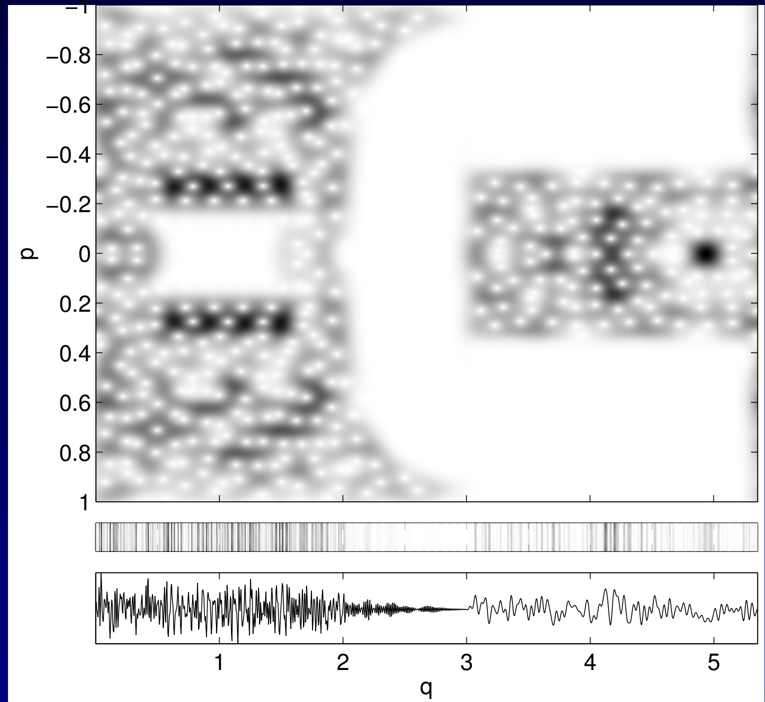




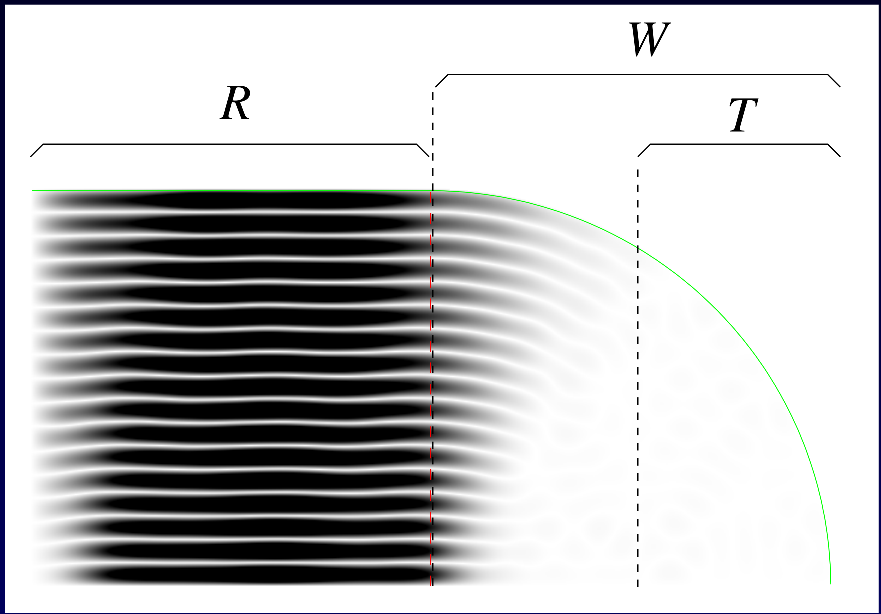


Husimi func on boundary: scarred

Bouncing ball modes

(ongoing, w/ A. Hassell, ANU)

seq. condensing on neutral family (region R): observed, but unproven



$\exists$ trivial $O(1)$ quasimode in R

Zworski's challenge:
construct $o(1)$ quasimode!
(mass in wing W must > 0)

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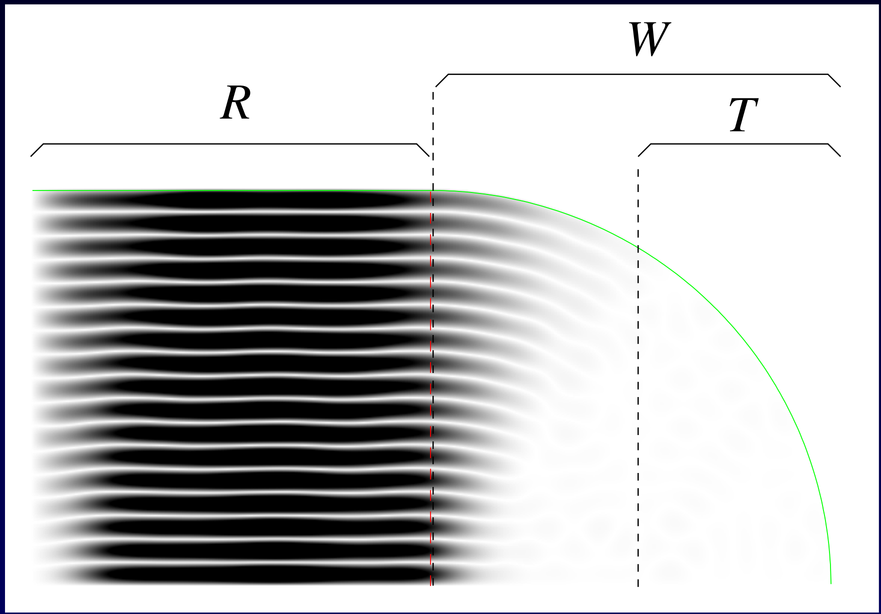

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(mass in wing W must > 0)

Proven: mass in W has lower bnd CE_j^{-2} (Burq-Hassell-Wunsch '07)

We conjecture (numerical evidence): lower bnd is actually $CE_j^{-3/4}$

- curious since matches Born-Oppenheimer adiabatic approx.
- architectural clues in modes w/ low mass in wing tip T: radial tendency

Conclusion

Global approx by fundamental solutions (MFS)...

- Spectral convergence, understand coeff. blow-up, 2 ppw

'Scaling' accel by $O(k)$: linearizing DtN map...

- Complexity $O(k^2) = O(N^2)$ per mode (w/ dense lin. alg.)
- Fastest eigenmode method known by factor 10^3 at high freq

Ongoing:

- MFS/MPS for scattering (w/ T. Betcke)
- photonic crystal band structure (w/ L. Greengard)
- MFS for graded-index materials: fund. soln. to $(\Delta + E + x_1)$ known

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P. Deift (NYU)
L. N. Trefethen (Oxford)
T. Betcke (Manchester)

Funding: NSF (DMS-0507614)

Preprints, talks, movies:
http://math.dartmouth.edu/~ahb

made with: Linux, LaTeX, Prosper

MPS is E-derivative of our DtN map!

Define operator $A(E)$ by $\langle U, AU\rangle = \|u\|^2_{L^2(\Omega)}$ bounded for $E \notin \sigma_D$

MPS can be written $t(E) =$ lowest inverse eigenvalue: $\lambda_A A(E)v = v$

Proposition: $A = -\frac{1}{w}\frac{dR(E)}{dE}$

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Fixing U, write $u' := du/dE$, u is interior soln. (trick from Friedlander '91)

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(\Delta + E)u' &= -u \qquad \text{mult by u and integrate} \\
\int_\Omega u(\Delta + E)u' &= -\int_\Omega u^2 \;:=\; -\langle U, AU\rangle \\
\text{LHS by Green's identity} &= \int_{\partial\Omega} u\partial_n u' - \int_{\partial\Omega} u'\partial_n u - \int_\Omega u'(\Delta + E)u \\
&= \int_{\partial\Omega} U \frac{d}{dE}\partial_n u \;=\; \langle U, \tfrac{1}{w}R'(E)U\rangle
\end{aligned}$$

- So A has 2nd-order pole at each E_j:

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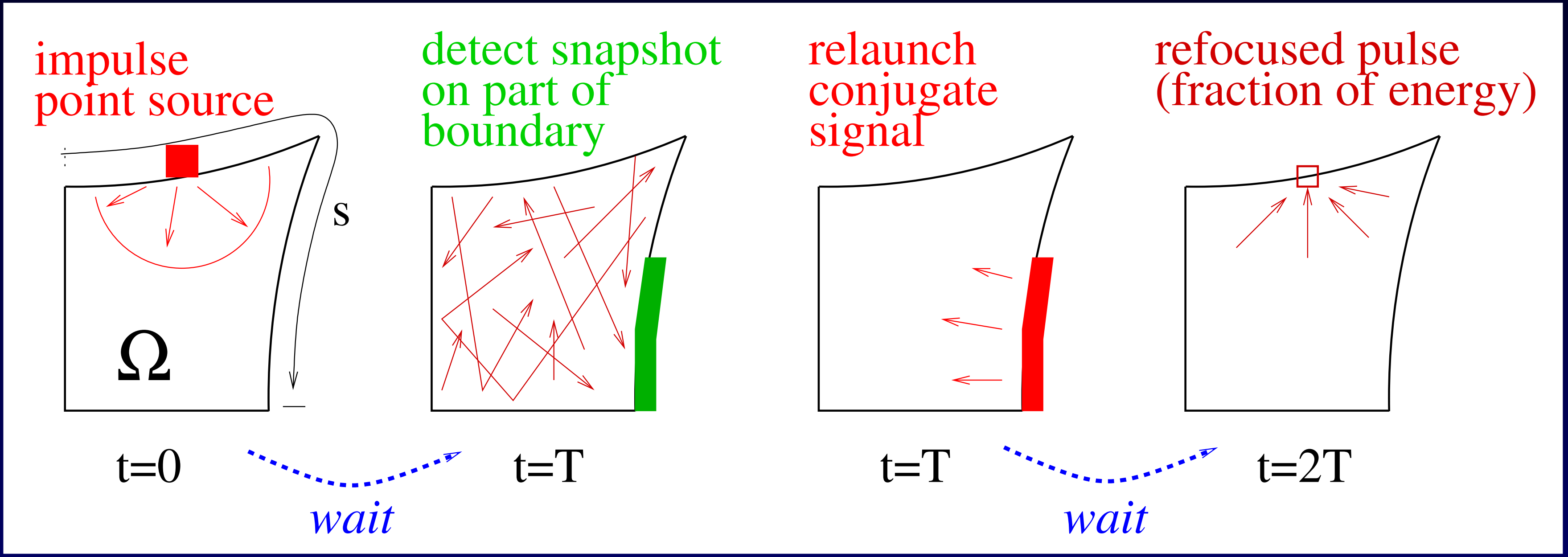
Thm (B '04): $\lambda_A(E) = \frac{1}{\|\psi_j\|^2_w}(E-E_j)^2 + O(E-E_j)^4$

pert. theory of $A(E)$ is easier than $R(E)$ since bnded in $L^2(\Omega)$

App: time-reversed waves in chaotic cavity

(idea of G. Bal)

Wave equation $u_{tt} = \Delta u$ in Ω, Dirichlet BCs



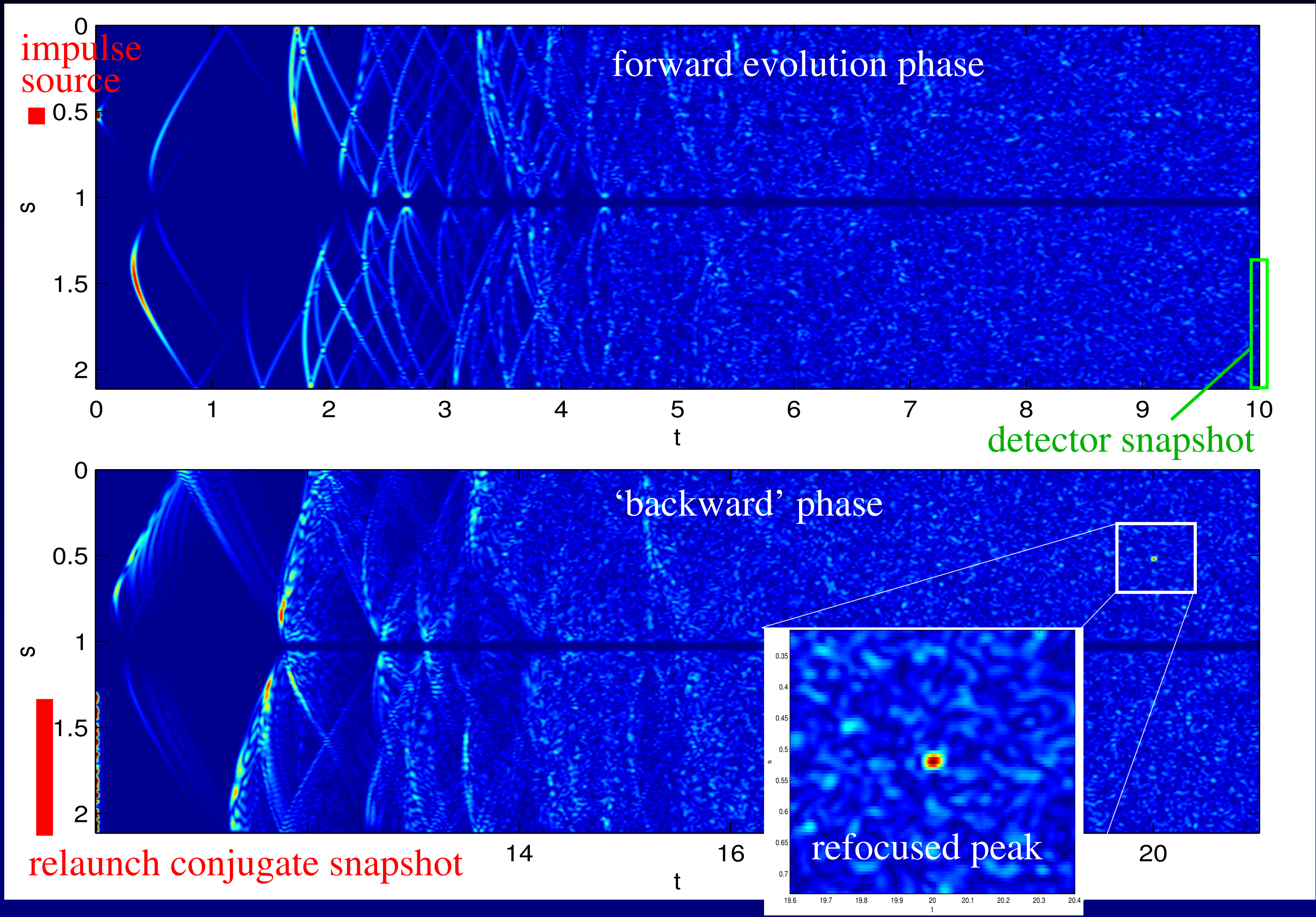
- Why? Disordered media, ultrasound, unscrambling, imaging…
- Chaotic Ω gives best resolution (1-channel expt, Draeger-Fink '99)

Eigenmodes cheap: use as basis expansion (a Victorian dream!)

- instant evolution for very long times, *no dispersion errors*

Numerical demonstration

basis of 4300 modes $\partial_n \phi_j$ via scaling



- intermediate times (and unused locations) need not be computed!

Issues: improve upon Draeger-Fink random-wave theory…