High-frequency cavity modes: efficient computation and applications

Oxford University Computing Laboratory, 9 June, 2005

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Thanks to J. Goodman, L. Greengard, P. Deift, P. Sarnak (NYU), H. Tureci (Yale), N. Trefethen, T. Betcke (Oxford), . . .

Dirichlet eigenproblem

Normal modes of elastic membrane or 'drum' (Helmholtz, Germain, 19^{th}C)
Eigenfunctions ϕ_j of Laplacian Δ in bounded domain $\Omega \subset \mathbb{R}^d$

$$-\Delta\phi_j = E_j\phi_j, \qquad \phi_j|_{\partial\Omega} = 0 \ \text{Dirichlet BC} \qquad \int_\Omega \phi_i\phi_j = \delta_{ij}$$

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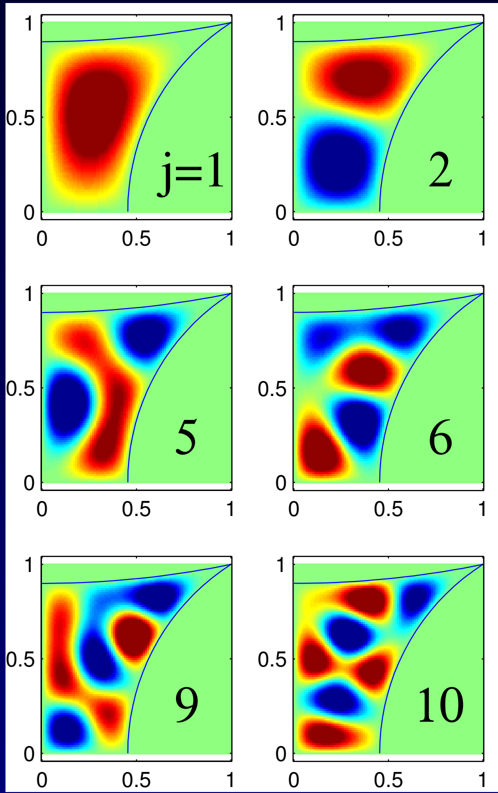

... ∞

mode $j = 1 \cdots \infty$

‘energy’ eigenvalue E_j

wavenumber $k_j = E_j^{1/2}$

wavelength $= 2\pi/k_j$

focus on d=2

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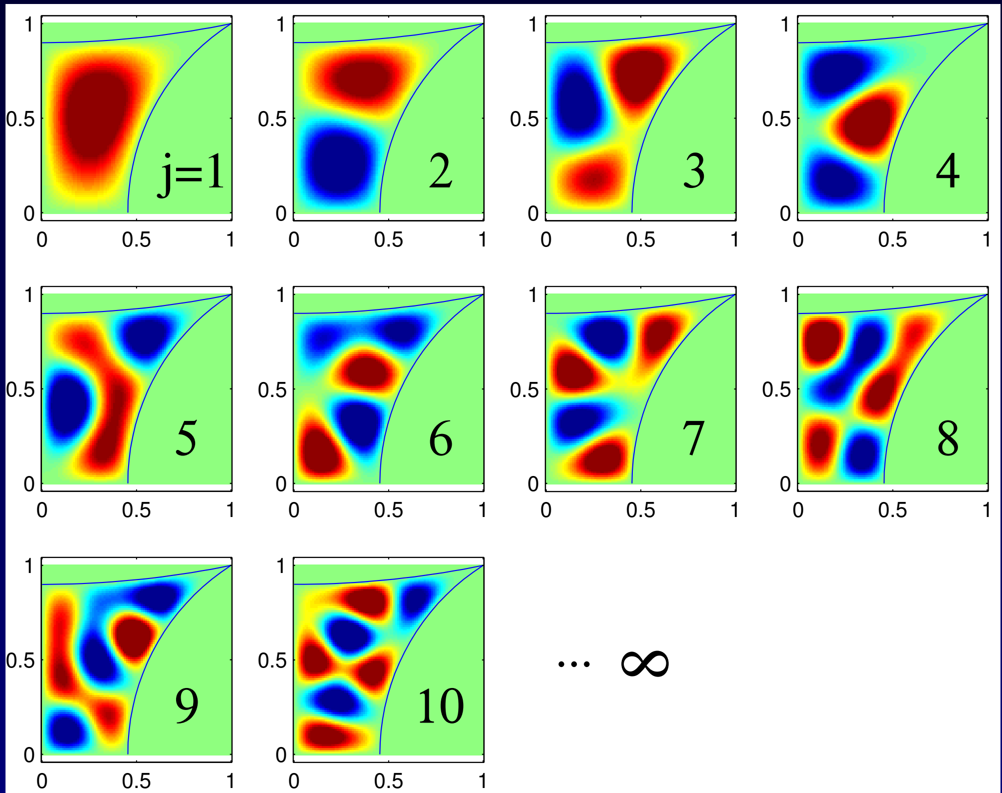

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focus on d=2

- Analytic solutions only if Δ separable (rectangle, ellipse…)
- How numerically compute large numbers of E_j & ϕ_j efficiently?

Motivation

- electromagnetic waveguides (TM modes: Dirichlet BC)
- eigenstates of quantum particles trapped in a cavity
- acoustic resonances and duct transmission (Neumann BC)
- paradigm for more general trapped wave problems

e.g. full Maxwell for microwave, optical resonators

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Modern questions & applications involve…

1. Complex geometry: corners, 3D structures
2. Higher frequencies: *multiscale* problem, $\lambda \ll$ system size

VIEW $j \sim 3000$: 45 wavelengths across

Mathematical questions

1. 'Quantum chaos': what happens in $E \to \infty$ (high freq) limit?
    - depends on classical (ray) dynamics . . . what if chaotic?
    - arose in quantum physics (Einstein 1917; Gutzwiller, Berry '80s)
    - eigenvalue E_j statistics $\leftrightarrow$ Random Matrix Theory
    - impact: atomic, molecular, electronic, chemical physics

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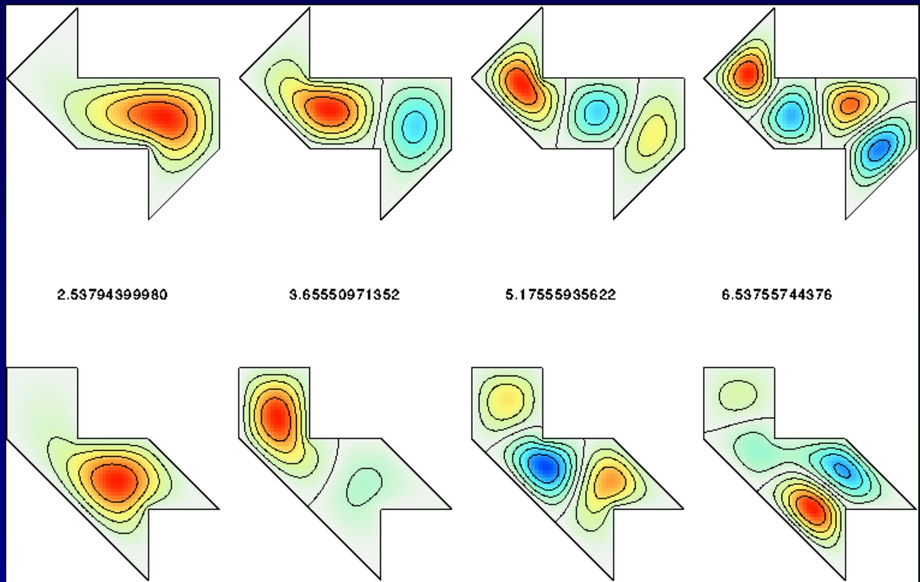
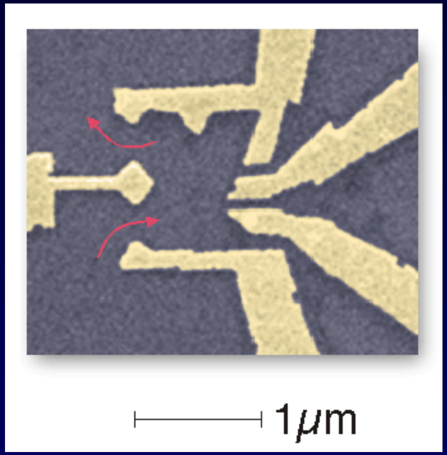
2. Spectral geometry, Riemann surfaces
   - can one hear the shape of a drum? (Kac '66, Gordon *et al.* '92)

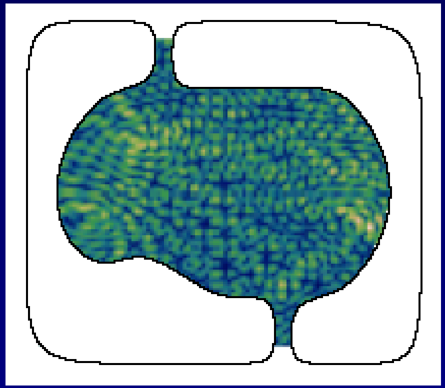


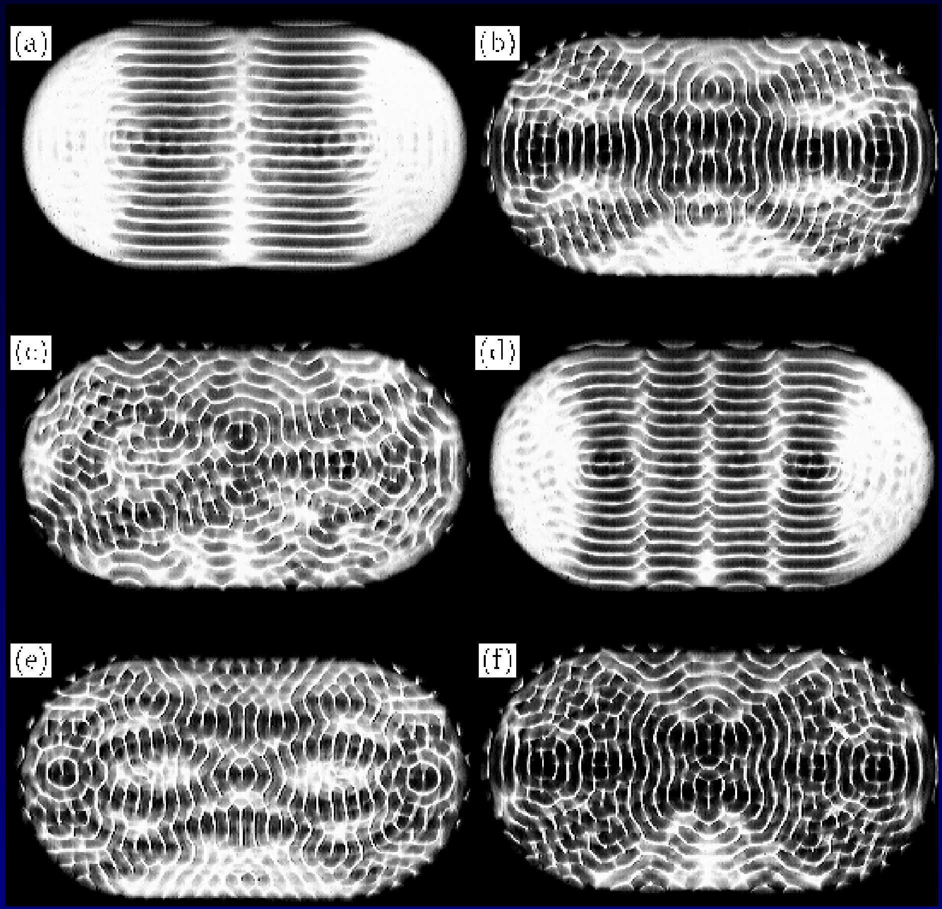
isospectral drums, numerics to 14 digits (Driscoll '97)

Modern applications

- ‘quantum dots’: $\sim 1\mu$m semiconductor labs for cold electrons
  —candidates for *quantum computers*
  —quantum chaos vital for statistics of resonances, conduction







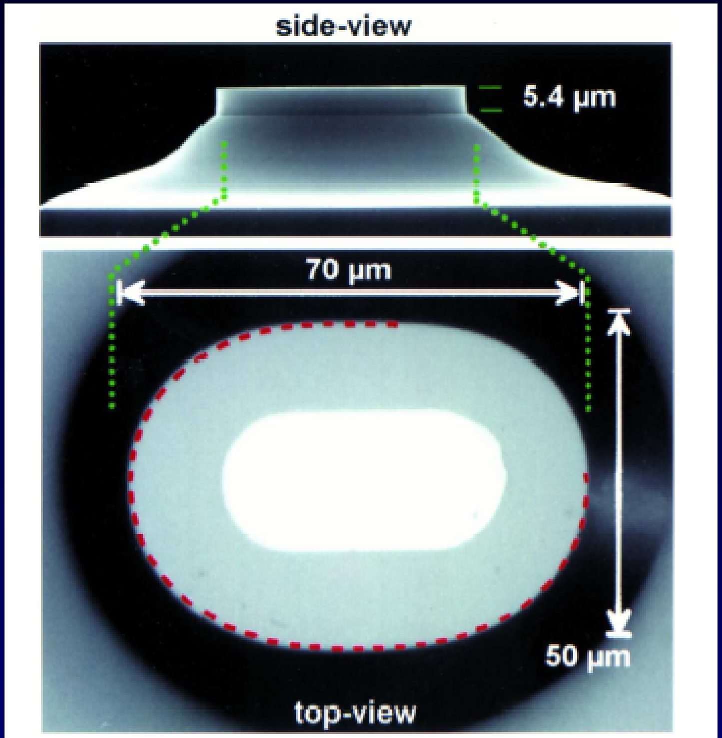
quantum dots (Marcus)

resonant liquid surfaces (Kudrolli)

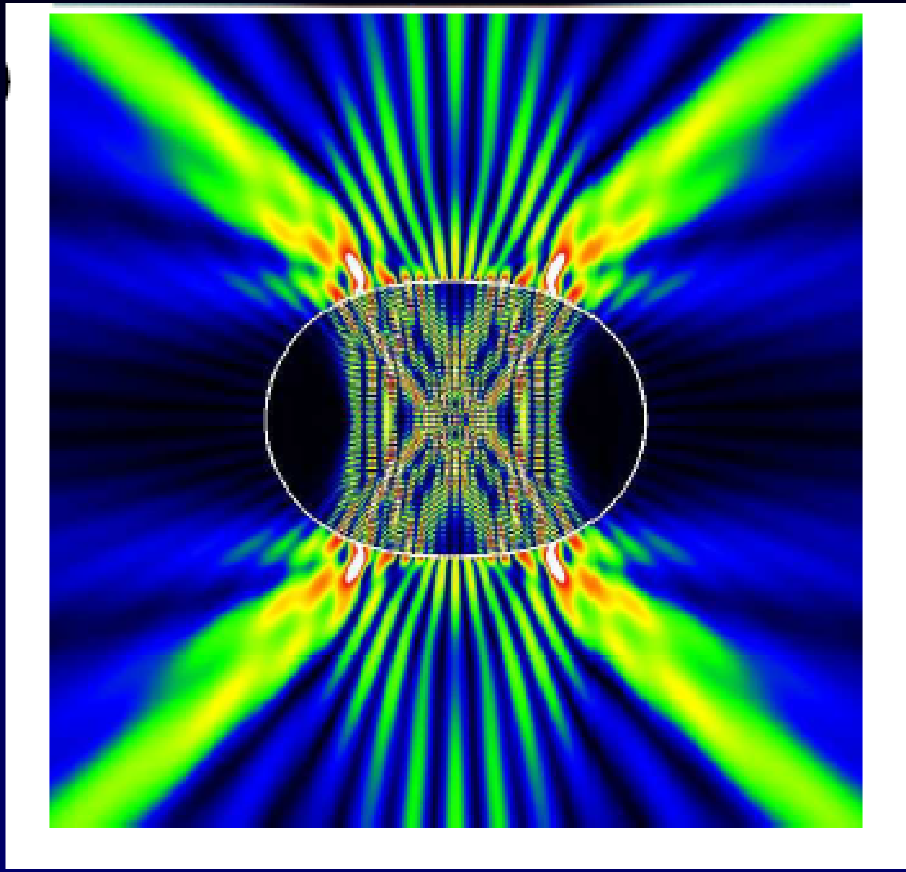
Dielectric micro-cavity lasers

leaky resonant cavities

e.g. quantum-cascade laser



'bowtie' mode, emission pattern



- 2D cavity confinement due to total internal reflection ($n = 3.3$)
- asymmetric cavity, 'scarred' modes $\rightarrow 10^3$ more power (Gmachl '98)
- design is hard: compute many modes for many shapes (Tureci '03)

Outline

I. variant of Method of Particular Solutions

II. basis sets

III. eigenvalue inclusion bounds & rigorous analysis

IV. acceleration by scaling

V. application to quantum chaos: high-frequency mode asymptotics

I. Boundary-Interior Method of Particular Solutions (B '00)

Task: find ϕ_j and E_j such that $(\Delta + E_j)\phi_j = 0$ and $\phi_j|_{\partial\Omega} = 0$

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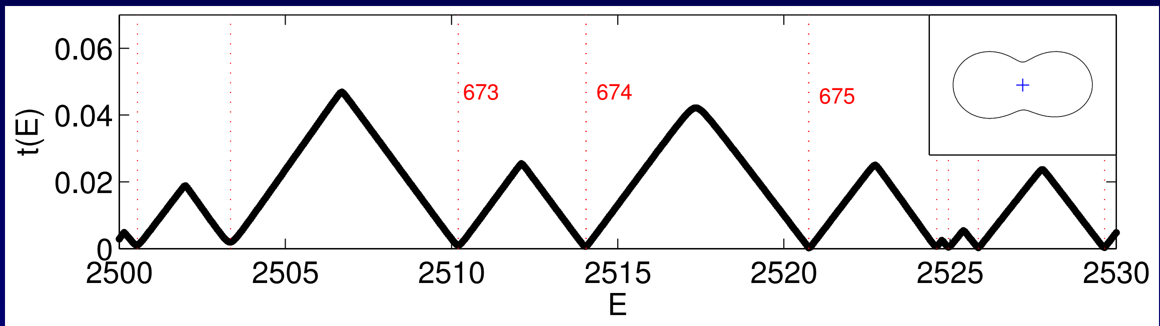
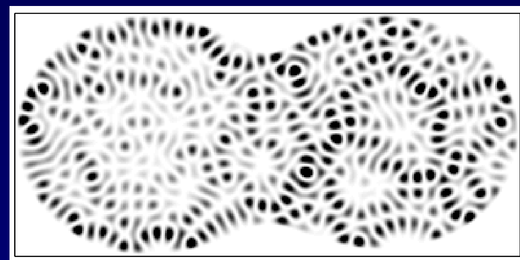
Define 'boundary error' $t(E) := \min_{u \in \mathrm{Span}\{\xi_i\}, u \neq 0} \dfrac{||u||_{L^2(\partial\Omega)}}{||u||_{L^2(\Omega)}}$



'peanut' cavity, $j \approx 700$



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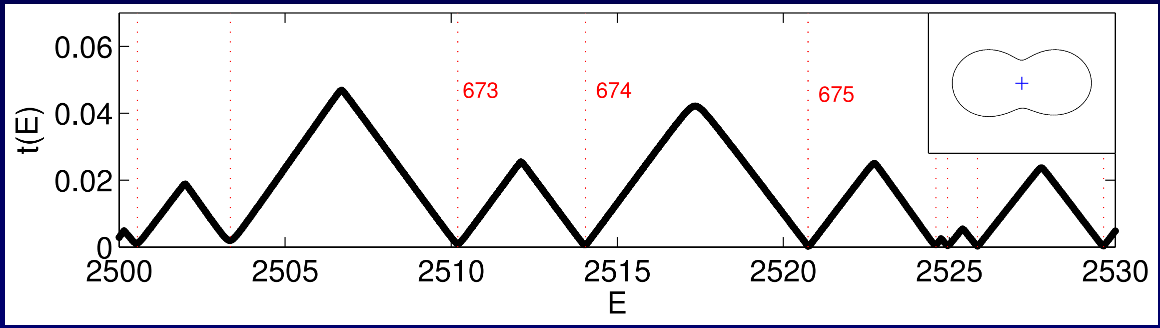

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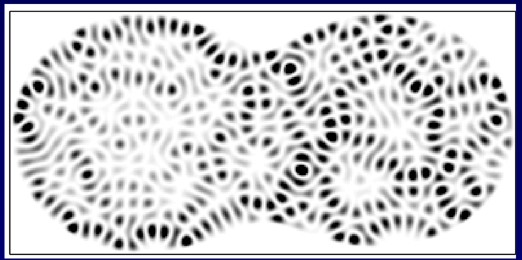

Search (Newton) in E for minima of $t(E)$

- Cures normalization problem plaguing original MPS (Fox '67, etc)

similar cure independently found (Betcke & Trefethen '04)

At each E, how is $t(E)$ computed?

defining bilinear forms

$$f(u,v) := \int_{\partial\Omega} uv \qquad \text{boundary}$$

$$g(u,v) := \int_{\Omega} uv \qquad \text{interior}$$

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Rayleigh quotient $t(E) := \min_{u \neq 0} \sqrt{\frac{f(u,u)}{g(u,u)}} = \min_{\mathbf{x}^T G \mathbf{x} \neq \mathbf{0}} \sqrt{\frac{\mathbf{x}^T F \mathbf{x}}{\mathbf{x}^T G \mathbf{x}}} = \sqrt{\hat{\lambda}_1}$

$\hat{\lambda}_1 =$ lowest generalized eigenvalue of order-N matrix eigenproblem

$$F\mathbf{x} = \hat{\lambda} G \mathbf{x}$$

elements $F_{ij} := \int_{\partial\Omega} \xi_i \xi_j$ quadrature on boundary (trapezium)

$G_{ij} := \int_{\Omega} \xi_i \xi_j$ oscillatory integrals over interior… (yuk)

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F, G dense symm positive-definite, numerically singular as N large

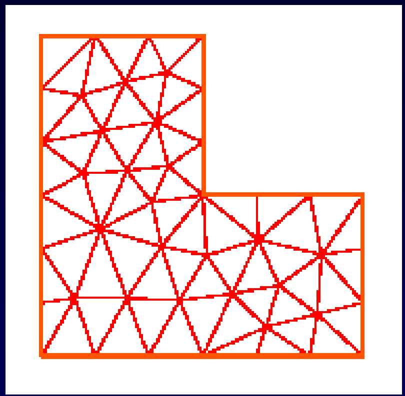
- F, G share common nullspace $\rightarrow$ $\exists$ both stable and unstable $\hat{\lambda}$'s
- Cholesky, QZ fail: use *regularized* (ϵ_{mach}-truncated) inverse of G

Compare to direct methods

Direct discretization (mesh)

finite differencing

finite element method (FEM)



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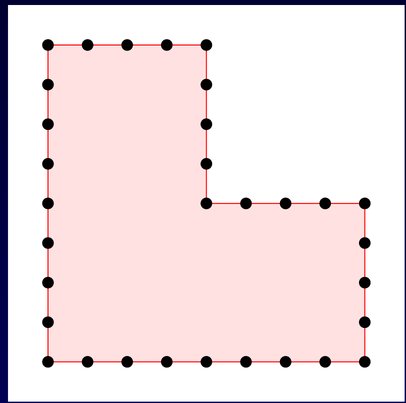
- basis satisfies BC
- find basis coeffs to solve PDE

Boundary methods

integral equation methods (BEM)

method of particular solutions (MPS)



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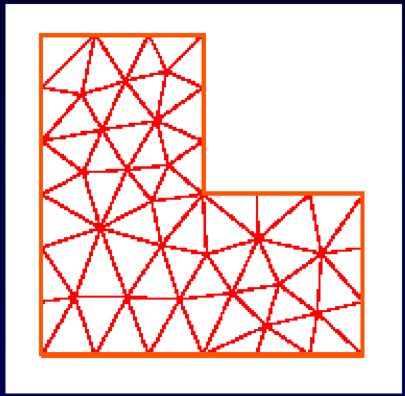

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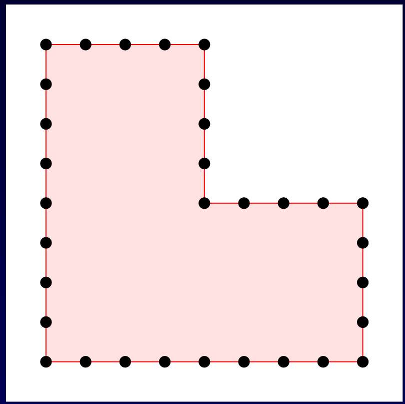

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Direct discretization: $N \sim$ # wavelengths in volume $\sim k^d$

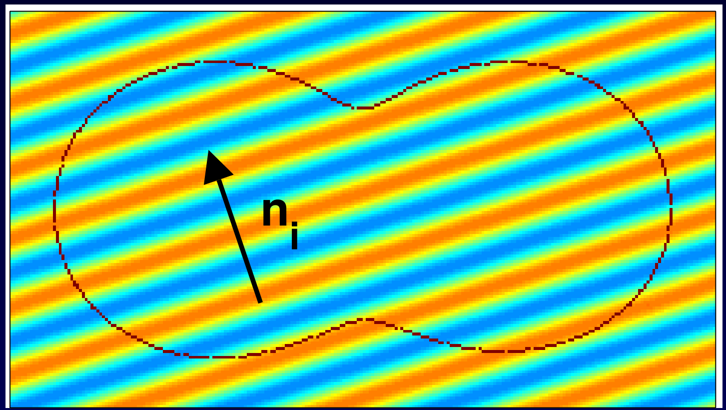
MPS has much smaller $N \sim$ # wavelengths on boundary $\sim k^{d-1}$

$\Rightarrow$ short wavelengths : huge advantage (even with loss of sparsity)

II. Types of MPS basis sets

Each ξ_i is *global* Helmholtz soln at energy E in the cavity...

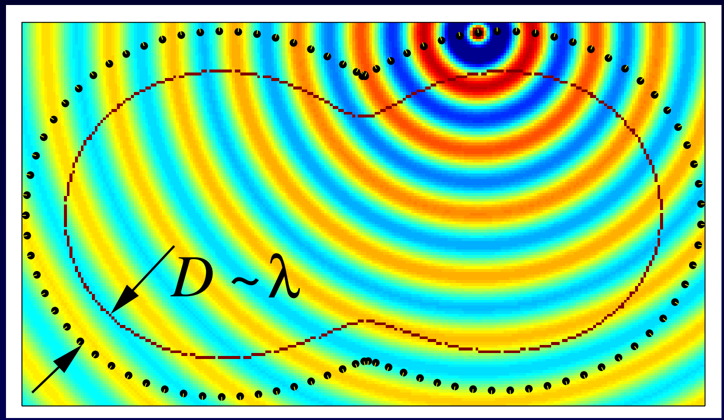
PLANE WAVES



$\xi_i(\mathbf{r}) = \sin(k\mathbf{n}_i \cdot \mathbf{r}), \quad k^2{=}E$

physics community (Heller '84)

FUNDAMENTAL SOLUTIONS



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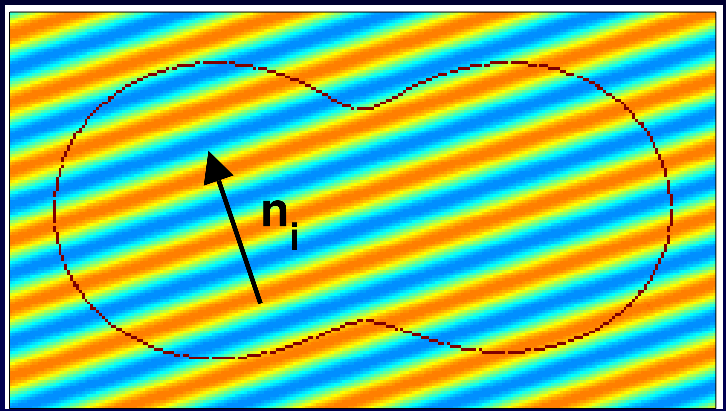

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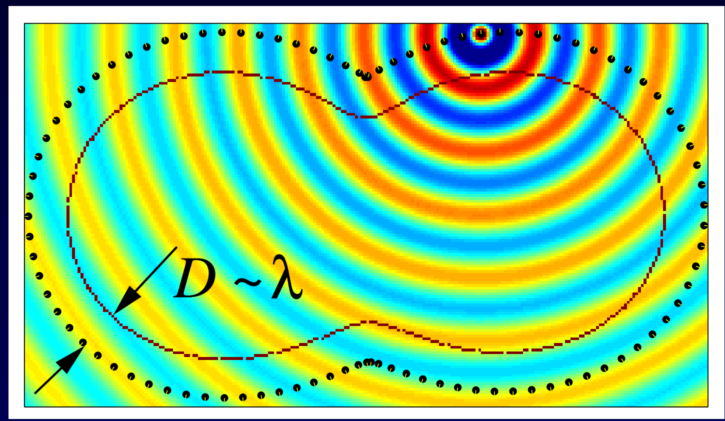

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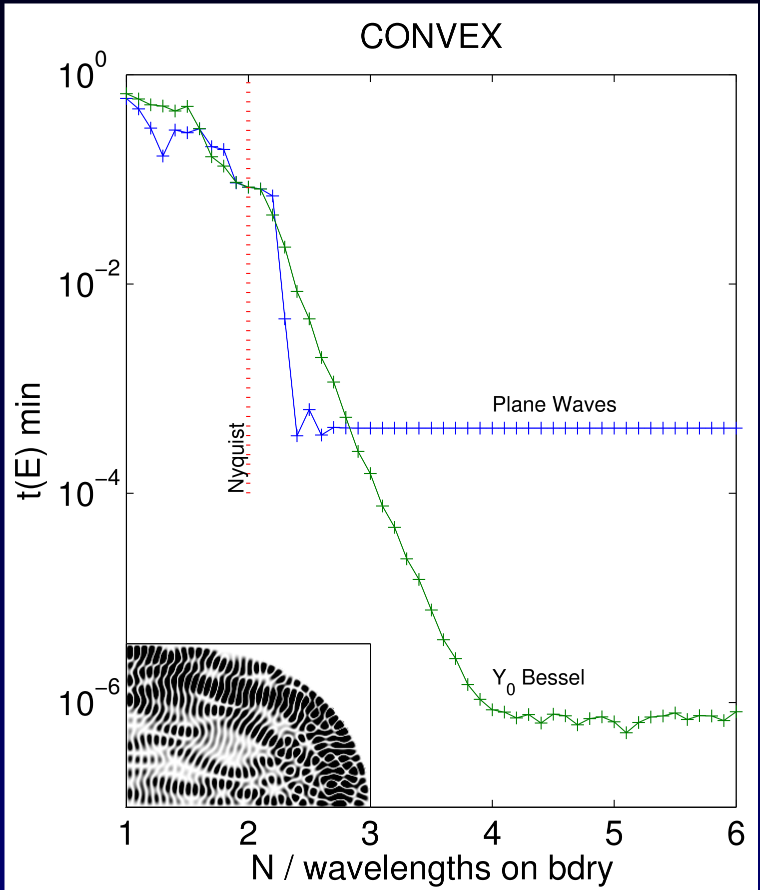
Note: set of $\{\xi_i\}$ recomputed, F, G refilled, at each E during search

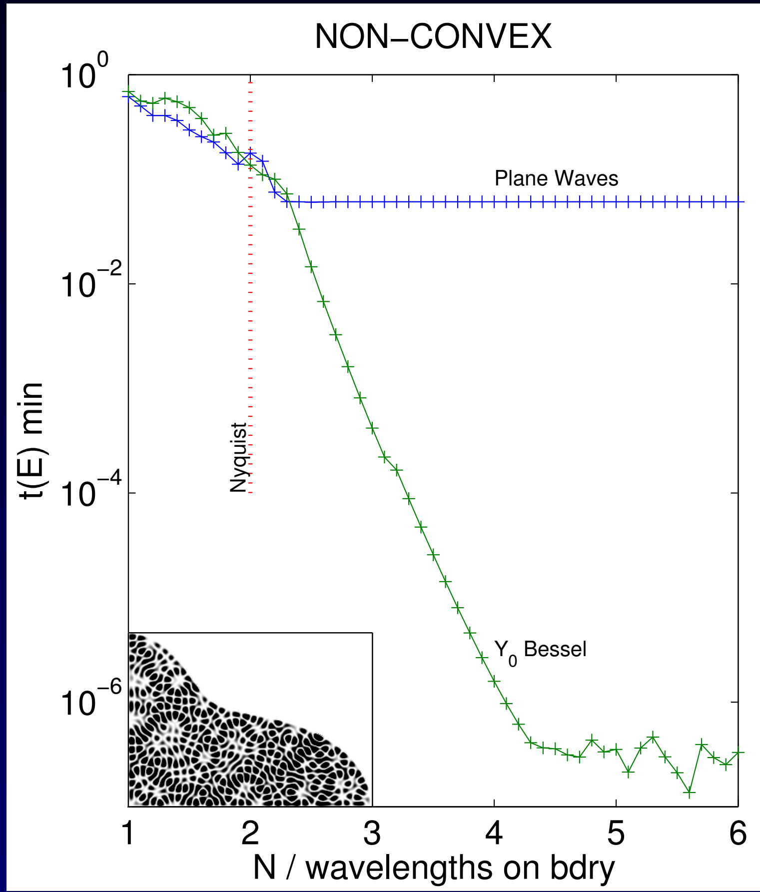
This is $O(N^2)$, dwarfed by $O(N^3)$ dense eigensolve

How well do these basis sets perform for different cavity shapes?

Convergence with basis size N

How small can we make bdry error $t(E)$, for a given mode ?





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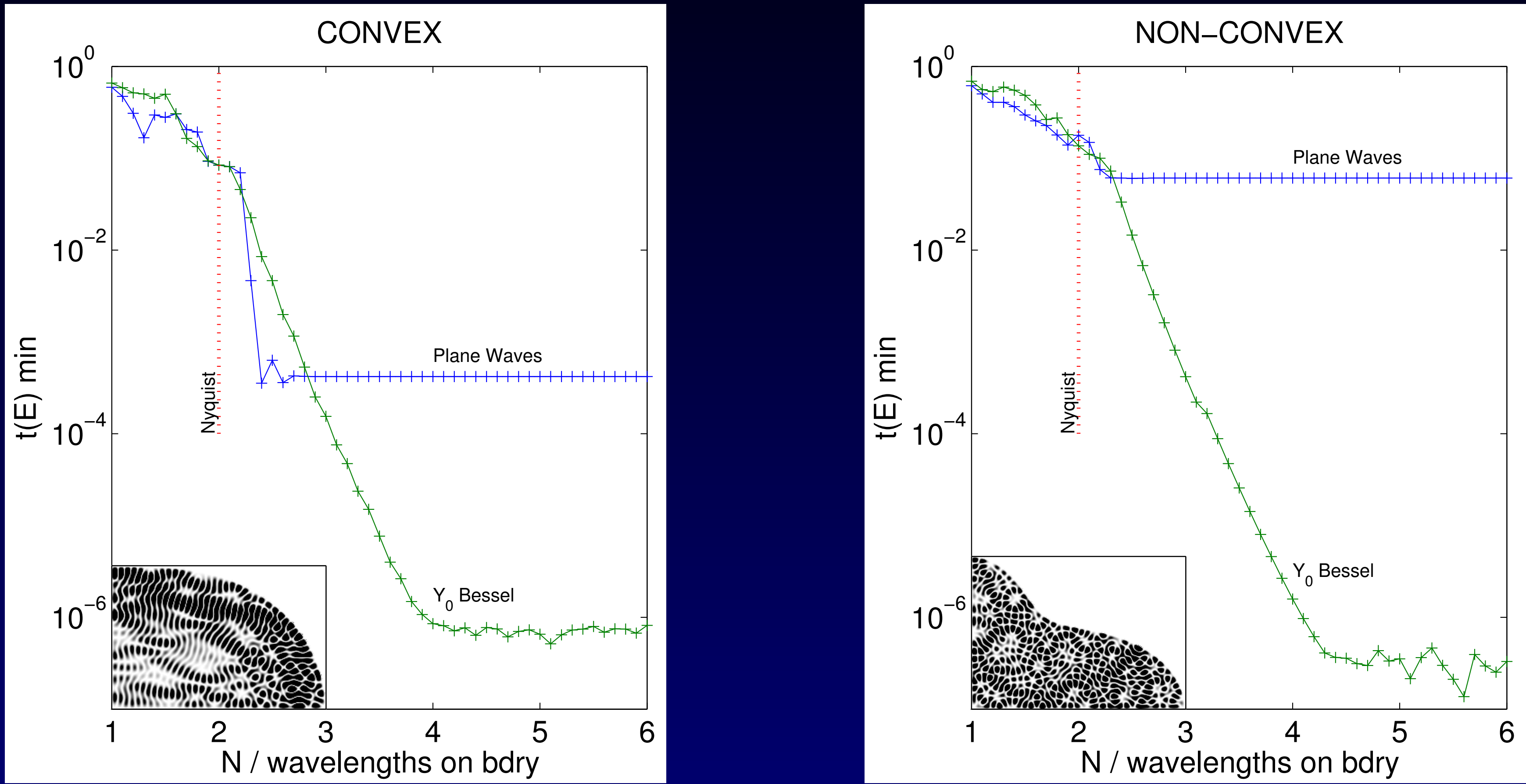

- 2 points per wavelength: $N_{sc} =$ Nyquist sampling limit at spatial freq k
- plane waves useless (fail to converge) for non-convex Ω
- Y_0's give exponential convergence, beyond N_{sc} (down to $\sqrt{\epsilon_{\text{mach}}}$)
- 3-4 points per wavelength, beats 10 usual for integral eqns, BEM

Mysteries of basis sets

Plane waves poor in practise (basis coeffs $\mathbf{x}$ too big), even though. . .

- Fourier-Bessels $J_l(kr)\left\{\begin{smallmatrix}\sin l\theta\\ \cos l\theta\end{smallmatrix}\right.$ complete in simply-connected Ω (Schryer '72)
- Map from Fourier-Bessel to plane-wave coeffs is well-conditioned (Discrete FT)
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Expect closed, closely-spaced wall of Y_0's to be good since. . .

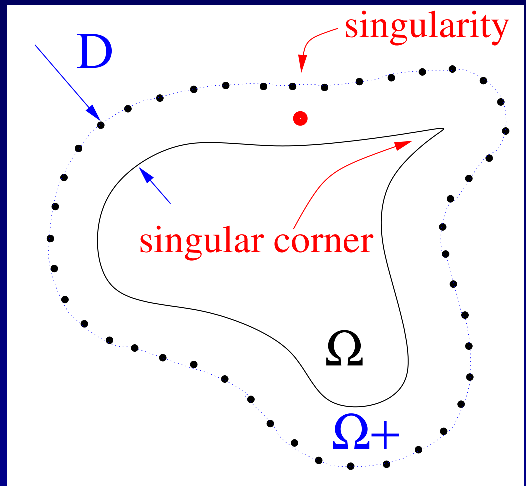
- single layer potential on $\partial\Omega^+$ complete when $E \neq$ Dir. eigenvalue of Ω^+
- Helmholtz solns regular in Ω^+ form dense subspace of those regular in Ω

(Lax '56, Runge approx property)

How big will Y_0 coeffs **x** be?

What if mode ϕ_j cannot be analytically continued to Ω^+? (Eckmann-Pillet '95)

In practise, coeffs not too big: MOVIE



III. New eigenvalue inclusion bounds

Recall $t(E) = \frac{||u||_{L^2(\partial\Omega)}}{||u||_{L^2(\Omega)}}$ for u some trial global Helmholtz soln at E

When $t(E)$ small, intuitively $E \approx E_j$, but can we bound this error?

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Thm (Fox '67, Moler-Payne '68): $$\min_j \frac{|E - E_j|}{E_j} \leq C_\Omega t(E)$$

- $t(E) = 10^{-6}$ means $E \approx E_j$ to 6-digit relative accuracy
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Actually can do better...

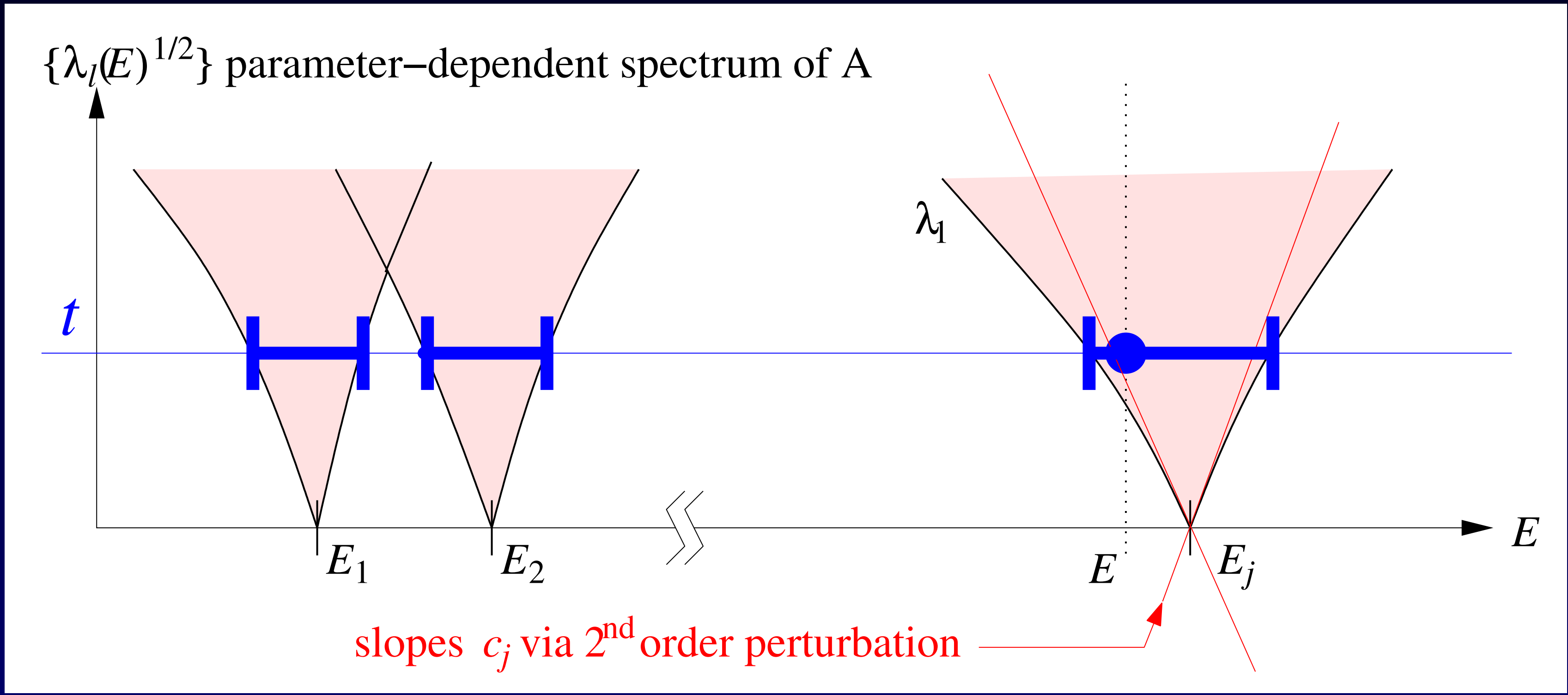
Thm (B '04): For some δ which vanishes as $t(E) \to 0$,

$$\min_j \frac{|E - E_j|}{E_j^{1/2}} \le C'_\Omega (1 + \delta) t(E)$$

- In practise δ is tiny and can be ignored
- At high freq $E \sim 10^6$: now $t(E) = 10^{-6}$ means 9-digit accuracy

Mechanism for improved inclusion

$\forall E$: $t(E)$ exceeds lowest eigenvalue $\sqrt{\lambda_1(E)}$ of some operator $A(E)$



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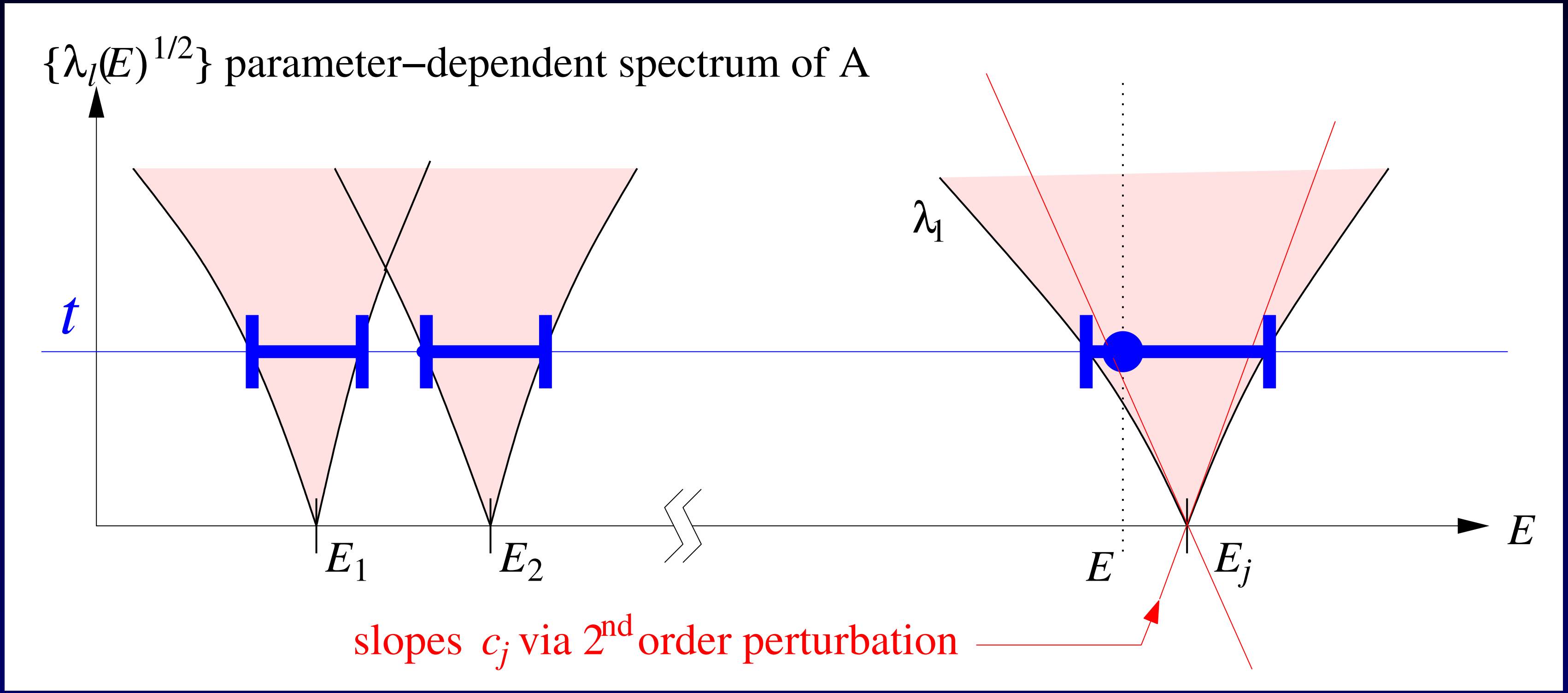

prove analytic perturbation series $\lambda_1(E) = c_j(E - E_j)^2 + O(E - E_j)^4$

- so as $t \to 0$, error $|E - E_j|$ must vanish linearly in t
- prove 'slope coeffs' c_j bounded from below by c/E_j, for all j

Rigorous analysis (sketch) (thanks: Deift, Goodman)

Work in ∞-dim space $\mathcal{H}_\Omega(E) := \{(\Delta+E)u=0 \text{ in } \Omega, \quad u|_{\partial\Omega}\in L^2(\partial\Omega)\}$

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- write boundary funcs $U = u|_{\partial\Omega}$. Choose f as inner product:

  $f(u,v) = \int_{\partial\Omega} w\, uv =: \langle U, V\rangle$ fixed weight func $w \in L^\infty(\partial\Omega)$, $w > 0$

  $g(u,v) = \int_\Omega uv =: \langle U, AV\rangle$ defines $A(E) : L^2(\partial\Omega) \to L^2(\partial\Omega)$

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A compact for $E \neq E_j$ — proof: Poisson kernel for Helmholtz eqn

Spectral problem $\boxed{V = \lambda A V}$ — discrete spectrum $\lambda_1 \le \lambda_2 \le \cdots \to \infty$

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A compact for $E \neq E_j$ proof: Poisson kernel for Helmholtz eqn

Spectral problem $\boxed{V = \lambda AV}$ discrete spectrum $\lambda_1 \leq \lambda_2 \leq \cdots \to \infty$

For E in neighborhood of E_j, isolate unbounded part of A:

$$A(E) = (\text{compact analytic}) + \frac{1}{(E - E_j)^2}(\text{constant rank-1})$$

- perturbation details: analyticity & Cauchy eigenvalue interlacing
- get $c_j^{-1} = \int_{\partial\Omega} w^{-1}(\partial_n \phi_j)^2$ has upper bound $O(E_j)$ in wide class of Ω

Rigorous analysis (sketch)

(thanks: Deift, Goodman)

Work in ∞-dim space $\mathcal{H}_\Omega(E) := \{(\Delta{+}E)u{=}0 \text{ in } \Omega, \quad u|_{\partial\Omega}{\in}L^2(\partial\Omega)\}$

- write boundary funcs $U = u|_{\partial\Omega}$. Choose f as inner product:

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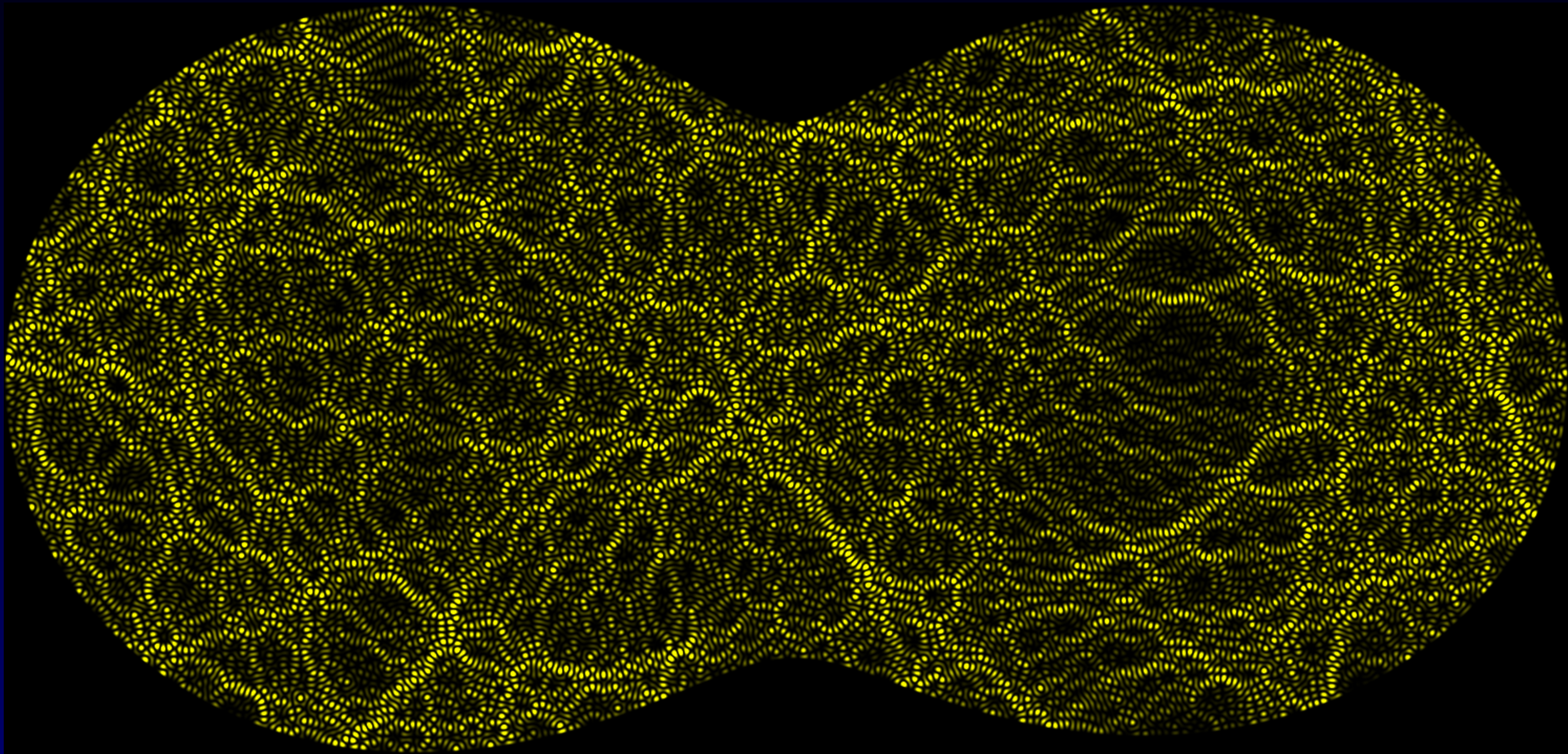
Finally, note $t(E)^2 = \hat{\lambda}_1 \geq \lambda_1$ since Span$\{\xi_i\} \subset \mathcal{H}_\Omega(E)$

RESULT: optimal symmetric bounds, tighter by factor $E^{1/2} = O(N)$

High-frequency peanut inclusion



Mode $j \approx 27000$. Given typical boundary error norm $t(E) = 1.2 \times 10^{-5}$, get…

Moler-Payne bounds: $10000^{6.1}_{0.5}$

New bounds: 100003.3^{32}_{17} 2.5 extra digits, no extra work!

IV. Acceleration by scaling

(back to numerical method, N-dim Span$\{\xi_i\}$)

Root search slow, close levels easily missed — can we do better?

We used $t(E) = \hat{\lambda}_1(E)^{1/2}$. Plot higher generalized eigenvalues…

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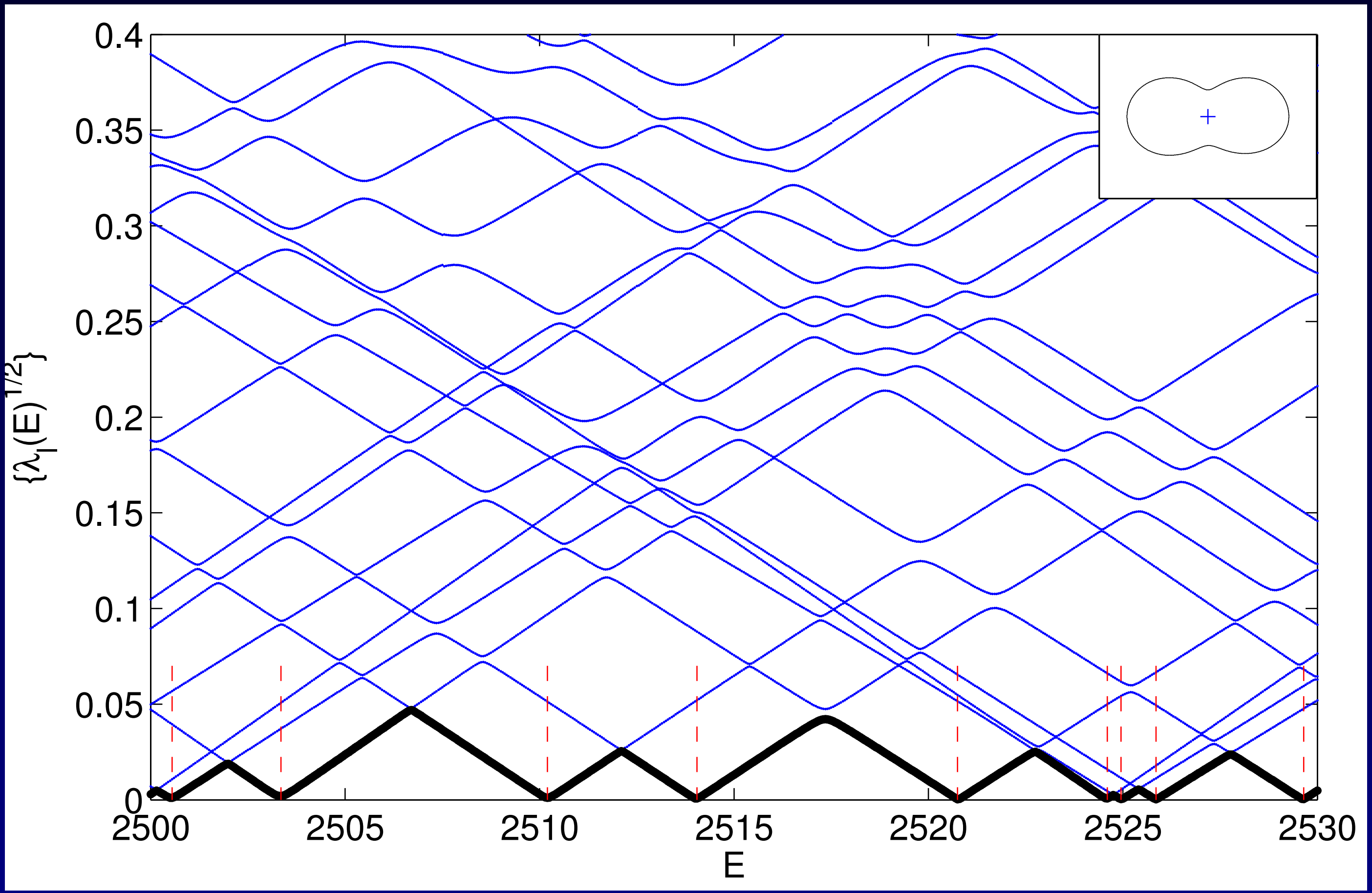

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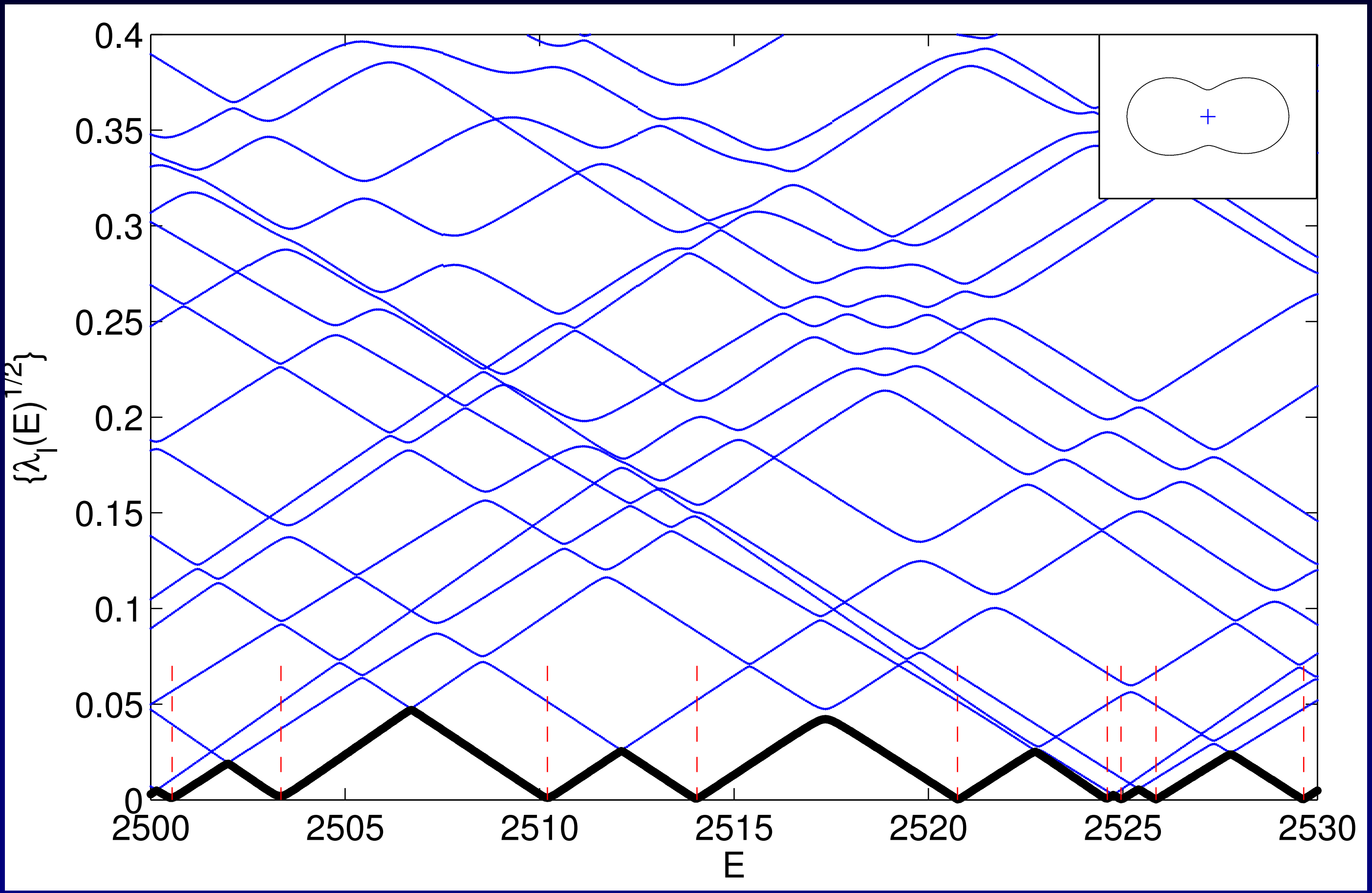

- Idea: spectrum at single E has info about many nearby $\hat{\lambda}_1$ minima

Special boundary weighting w

For f, change from $w=1$ to $w=(\mathbf{r} \cdot \mathbf{n})^{-1}$ (requires Ω star-shaped)

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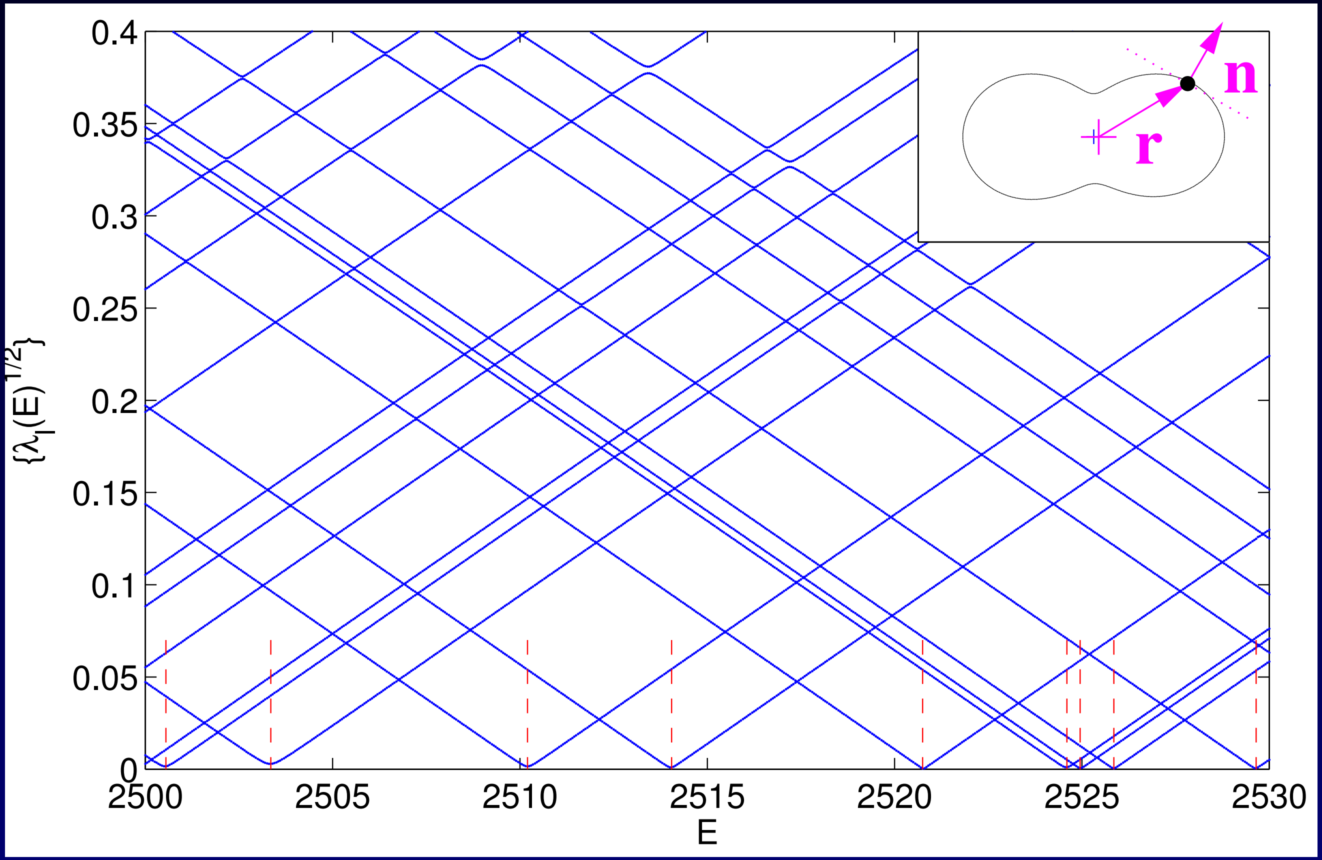


- beautiful clean quadratic structure, tiny avoided crossings
- no 'slope' variation: prove $c_j E_j\!=\!\frac{1}{2},\ \forall j$ $\quad\longrightarrow$ accurate prediction!

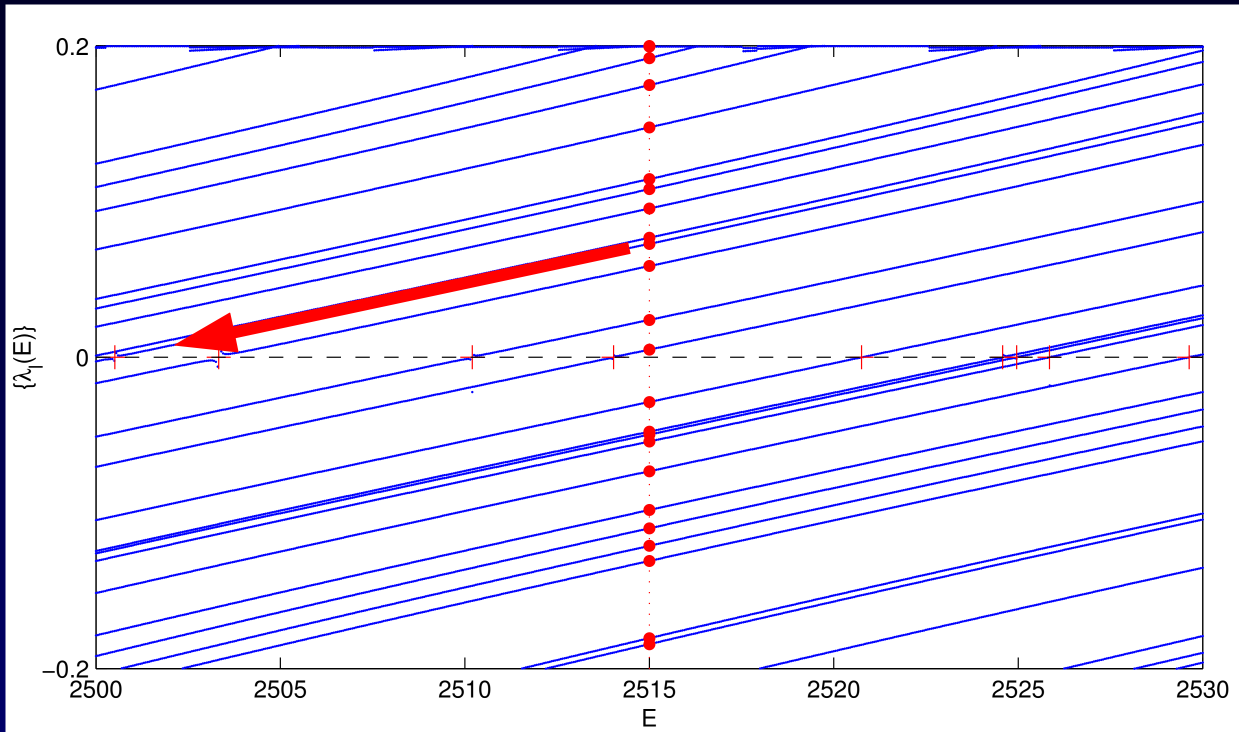
Can do even better…

Scaling method

(Vergini '94, B '00, '04)

Invented in physics community... a correct explanation was lacking!

Use f as before, but new $g(u,v) = \int_{\partial\Omega} (\mathbf{r}\cdot\mathbf{n})^{-1}(u\mathbf{r}\cdot\nabla v + v\mathbf{r}\cdot\nabla u)$



- solving $F\mathbf{x} = \hat{\lambda} G\mathbf{x}$ at single E value gives *all* nearest $O(N)$ modes
- no root search, no missing levels, efficiency gain $O(E^{\frac{d-1}{2}})$, in 3D too
- eigenvectors $\mathbf{x}$ give *dilated* (scaled) approximations to modes ϕ_j
- errors grow like $t \sim |E_j - E|^3$ (3^{rd}-order convergence with effort)

Scaling relies on quasi-orthogonality

modes exactly orthogonal in interior $\int_\Omega \phi_i \phi_j = \delta_{ij}$

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

It's known $\quad Q_{ij} = 2\delta_{ij} E_j + q_{ij} \quad$ with $q_{jj} = 0$ (Rellich '40)

- conjecture (Vergini '94): off-diag terms grow $|q_{ij}| \sim |E_i - E_j|$
- semiclassics (B-Cohen-Heller '00): for Ω ergodic, $|q_{ij}| \sim (E_i - E_j)^2$

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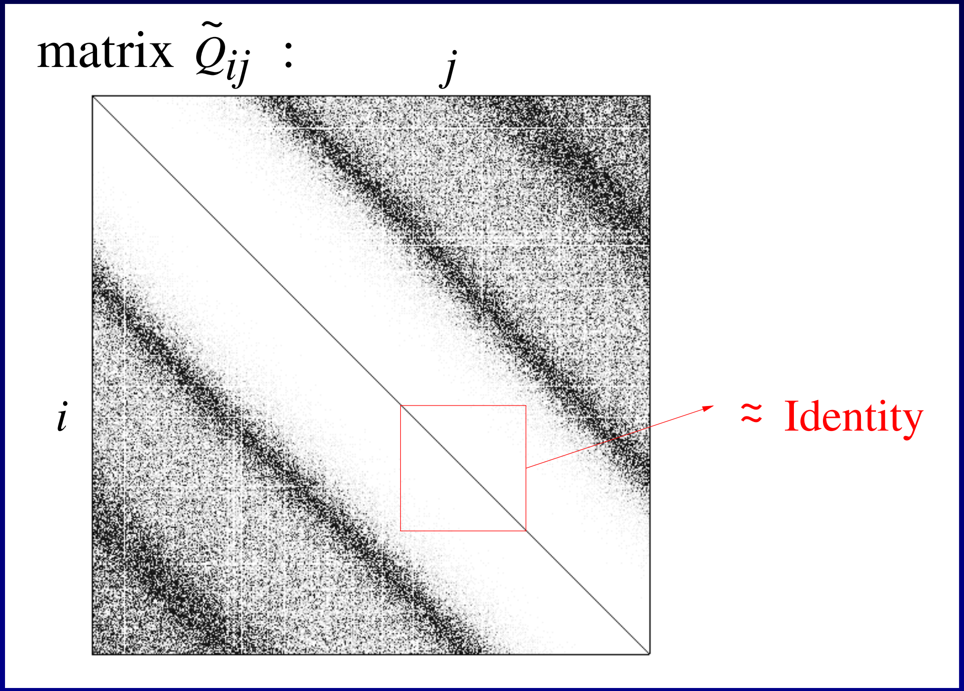
- semiclassics (B-Cohen-Heller '00): for Ω ergodic, $|q_{ij}| \sim (E_i - E_j)^2$
- Thm (B '04): for *all* Ω, ergodic or not, $|q_{ij}| \leq C_\Omega (E_i - E_j)^2$



Algebra shows the set of dilated ϕ_j with E_j near E approx diagonalize f and g

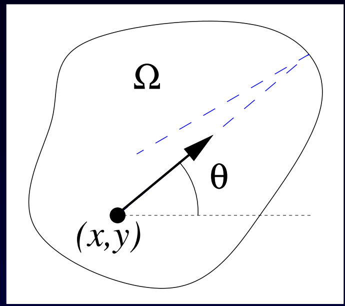
$\Rightarrow$ scaling works

V. Application: Quantum chaos & cavity shape

Drum problem is *quantized* equivalent of ‘billiards’

dynamical system: point particle, elastic reflection from $\partial\Omega$

phase space $= (x, y, \theta)$



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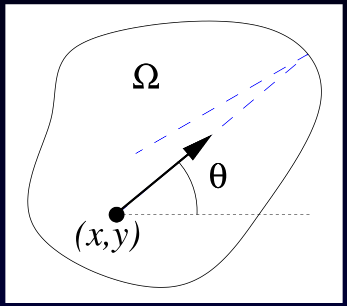
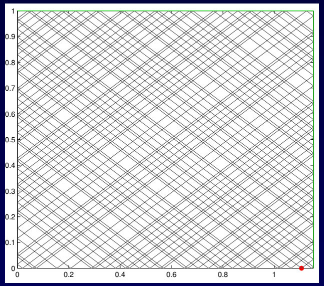
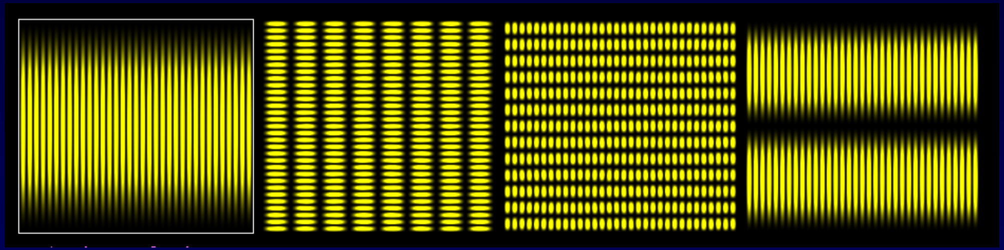


classical | eigenfunctions ϕ_j: ‘quantum’

Integrable:

conserved quantities

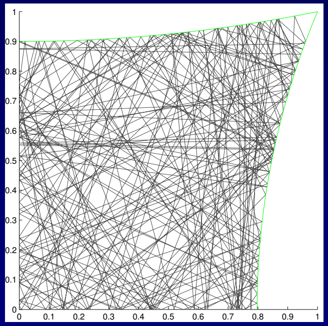


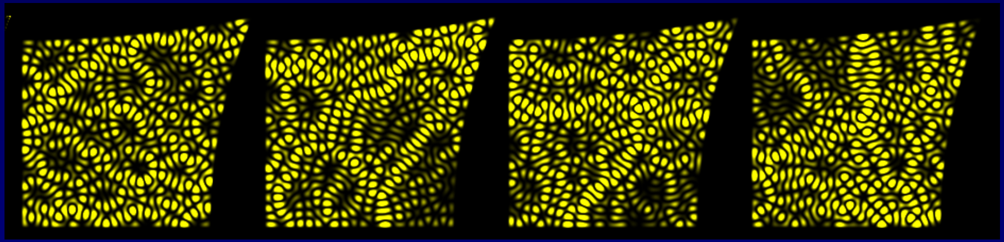


localization (tori in phase space: EBK)

Ergodic:

covers all phase space





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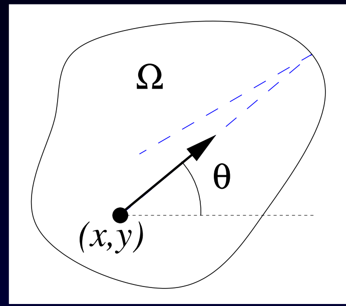

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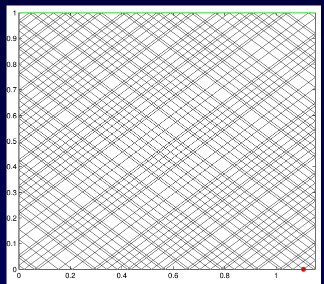

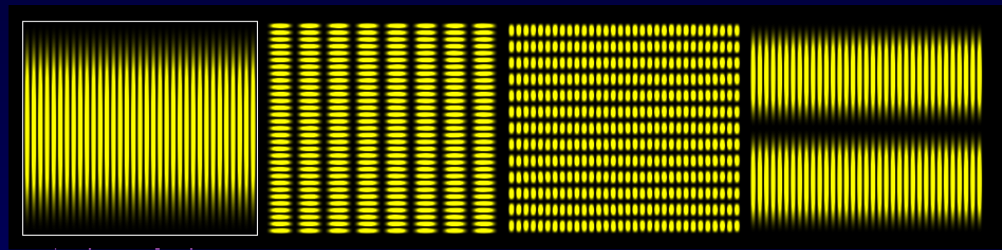

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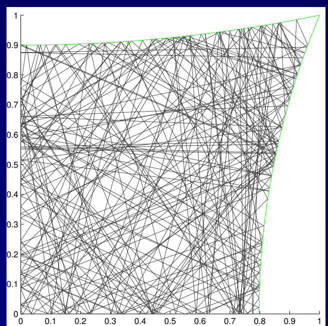
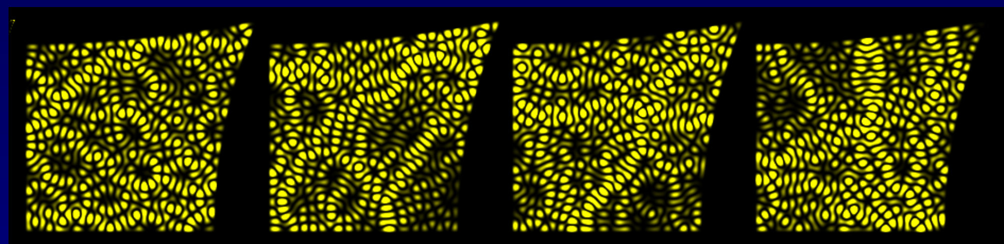




‘quantum chaos’

- We examine mode intensity ϕ_j^2 for ergodic Ω in $E \to \infty$ limit

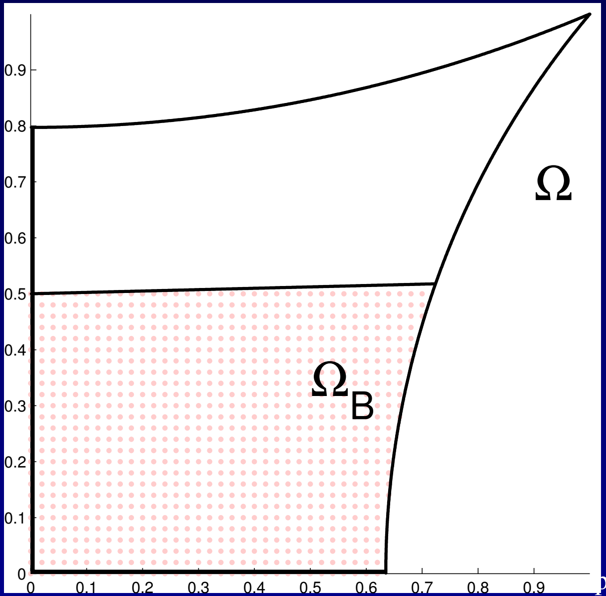
Do modes become spatially uniform?

Quantum Ergodicity Theorem: For ergodic cavity $\Omega \supset \Omega_B$,

$$\lim_{E_j \to \infty} \int_{\Omega_B} \phi_j^2 = \frac{\mathrm{vol}(\Omega_B)}{\mathrm{vol}(\Omega)} \qquad \forall j \text{ except subseq. of vanishing density}$$

(Schnirelman '74, Colin de Verdière '85, Zelditch '87, Z-Zworski '96)

Gives no prediction of convergence rate or density of subsequence



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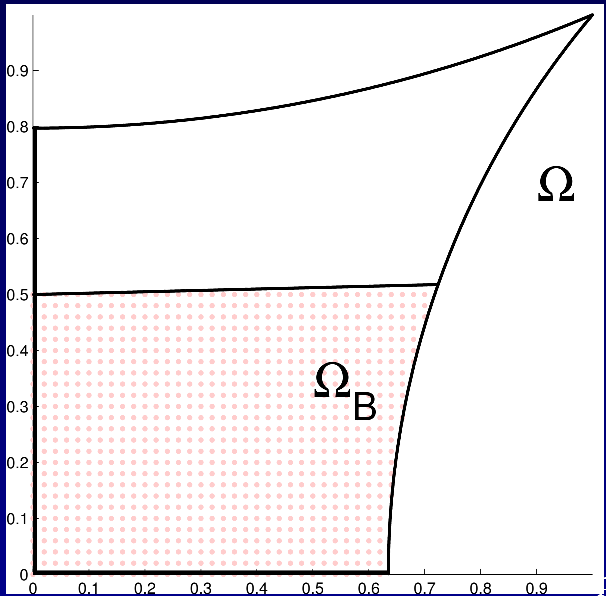
Large-scale numerical study of $\int_{\Omega_B} \phi_j^2$:

- Sinai-type cavity (chaotic: uniformly hyperbolic)
- 30,000 modes, level numbers $j \sim 10^4$ to 10^6

  ... 100 times higher than other studies
- only a few CPU-days total (B '04)



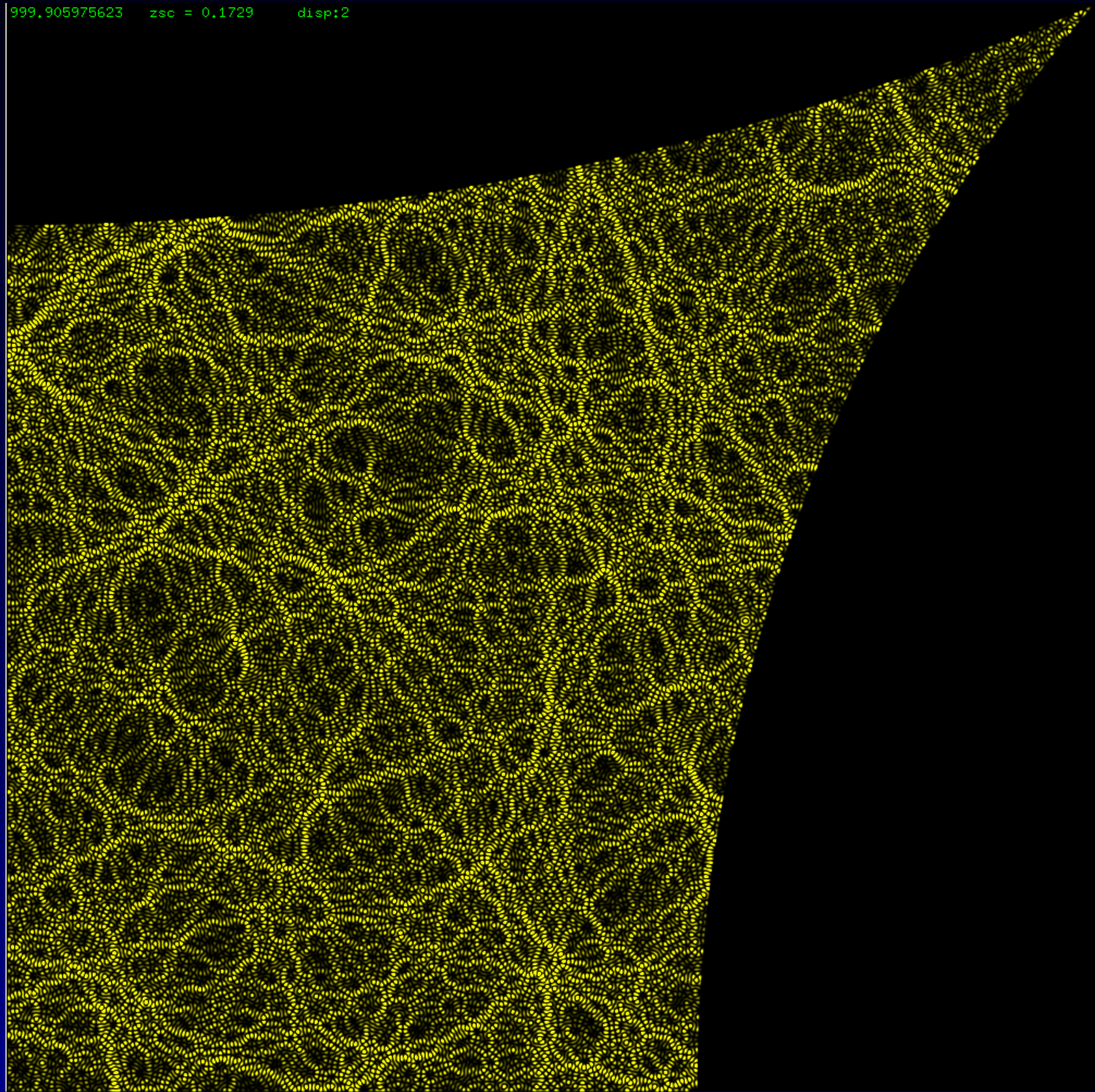
High-frequency chaotic mode

225 wavelengths across system

level number $j \approx 5 \times 10^4$

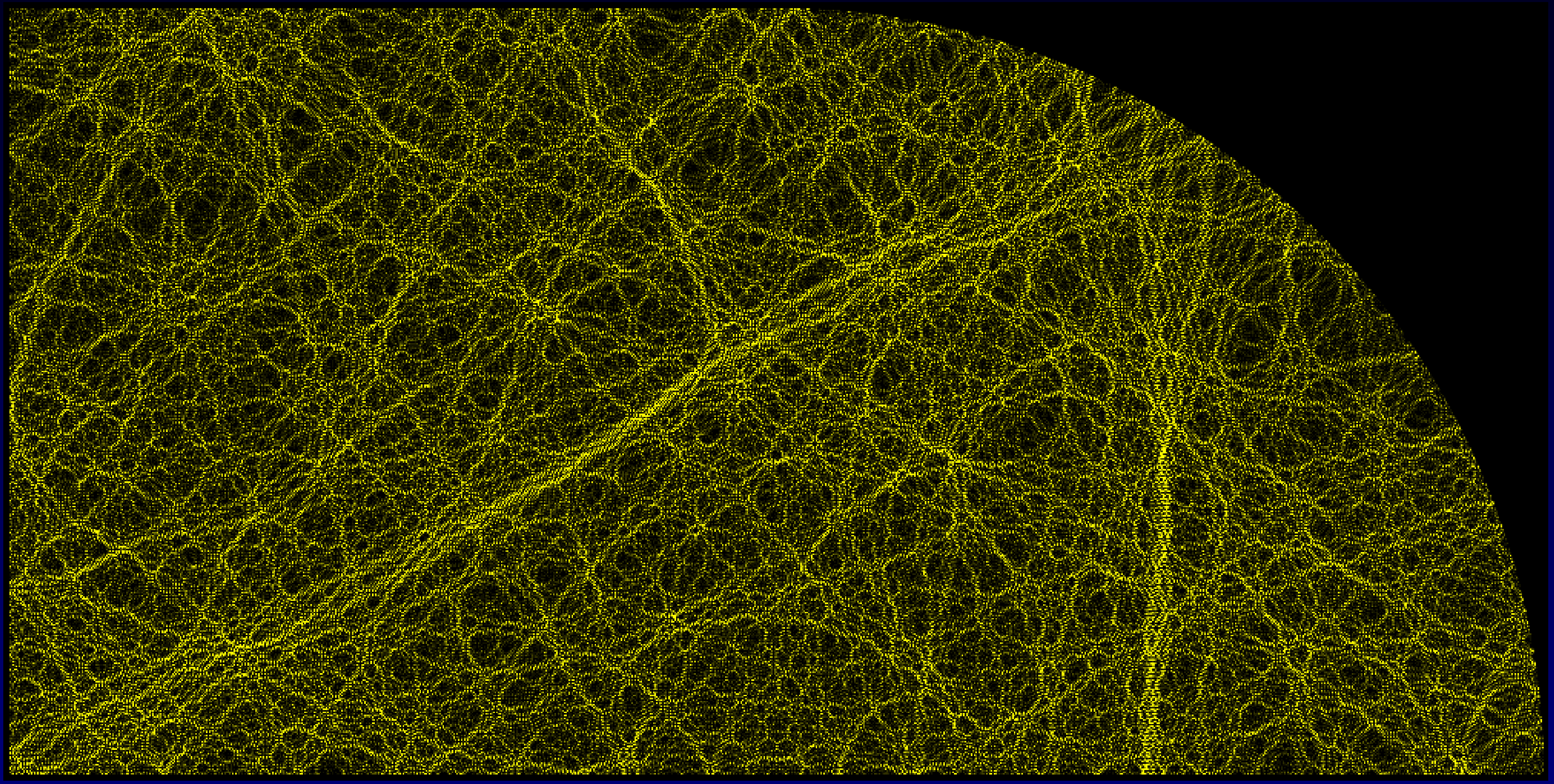
$E \approx 10^6$

here scaling method is 10^3 times faster than MPS! (or BEM)



Scarred mode (stadium cavity)

'Scar' is: enhanced intensity ϕ_j^2 on unstable periodic (ray) orbit



- discovered in physics, predict width dies $E \sim E^{-1/4}$ (Heller '84)

But do scars die out in the $E \to \infty$ limit, or persist as subsequence?

Result: asymptotic convergence rate with E

local variance $\quad V_B(E) := \frac{1}{E^{1/2}} \sum_{E_j \in [E, E+E^{1/2}]} \left(\int_{\Omega_B} \phi_j^2 - \frac{\mathrm{vol}(\Omega_B)}{\mathrm{vol}(\Omega)} \right)^2$

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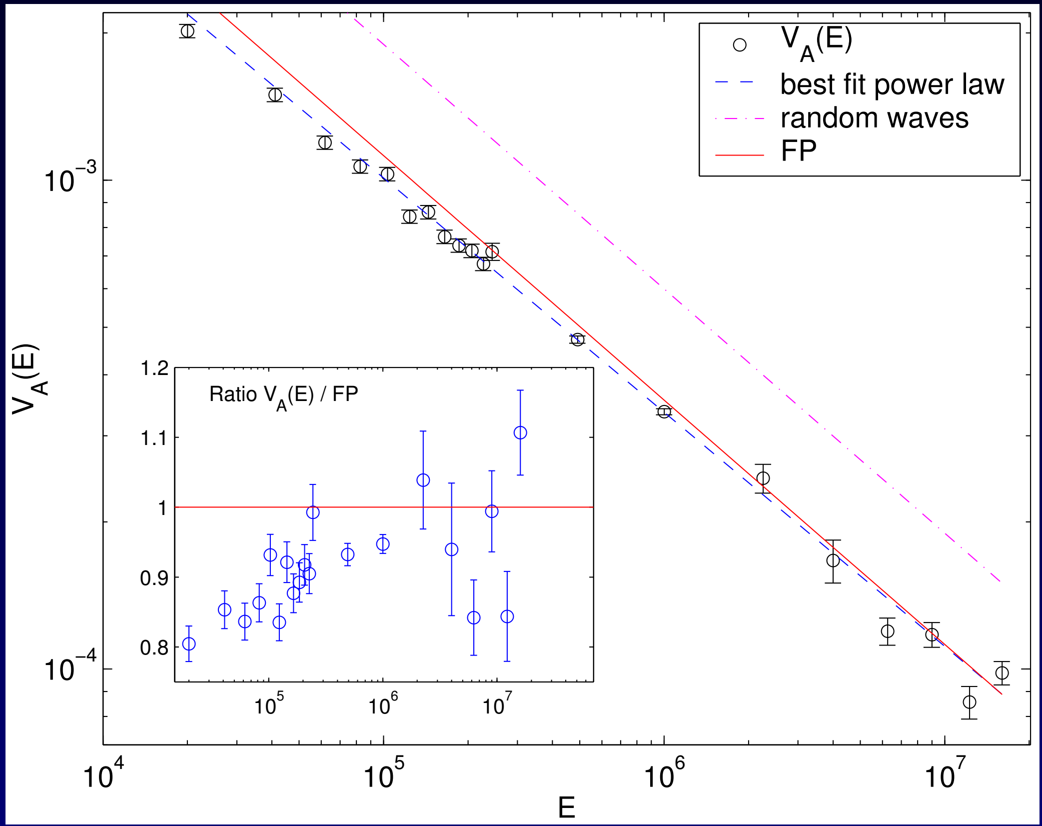


consistent with power law model $V_B(E) = aE^{-\gamma}$

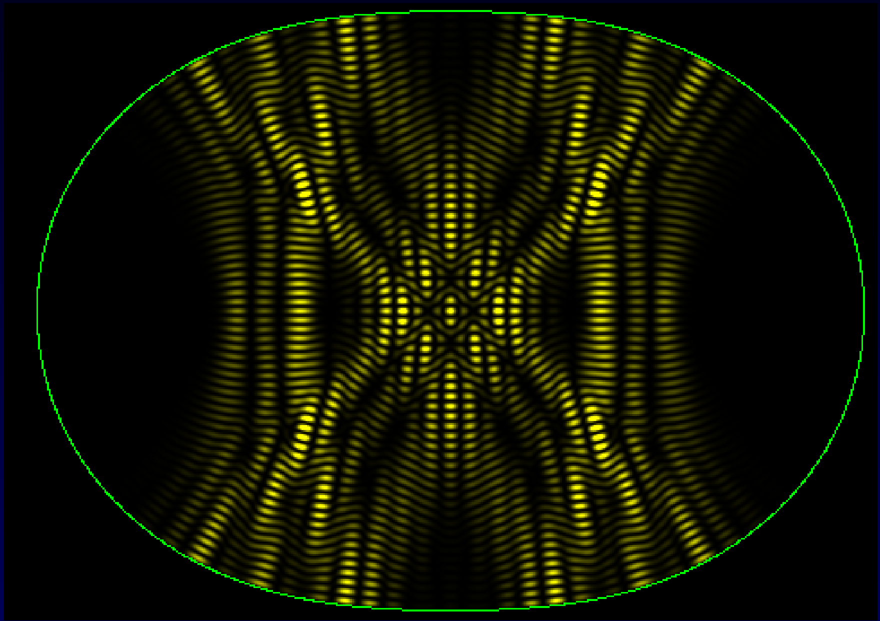
fit $\gamma = 0.48 \pm 0.01$

random waves, scar theory predict $\gamma = 1/2$

- large numbers of modes $\longrightarrow$ highly accurate statistics ($< 1\%$)
- convergence slow; prefactor a not explained by random wave model
- no exceptional modes: supports Quantum Unique Ergodicity (Sarnak *et al.*)

Laser results: closed cavity modes

$E = 16417.2$ MODES



CPU / mode	method
60 s	MPS, root search
10 s	scaling, output 2d grid
0.6 s	scaling, bdry vals only

Conclusions

Dirichlet eigenmode problem: global (meshless) methods excel

At high frequencies *e.g.* ~ 100 wavelengths across...

- made eigenvalue inclusion 10^3 times more accurate
- scaling: 10^3 faster computation than any other known method

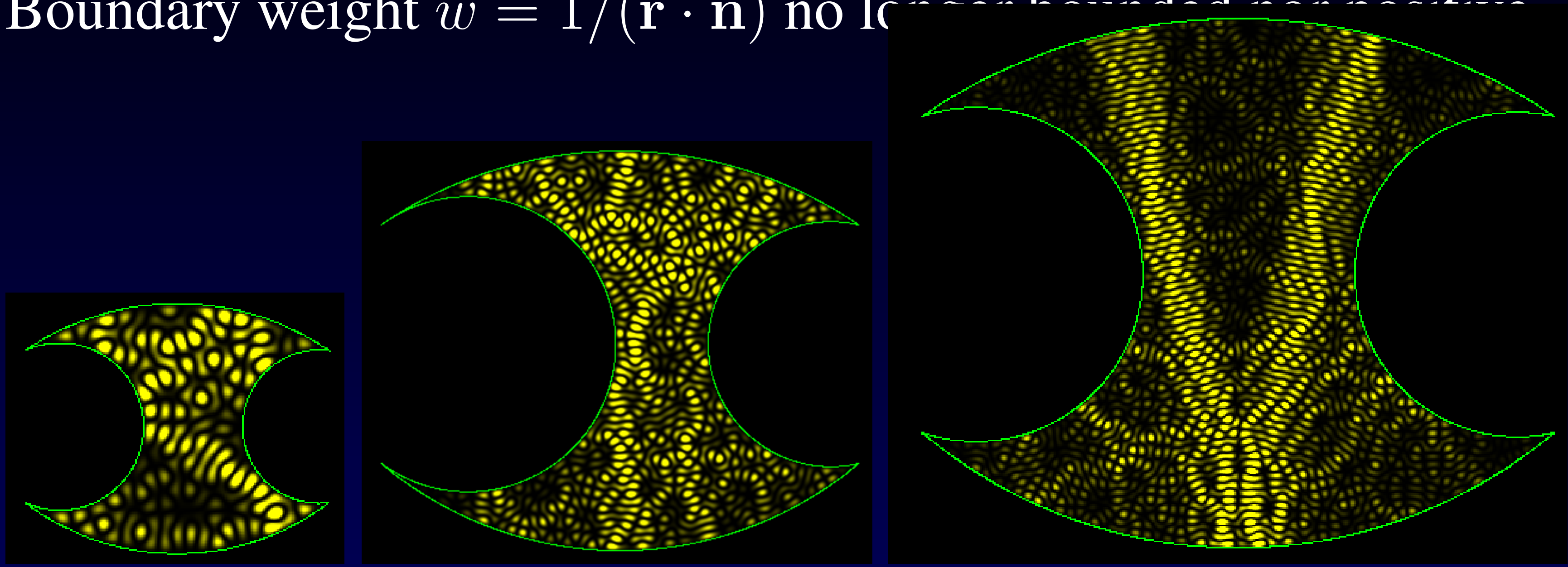
Future:

- scaling method rigorous error analysis
- basis sets for corners, mixed boundary conditions, 3D
- accelerate integral equation methods: open systems

Preprints/talks: http://www.cims.nyu.edu/∼barnett

Non-star-shaped domains: initial results

Boundary weight $w = 1/(\mathbf{r} \cdot \mathbf{n})$ no l

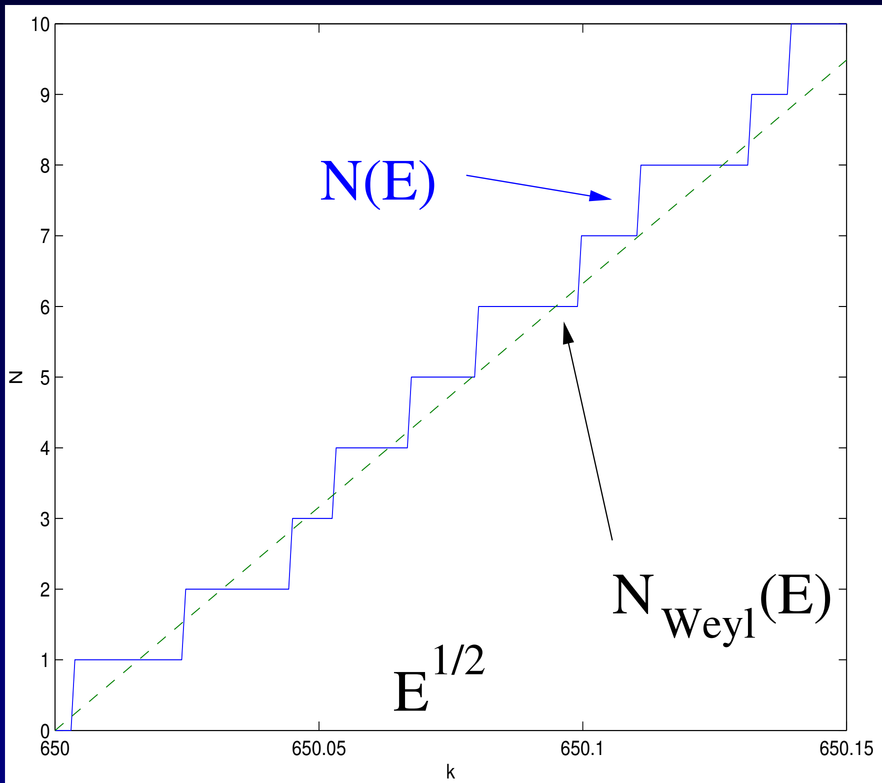


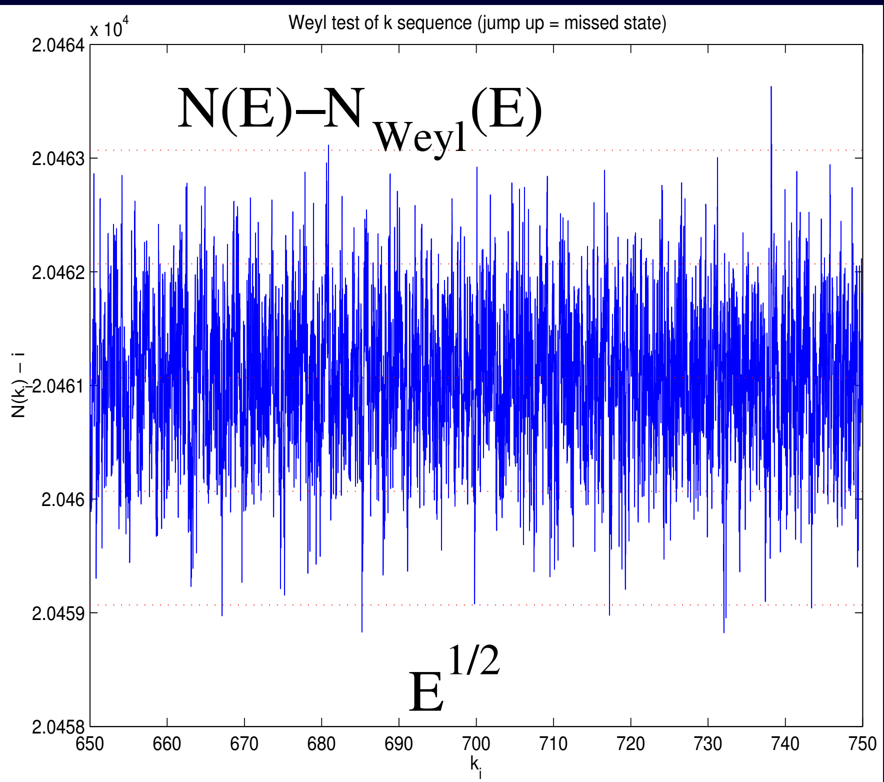
- scaling method *still works*: not great accuracy, $t \sim 10^{-2}$.
- promising for complex geometries…

Missing levels?

Weyl's estimate for $N(E)$, the # eigenvalues $E_j < E$:

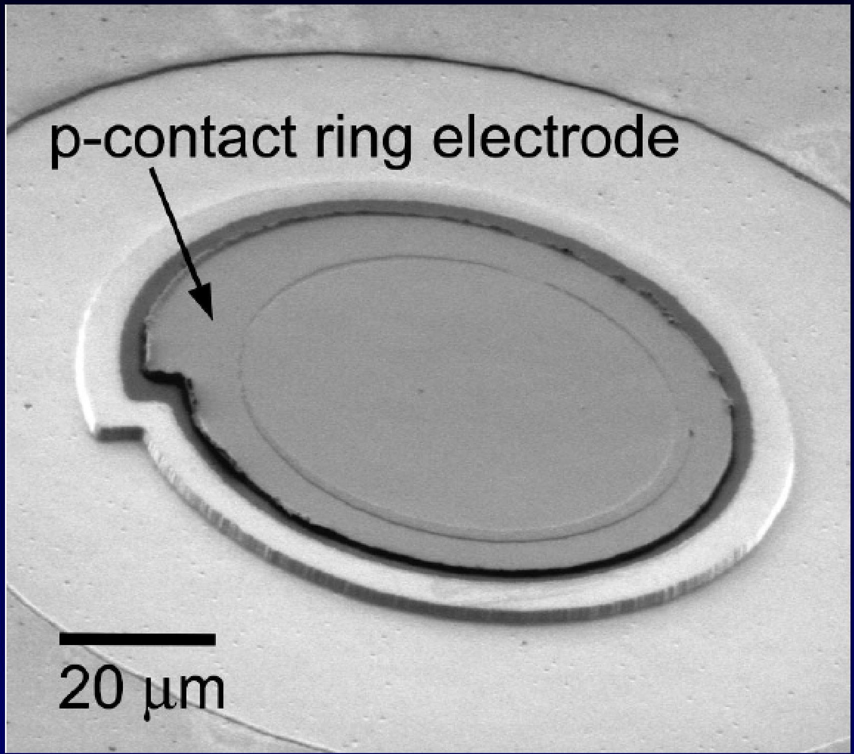
$$N_{\text{Weyl}}(E) = \frac{\text{vol}(\Omega)}{4\pi} E - \frac{L}{4\pi}\sqrt{E} + O(1) \cdots$$

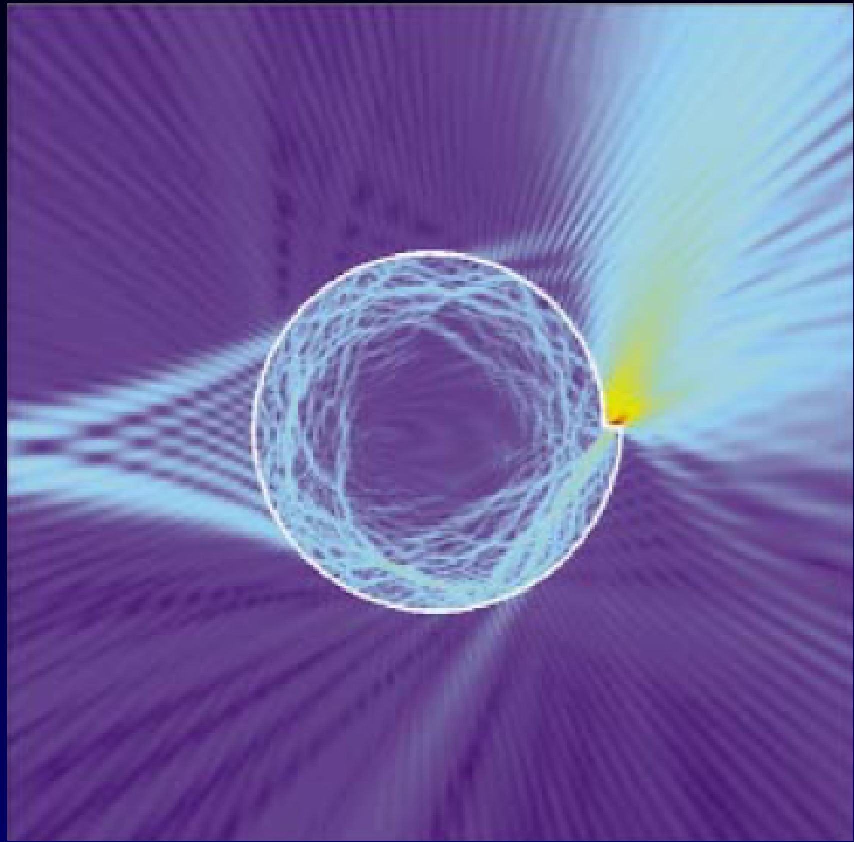




- not one level missing in sequence of 6812

Future laser plans: spiral cavity?





micrograph (Kneissl *et al.* '04) numerics (Chern *et al.* '03)

- Optimal shape? Where best to pump (spatially)?
- So far computations hard & limited in wavenumber
- Coupled MPS inside & outside