Quantum mushrooms, scars, and high frequency cavity eigenmodes

UMass Amherst, CAM Seminar, 28 Nov, 2006

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Dirichlet eigenproblem

Normal modes of elastic membrane or ‘drum’ (Helmholtz, Germain, 19^{th}C)

Eigenfunctions ϕ_j of Laplacian $\Delta := \frac{\partial^2}{\partial x^2} + \frac{\partial^2}{\partial y^2}$ in bounded domain $\Omega \subset \mathbb{R}^2$

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

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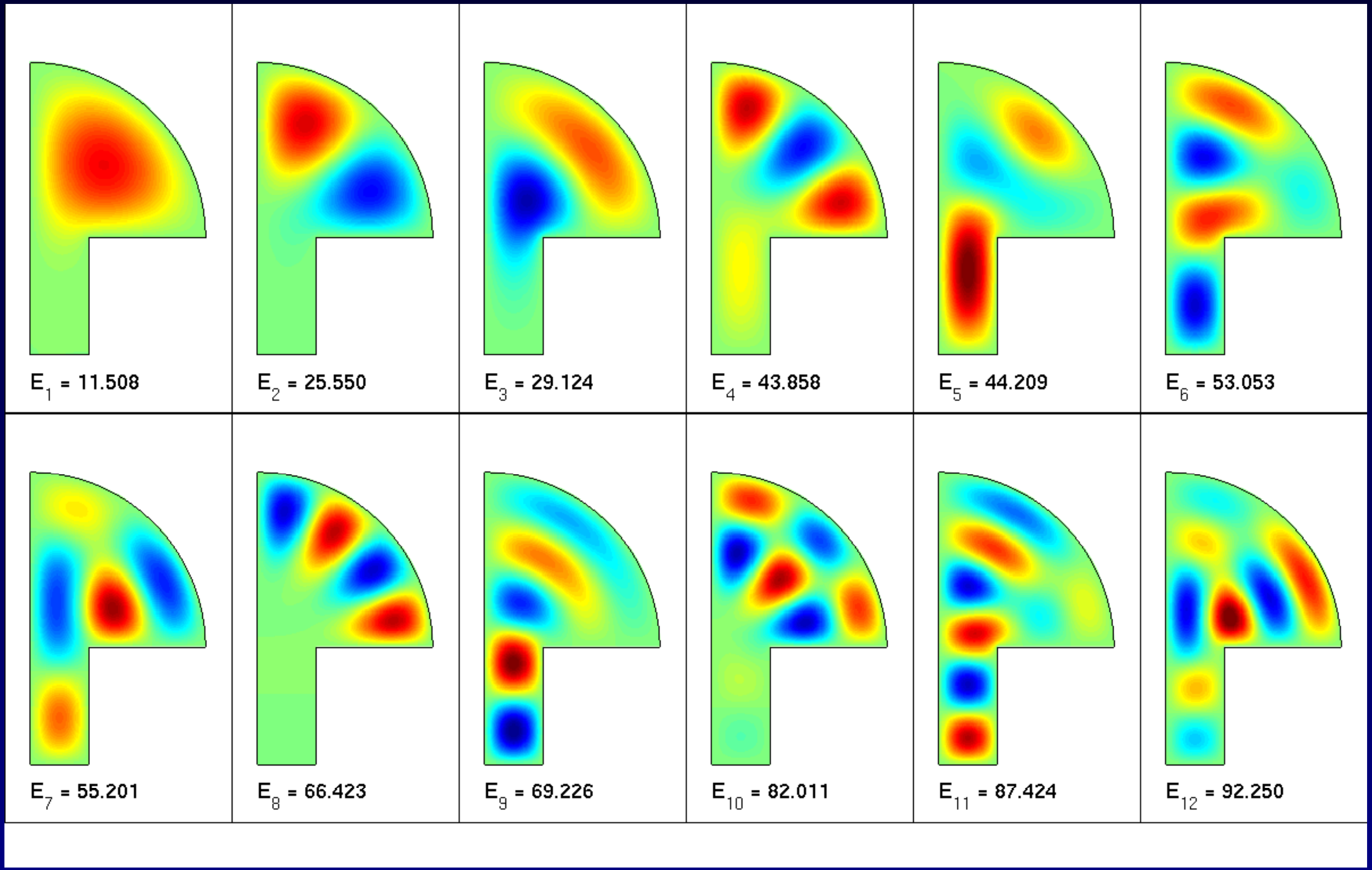

mode $j = 1 \cdots \infty$

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

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

wavelength $\frac{2\pi}{k_j}$

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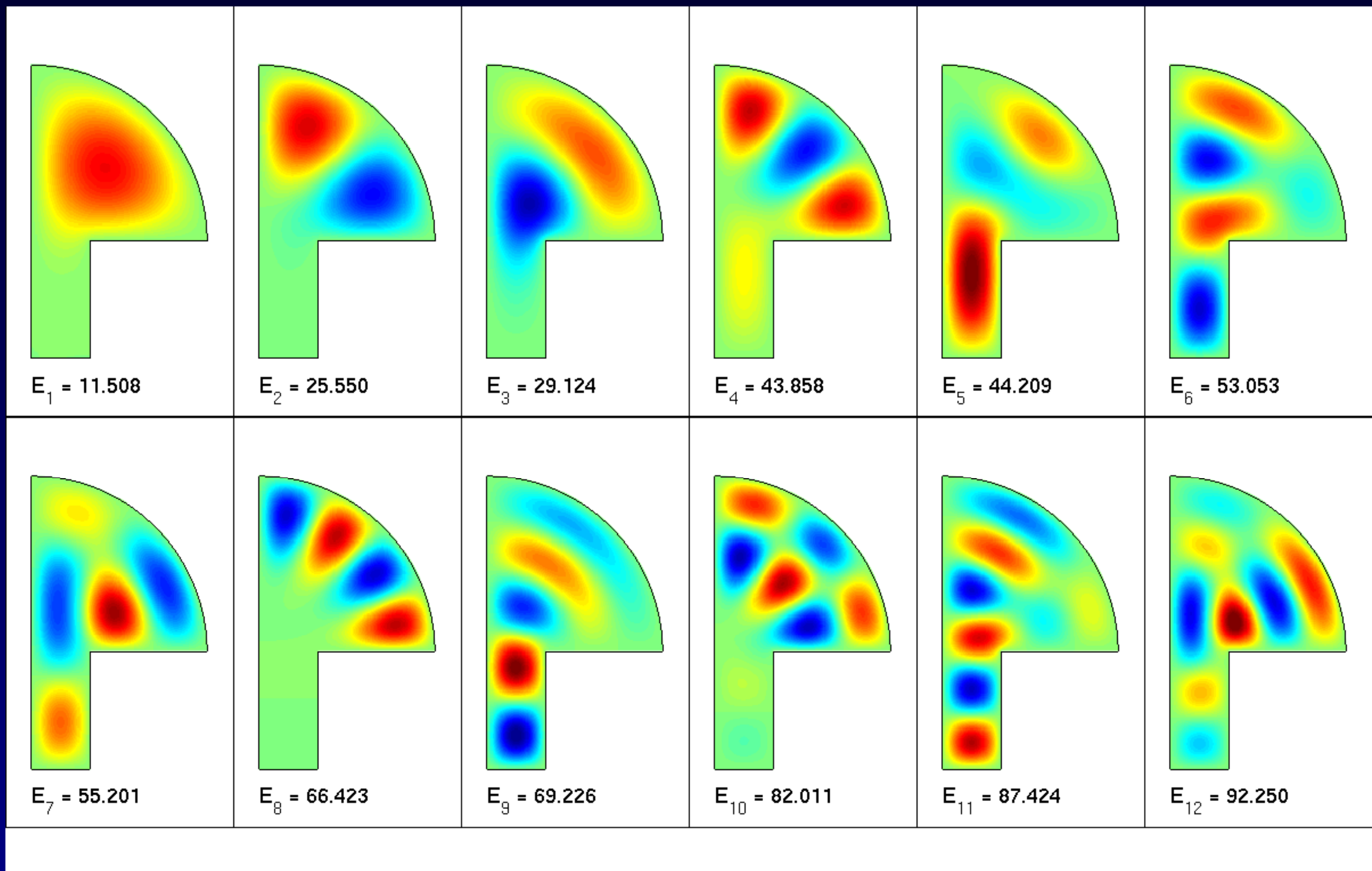

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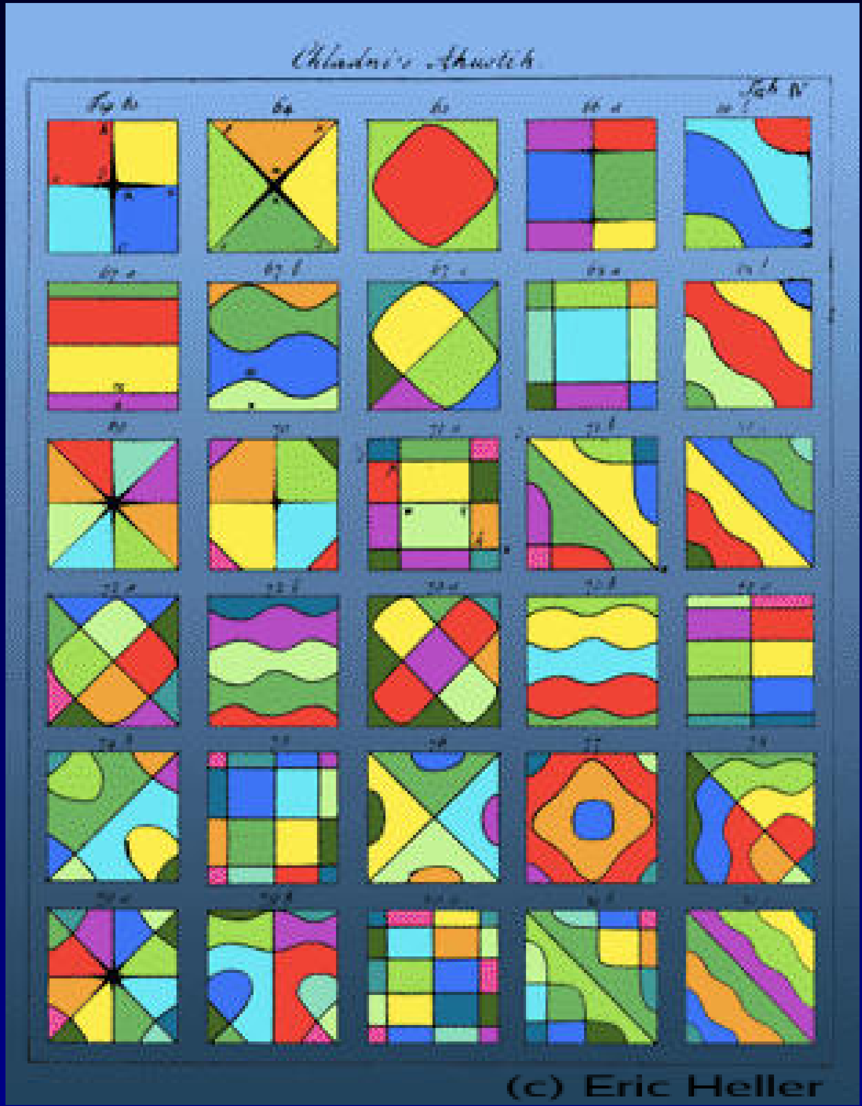
- What are asymptotic properties of modes in $E_j \to \infty$ limit ?

Some history of (related) normal modes

Ernst Chladni (1756–1827) sprinkles sand on metal plates
'Plays' them with violin bow: visualizes nodal lines ($\phi = 0$)



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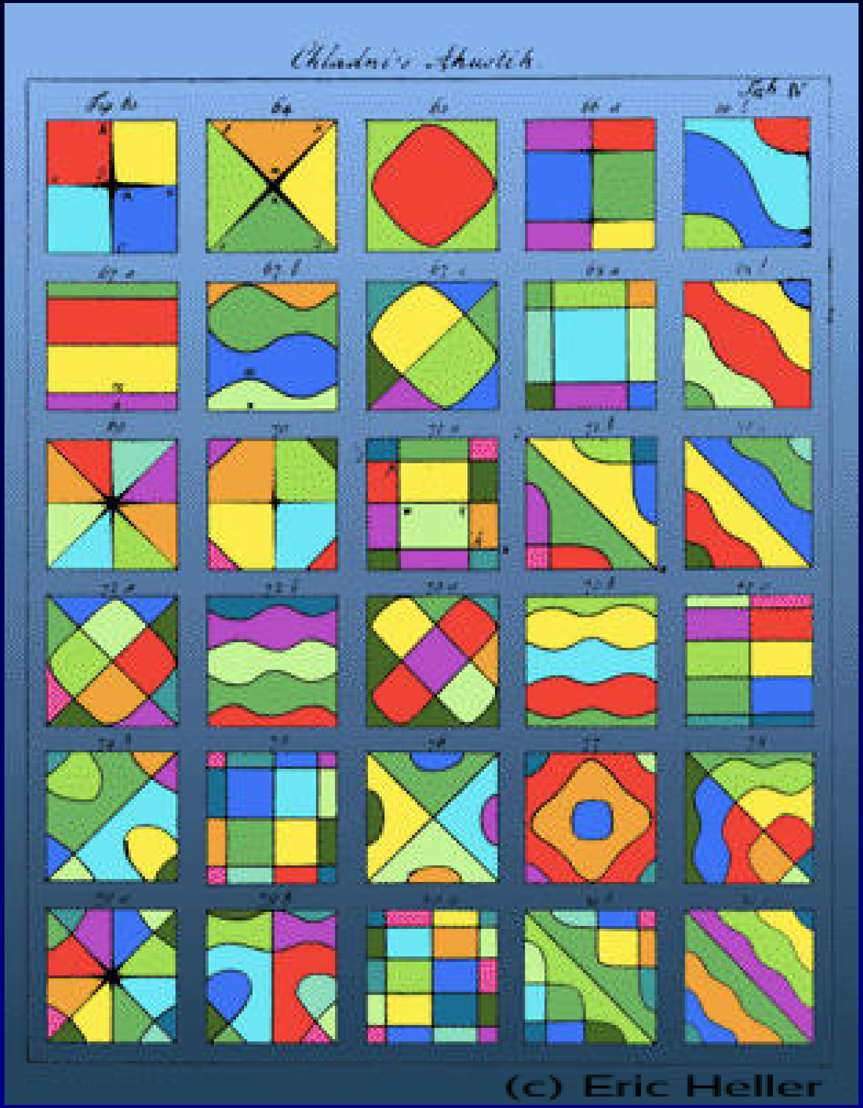

- popular lectures all over Europe
- Napoleon impressed: offers 1 kg gold to explain patterns
- Napoleon realised: irregularly shaped plate harder to understand!
- Sophie Germain got prize in 1816

Note: rigid plate $\neq$ membrane
(biharmonic Δ^2 rather than Laplacian Δ)

Modern applications

- electromagnetic waveguides (TM modes)
- acoustic resonances (Neumann BCs) *e.g.* aircraft cabin design
- paradigm for trickier resonance problems *e.g.* 3D RF/optical cavities

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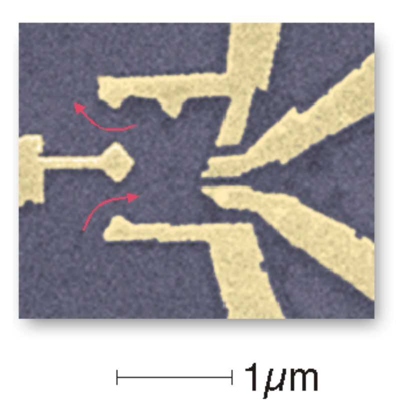
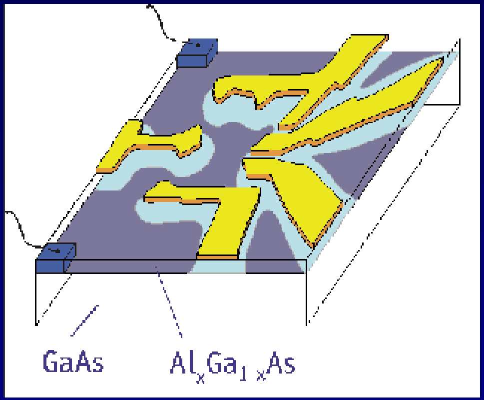
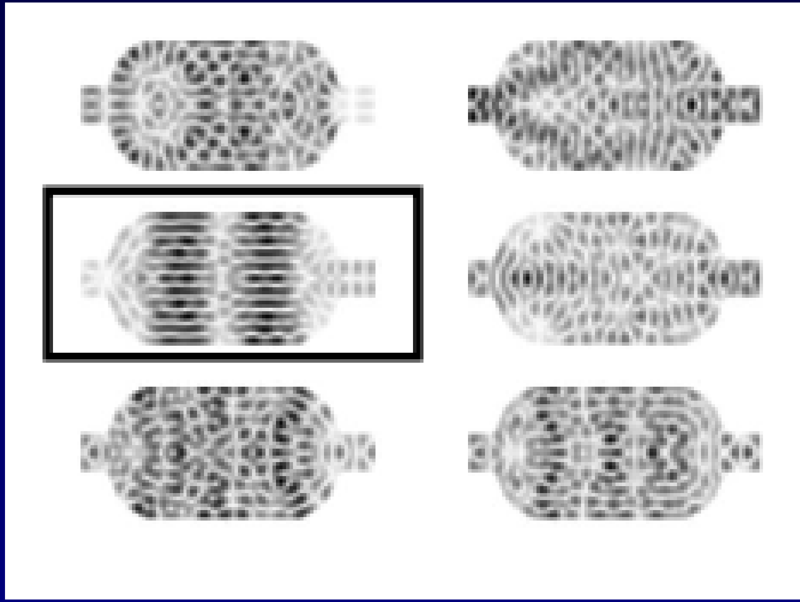
- single-particle quantum mechanics *e.g.* modeling quantum dots





quantum dots (Marcus)

resonant transmission, often single closed-dot mode responsible

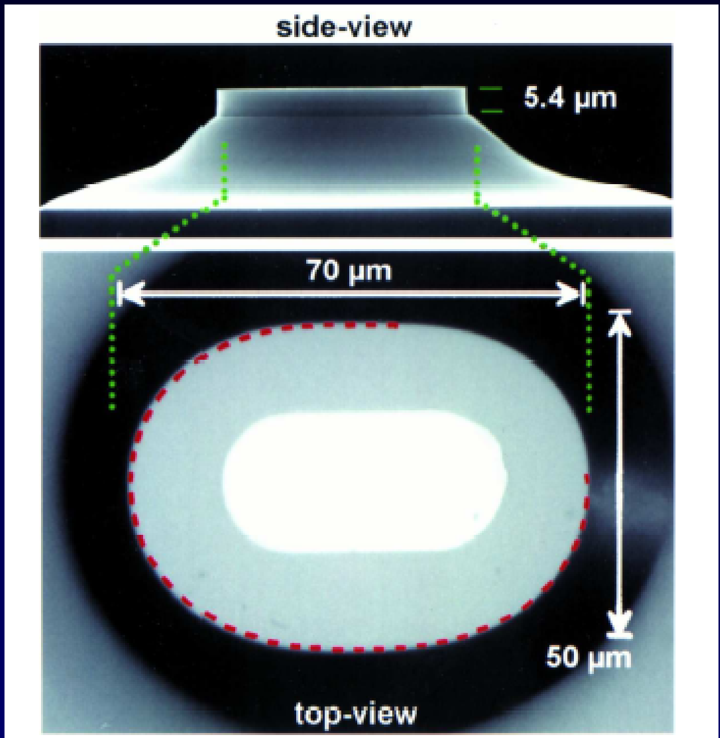


transport statistics (Akis)

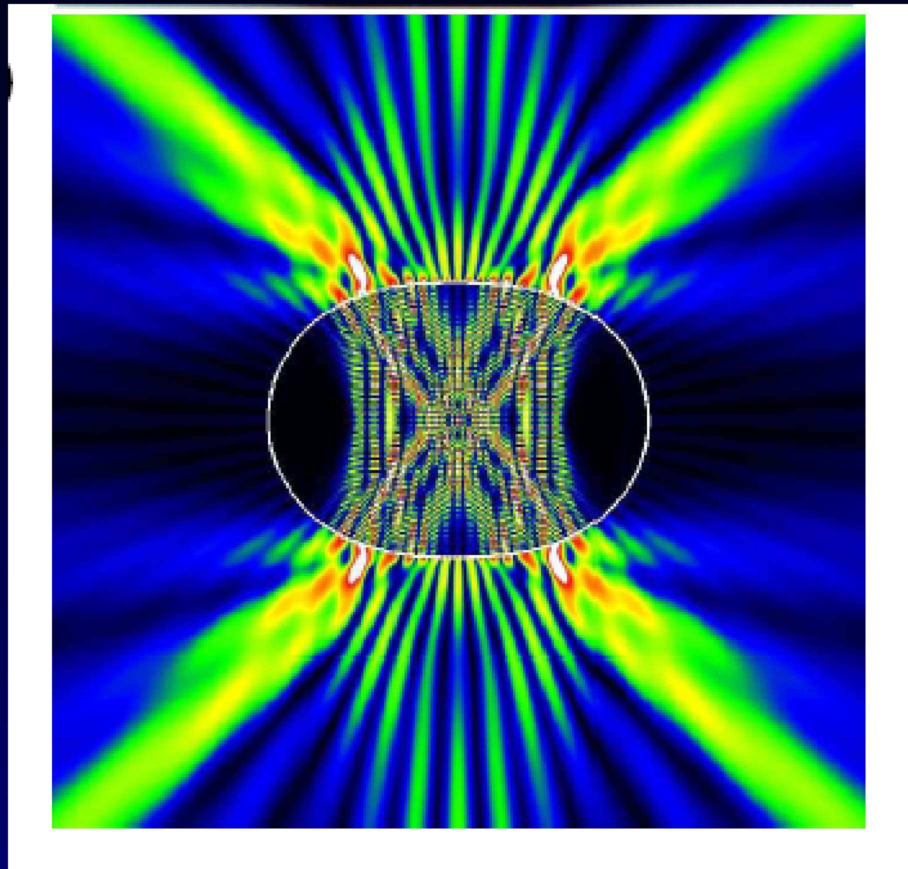
Dielectric micro-cavity laser design

leaky resonant cavities

quantum-cascade laser (Gmachl)



mode and emission pattern



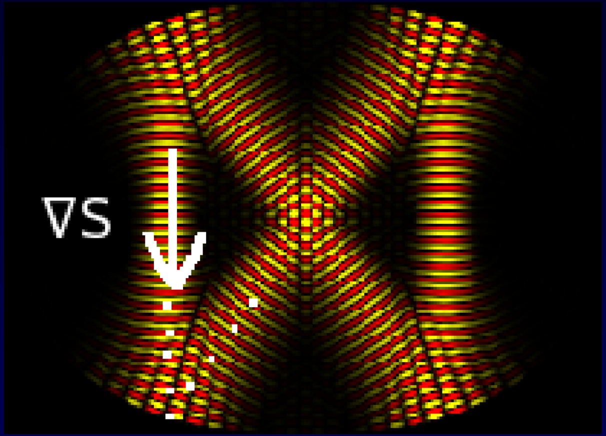
- 2D cavity confinement due to total internal reflection ($n = 3.3$)
- approximated by Dirichlet eigenmodes; system size 10–50 λ
- optimize design: need many modes for many shapes (Tureci '03)

Einstein-Brillouin-Keller (EBK) **(Keller '60)**

Recall $\{\phi_j\}$ are products of 1D modes if Δ separable (ellipse, rectangle)

If not, can use short wavelength asymptotic mode approximation:

$$\phi(x,y) \;\approx\; \sum_{m=1}^{M} A_m(x,y)\, e^{ikS_m(x,y)}$$



mode ≈ sum of traveling waves, 'rays'

S_m = phase function

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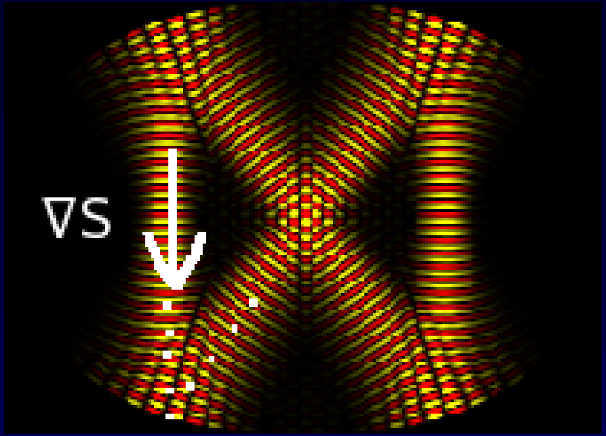

Substitute into $-\Delta\phi = E\phi$ gives

$|\nabla S_m| = 1$ eikonal: phase grows along straight rays

For such modes to exist:

i) rays reflect off boundary, giving ray families which must close

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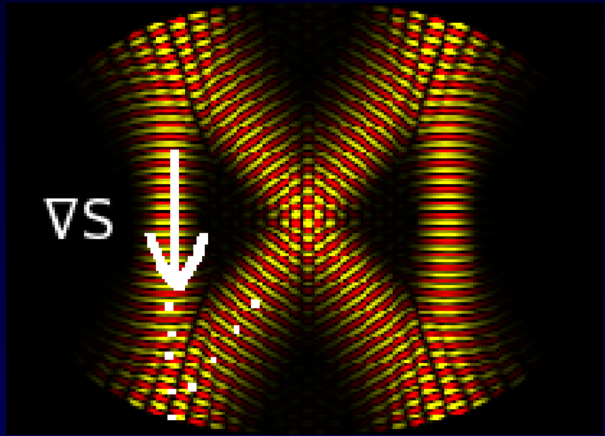

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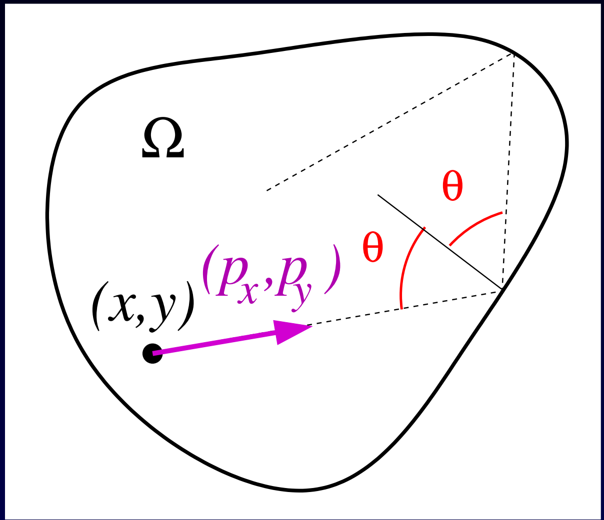
But, do bouncing ray paths always form closed families. . . ?

Bouncing rays: the game of billiards



phase space: (x, y, p_x, p_y)

$(x, y) = \mathbf{x} =$ position

$(p_x, p_y) = \mathbf{p} =$ momentum

trajectory $\mathbf{x}(t)$

free motion with reflection

Hamiltonian dynamical system: energy $H(\mathbf{x}, \mathbf{p}) = |\mathbf{p}|^2$ conserved

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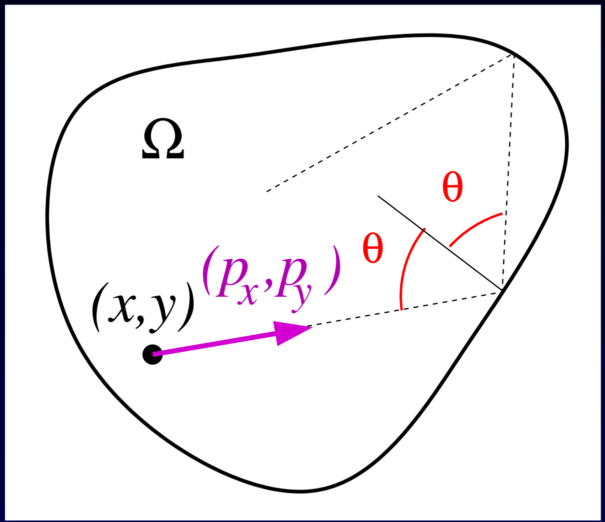

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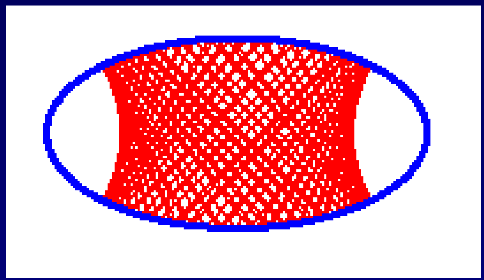
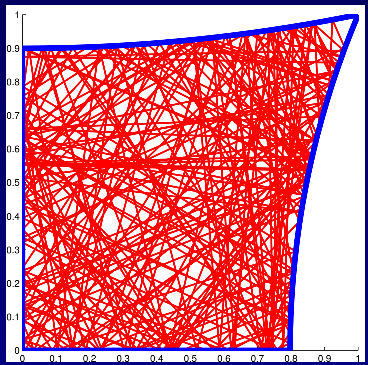
TWO BROAD CLASSES

integrable: 

d conserved quantities ($d = 2$)

(tori → closed ray families)

ergodic: 

energy alone conserved: chaos!

Quantum chaos

Class of ray dynamics in Ω has profound effect on eigenmodes. . .

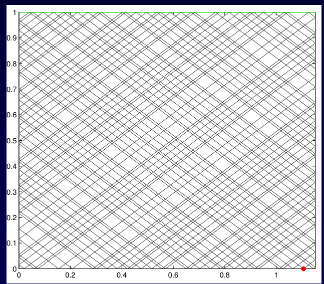
Quantum chaos

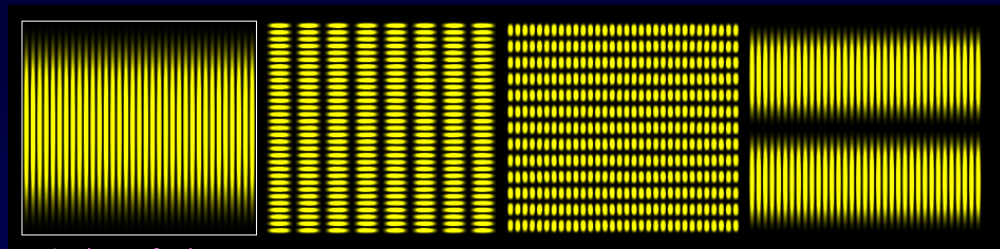
Class of ray dynamics in Ω has profound effect on eigenmodes…

rays (classical) eigenmodes ϕ_j (quantum)

Integrable:

d conserved quantities

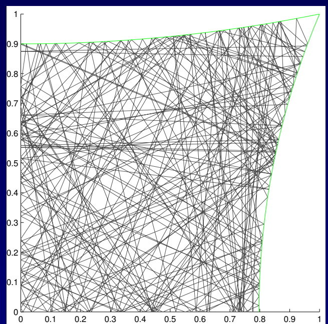


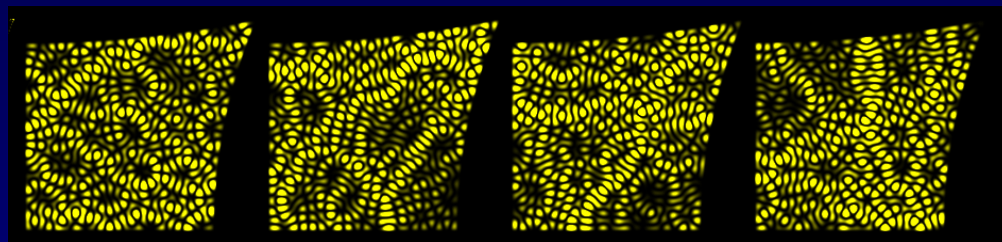


regular modes: separable or EBK

Ergodic:

covers whole energy shell





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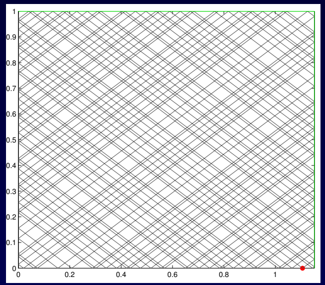

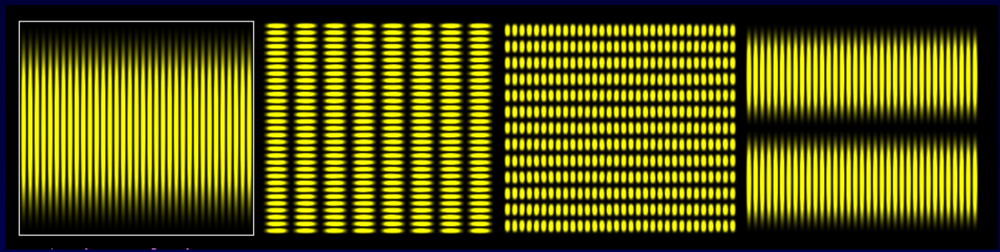

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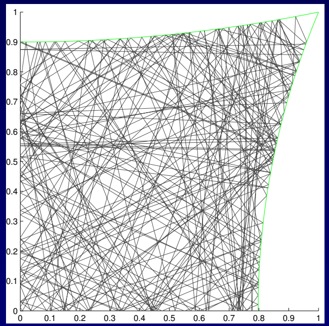

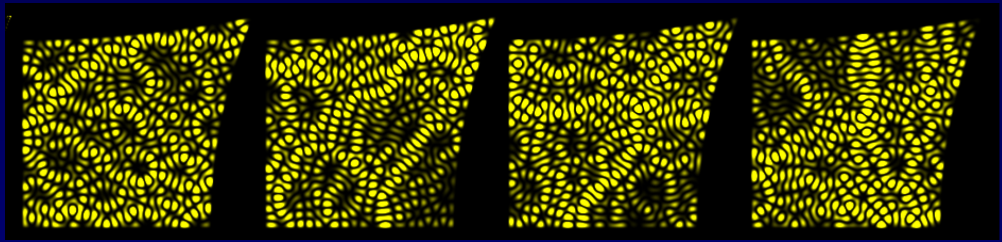

irregular modes: ‘quantum chaos’

(phase space may contain both integrable and ergodic pieces, other subtle categories)

Mathematical questions

1. Quantum chaos: what happens in $E \to \infty$ semiclassical limit?

(Einstein 1917; Gutzwiller, Berry '80s; Zelditch…)

- impact: atomic, molecular, mesoscopic physics…
- more general Riemann surfaces: modular forms, number theory
- eigenvalue E_j statistics $\leftrightarrow$ Random Matrix Theory (unproven!)

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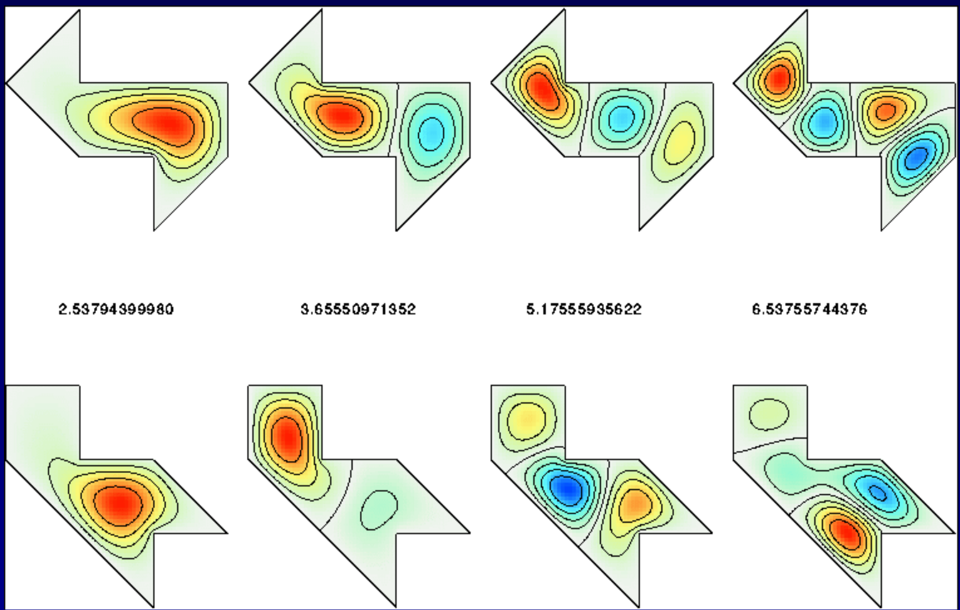
2. Spectral geometry: can one hear the shape of a drum? (Kac '66)



Answer: no !

(Gordon *et al.* '92)

Isospectral drums, numerics to 14 digits

(Driscoll '97)

Engineering, physics, and mathematical questions all pose the following *numerical* challenges:

1. Complex geometry and cavity shapes, *e.g.* corners, 3D
2. Higher frequencies: multiscale problem (wavelength $\ll$ system size)

Outline of rest of talk

I. Quantum ergodicity

II. A new type of ‘scarring’ of eigenmodes

III. The numerical methods that make it all possible

I. Quantum ergodicity

Quantum Ergodicity Theorem (QET)

If Ω ergodic, $A(\mathbf{x})$ 'well-behaved' function on Ω, with mean value $\overline{A} := \frac{1}{\mathrm{vol}(\Omega)} \int_\Omega A(\mathbf{x}) d\mathbf{x}$, then

$$\lim_{E_j \to \infty} \langle \phi_j, A\phi_j \rangle - \overline{A} \;=\; 0 \qquad \forall j \text{ except subseq. of vanishing density}$$

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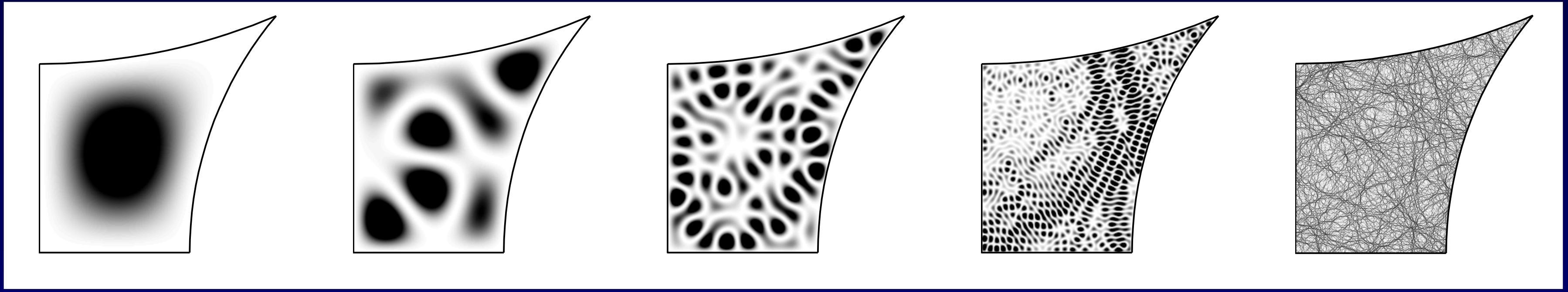

$j = 1$ $\quad$ $j = 10$ $\quad$ $j = 10^2$ $\quad$ $j = 10^3$ $\quad$ $j \approx 5 \times 10^4$

Proof: Egorov's Thm (microlocal analysis, time propagation of wave eqn)

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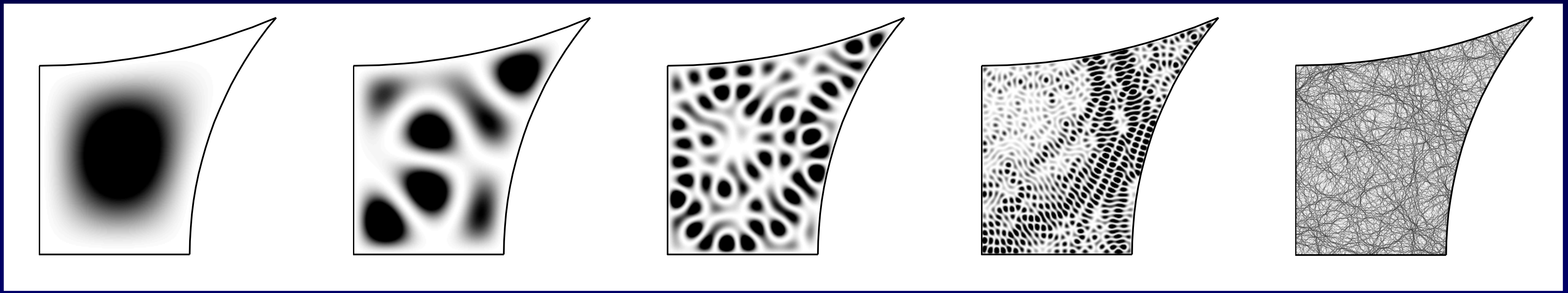

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Of practical importance: At what *rate* is limit reached?
How fast does the density of excluded subsequence vanish?

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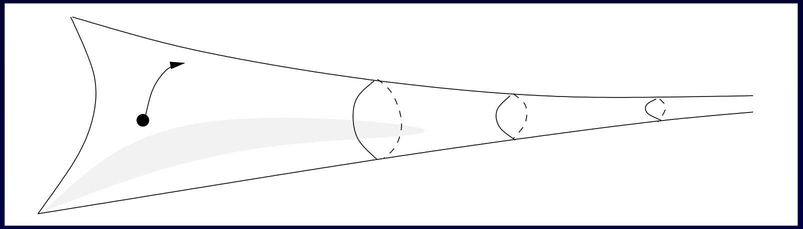

Recent rigorous analytic results:

- QUE proven for *arithmetic* manifold $SL_2(\mathbb{Z}) \setminus \mathbb{H}$ (Lindenstrauss '03)
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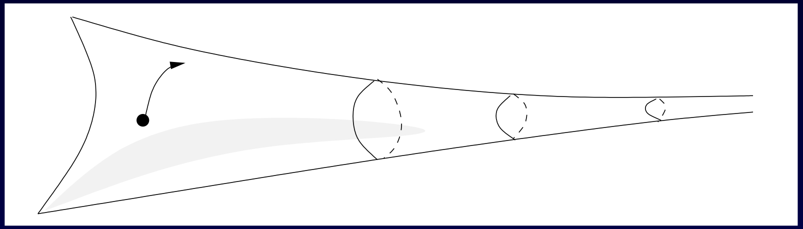

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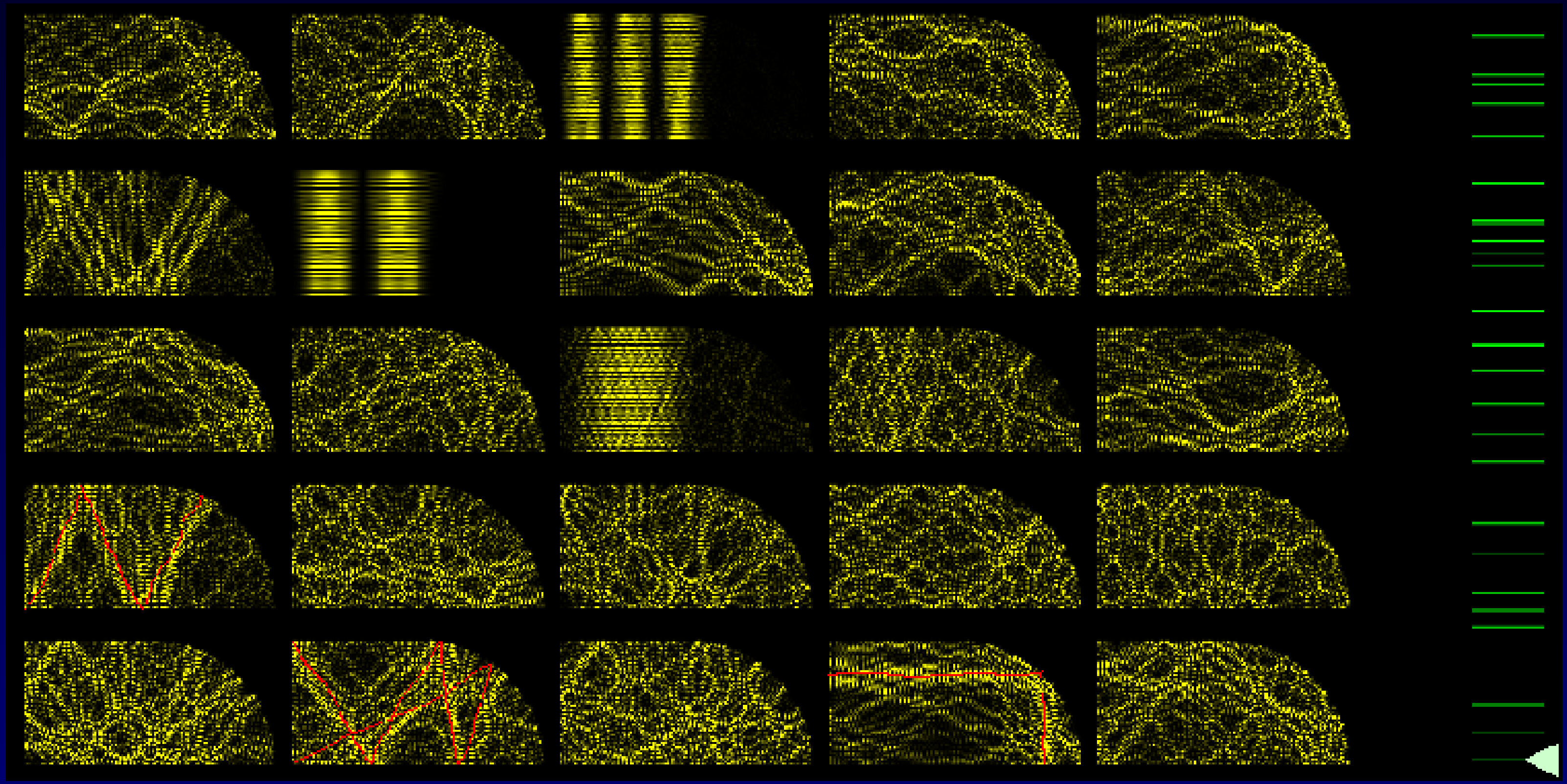
QUE might be a surprise for chaotic cavity eigenmodes because of…

Scars: an exceptional subsequence?

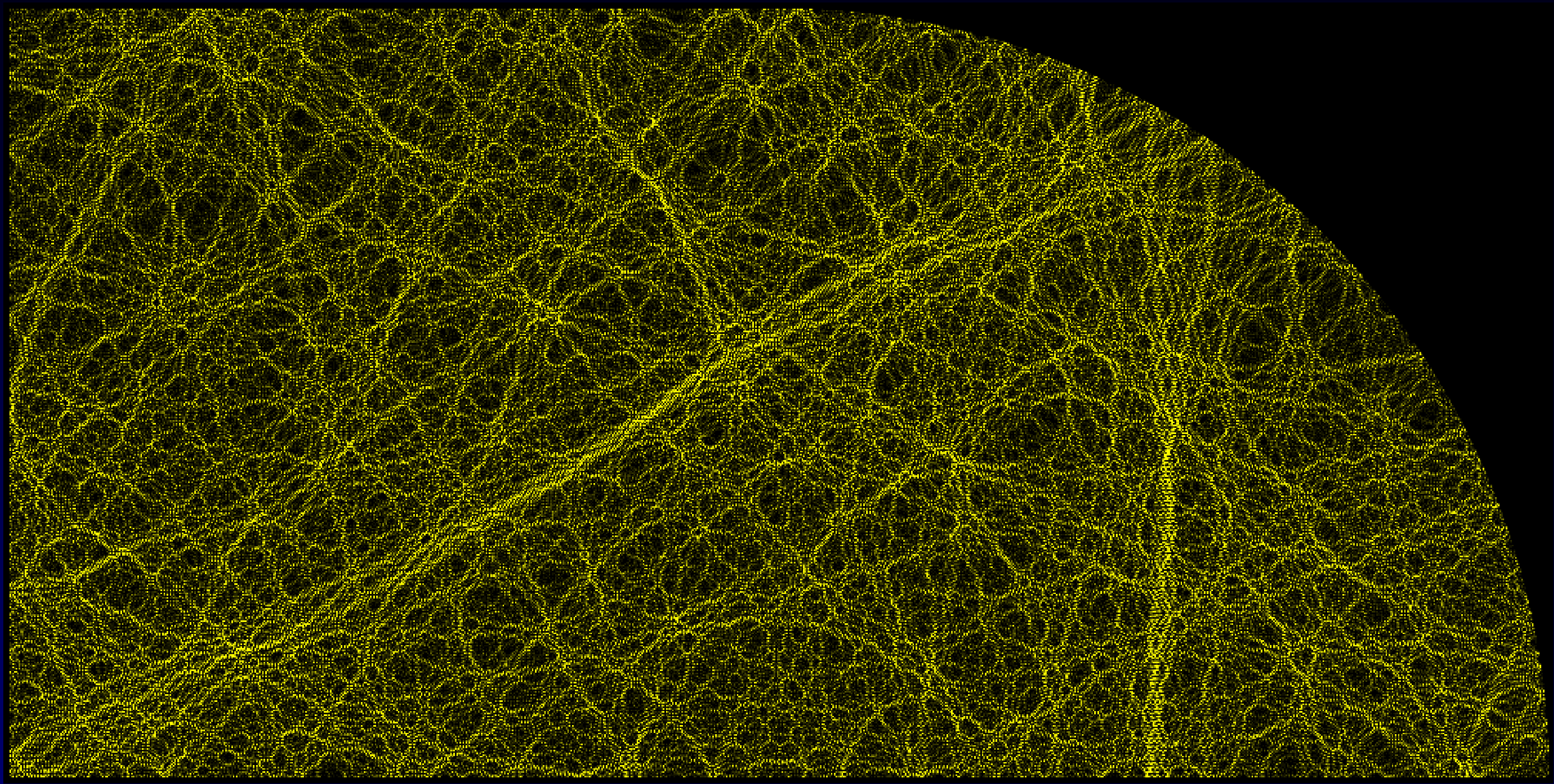
High-j modes $|\phi_j|^2$ sometimes localize on unstable periodic orbits (UPO)

- discovered by *numerical* study of quarter-stadium modes (Heller '84)



- Wavepacket arguments $\Rightarrow$ transverse width dies as $\sim E^{-1/4}$
- Note here also exceptional 'bouncing ball' sequence (neutrally stable)

High-eigenvalue scarred stadium mode

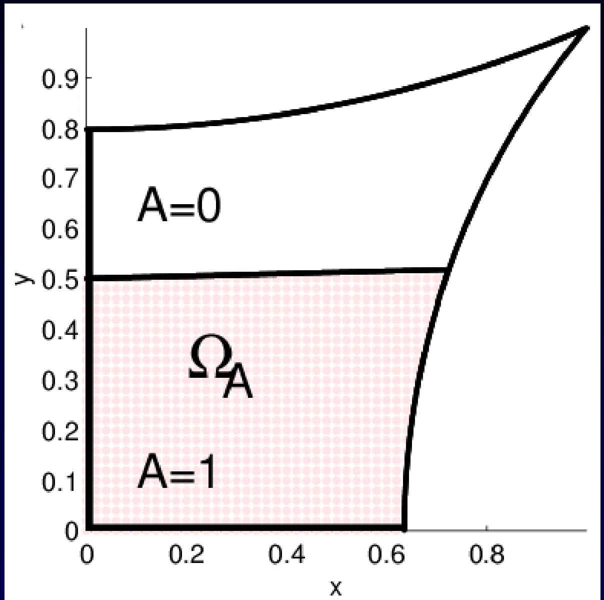


- ‘strong’ scar if there is a sequence $\{\phi_{j_n}\}$ with $O(1)$ mass on UPO
- QUE implies ‘weak’ scarring: mass on UPO vanishes as $E \to \infty$

Which occurs? No analytic results in 2D cavities…

Numerical experiments

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



dispersing billiard, proven chaotic (Sinai '70)

$$\text{test function } A = \begin{cases} 1 & \text{in } \Omega_A, \\ 0 & \text{otherwise} \end{cases}$$

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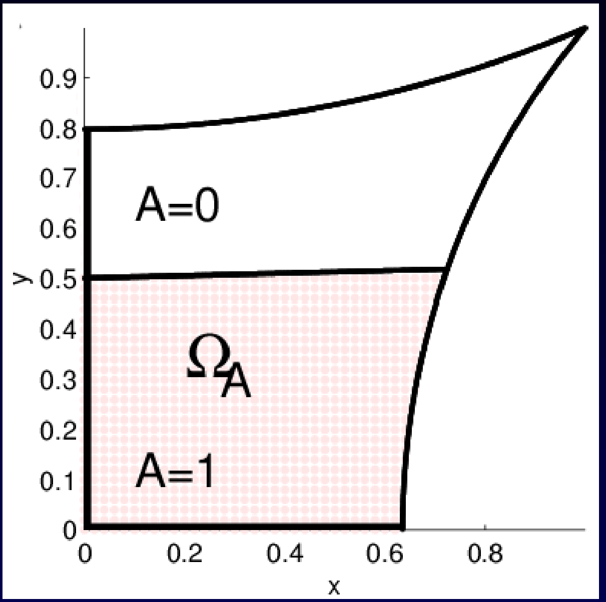


test function $A = \begin{cases} 1 & \text{in } \Omega_A, \\ 0 & \text{otherwise} \end{cases}$

Large-scale study, 30,000 modes in range $j \sim 10^4$ to 10^6, enabled by:

1. Efficient boundary-based numerics for ϕ_j: 'scaling method'
2. matrix elements $\langle \phi_j, A\phi_j \rangle = \int_{\Omega_A} \phi_j^2 d\mathbf{x}$ via boundary integrals

- 100 times higher in j than any previous studies (*e.g.* Bäcker '98)
- only a few CPU-days total

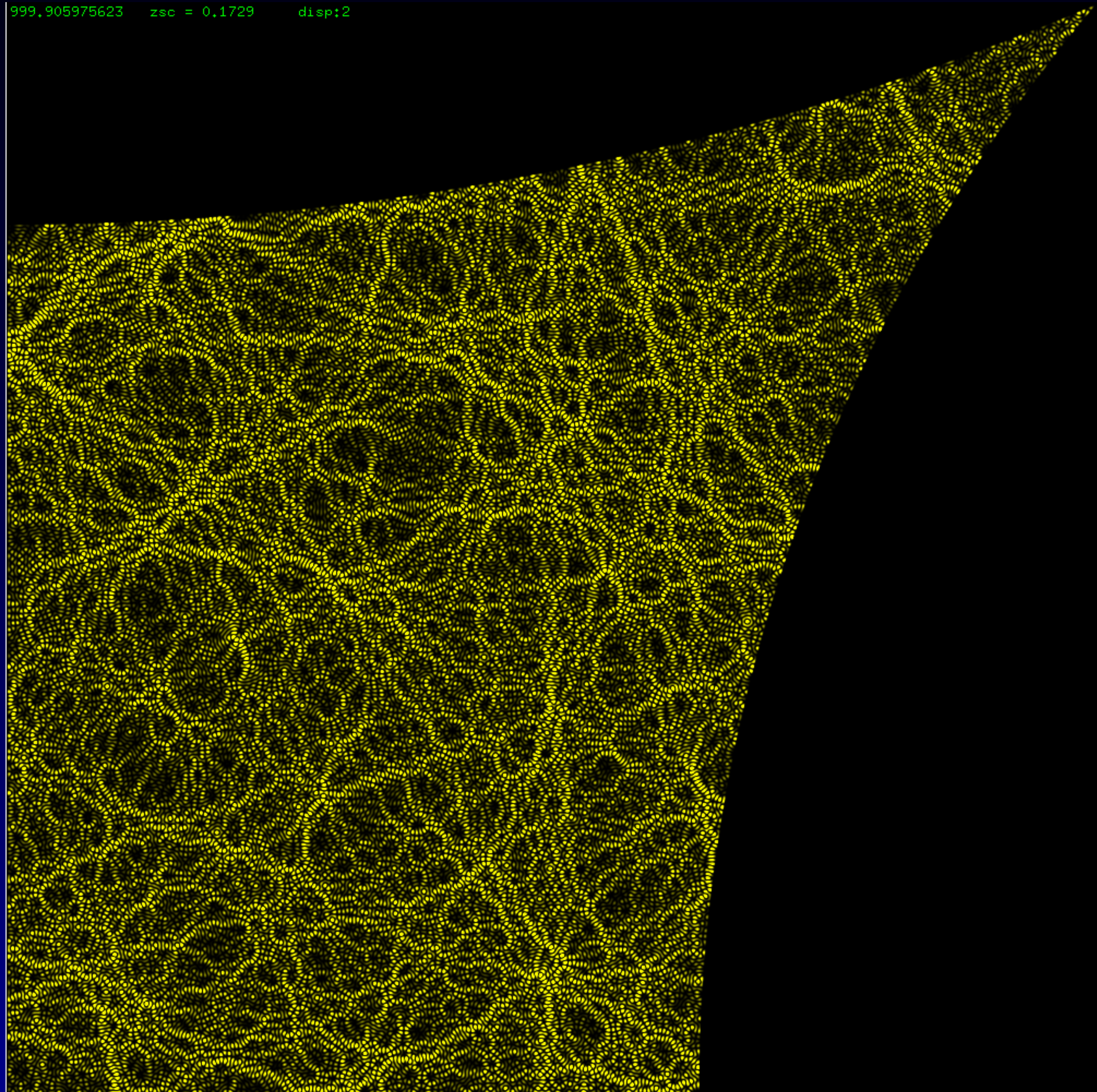
Typical high-frequency ergodic mode

225 λ across

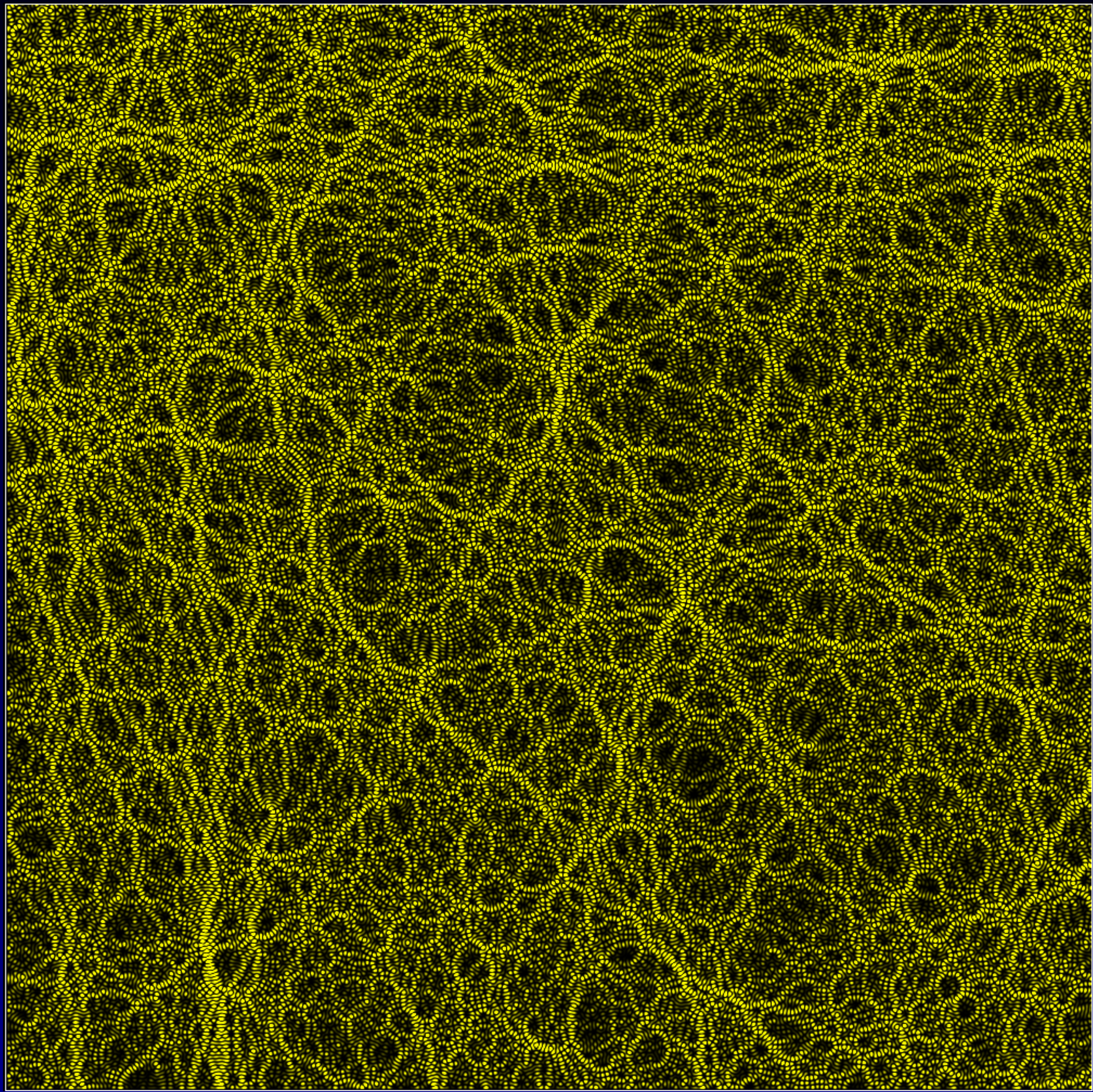
quantum number
$j \approx 5 \times 10^4$

$E_j \approx 10^6$

not very uniform,
rather, stringy…



(compare: random sum of plane waves)



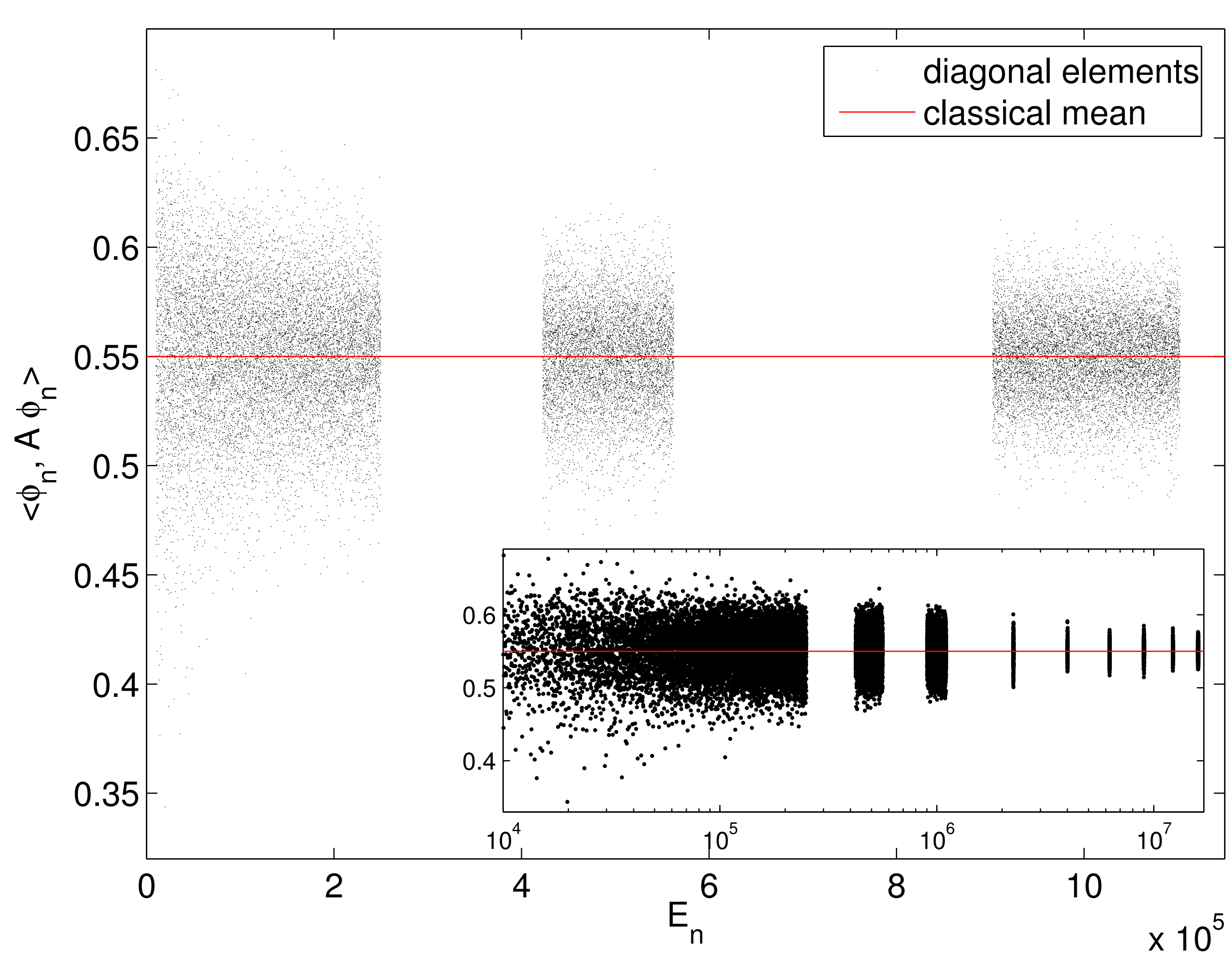
$\mathrm{Re}\sum_m a_m e^{i\mathbf{k}_m\cdot\mathbf{x}}$

all wavenumbers
$|\mathbf{k}_m| = \sqrt{E} = \text{const.}$

also stringy…
interesting
to the eye only?
(a mystery)

Raw diagonal matrix element data

To reach high E, calculate $\langle \phi_j, A\phi_j \rangle$ only in certain eigenvalue intervals



- strong evidence for QUE (exceptional fraction $< 3 \times 10^{-5}$)

Rate of quantum ergodicity

E-dependent variance $\quad V_A(E) :=$ local average of $\left|\langle \phi_j, A\phi_j \rangle - \overline{A}\right|^2$

At what rate does this 'quantum variance' die as $E \to \infty$?

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Conjecture (Feingold-Peres '86): $V_A(E) \sim \dfrac{2\tilde{C}_A(0)}{\mathrm{vol}(\Omega)} E^{-1/2}$

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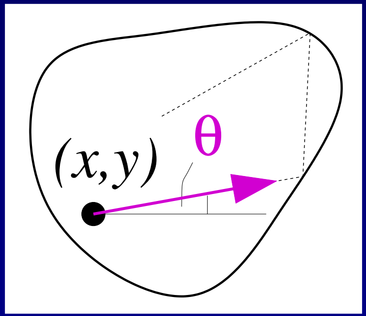
E-dependent variance $\quad V_A(E) :=$ local average of $\left|\langle\phi_j, A\phi_j\rangle - \overline{A}\right|^2$

At what rate does this 'quantum variance' die as $E \to \infty$?

Conjecture (Feingold-Peres '86): $\qquad V_A(E) \sim \dfrac{2\tilde{C}_A(0)}{\mathrm{vol}(\Omega)} E^{-1/2}$

- prefactor involves classical quantity $\tilde{C}_A(\omega) := \int_{-\infty}^{\infty} C_A(\tau) e^{i\omega\tau} d\tau$
- autocorrelation $C_A(\tau) := \frac{1}{2\pi \mathrm{vol}(\Omega)} \int_\Omega \int_0^{2\pi} A(\mathbf{x}_0(0)) A(\mathbf{x}_0(\tau)) d\mathbf{x}_0 d\theta_0 - \overline{A}^2$



notation: $\mathbf{x}_0(t)$ is the unit-speed trajectory launched at position $\mathbf{x}_0$, angle θ_0

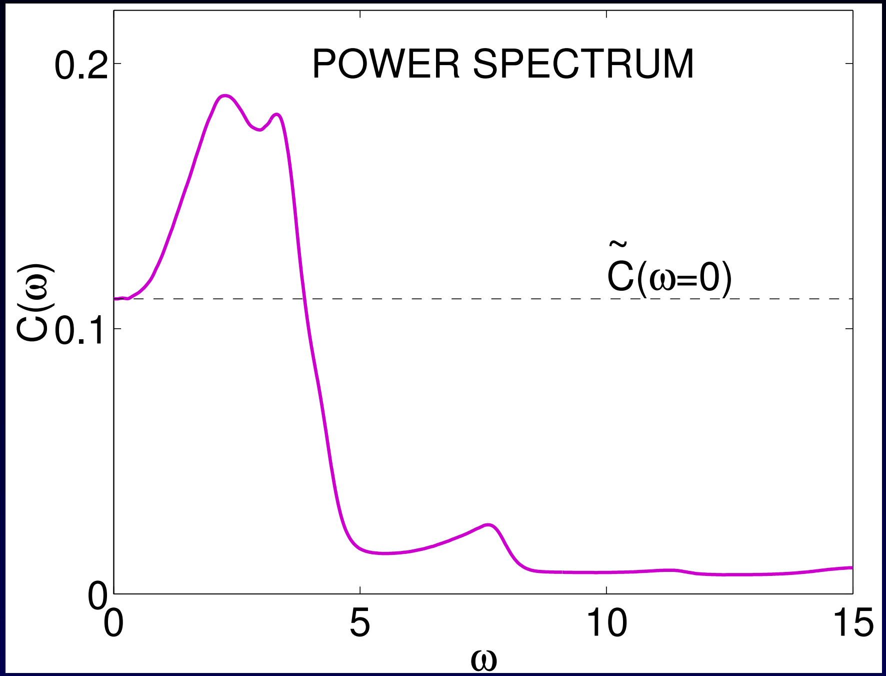
The integral is over the energy shell

Classical variance

$$\tilde{C}_A(\omega) := \int_{-\infty}^{\infty} C_A(\tau) e^{i\omega\tau} d\tau$$

FT of autocorrelation = power spectral density of noisy signal $A(\mathbf{x}(t))$ along ergodic trajectory

LISTEN to it!



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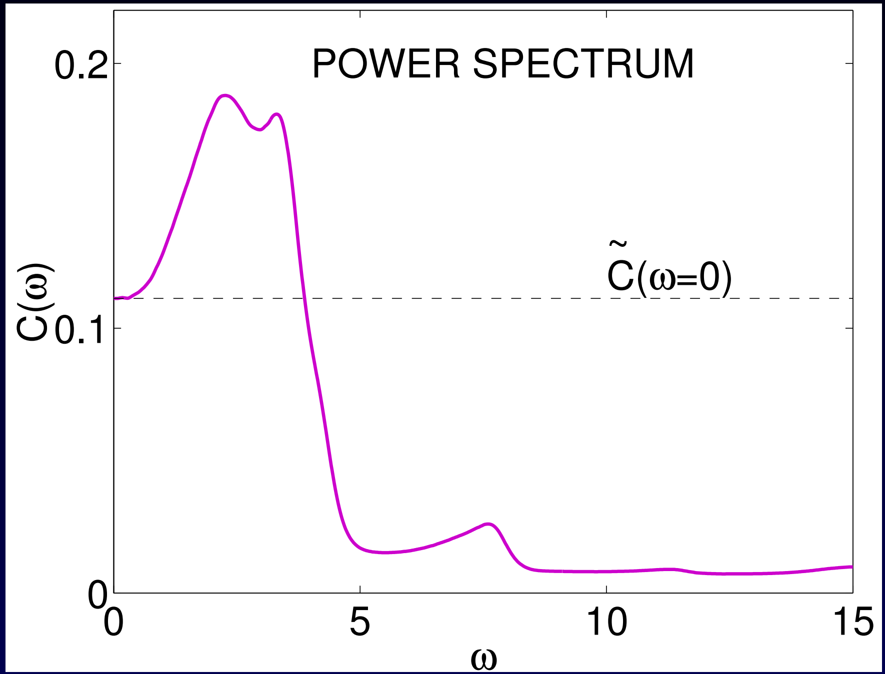


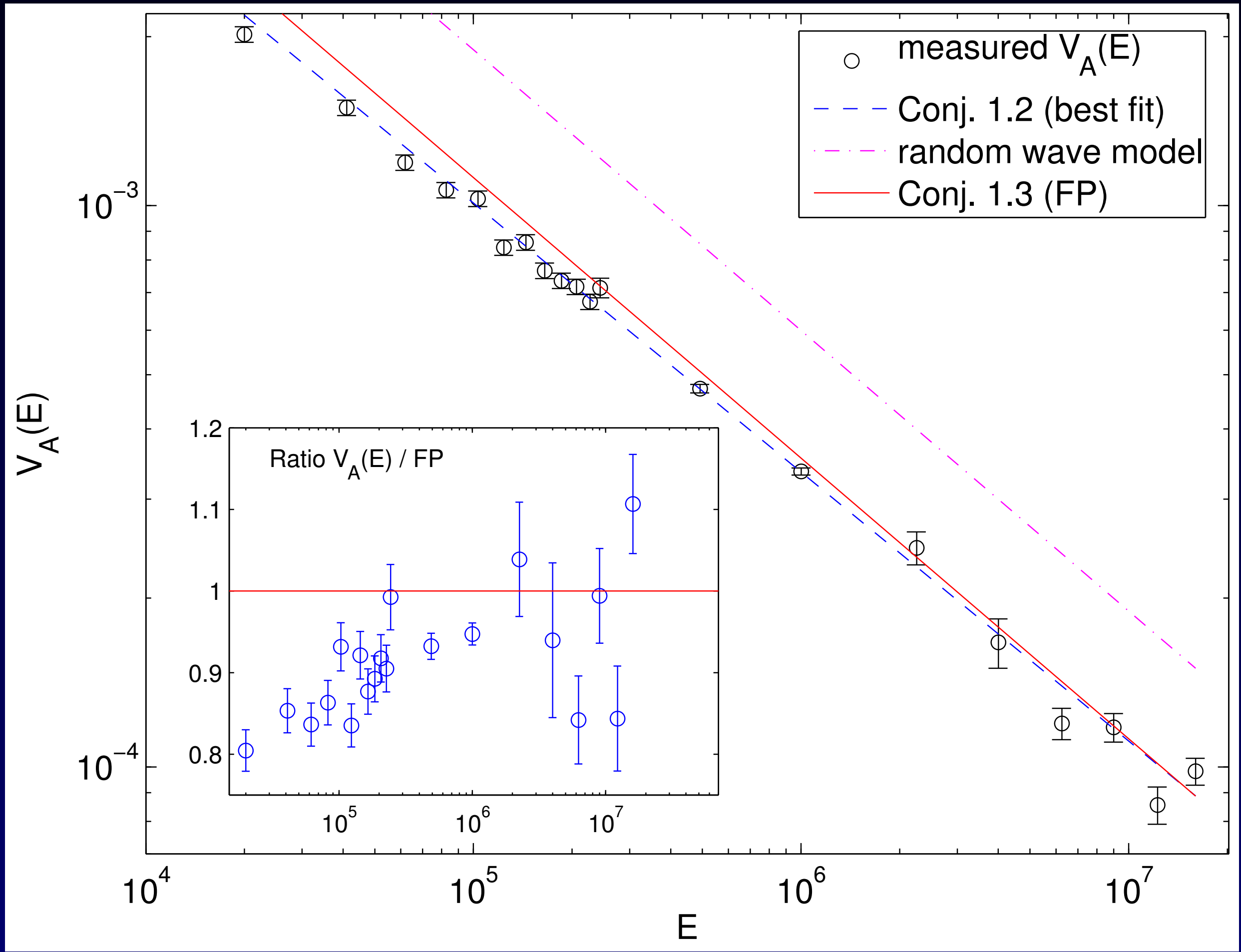
Physically: $\tilde{C}_A(\omega)$ is heating rate due to periodic driving of classical system, at frequency ω, by external field A (Cohen '99, B '00)

- $\tilde{C}_A(\omega)$ gives band profile of off-diagonal elements $\langle \phi_i, A\phi_j \rangle$

FP Conj.: $\omega \to 0$ limit gives prefactor for quantum ergodicity rate

Numerical test: does FP Conj. hold in this ergodic cavity?

Results on ergodicity rate



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

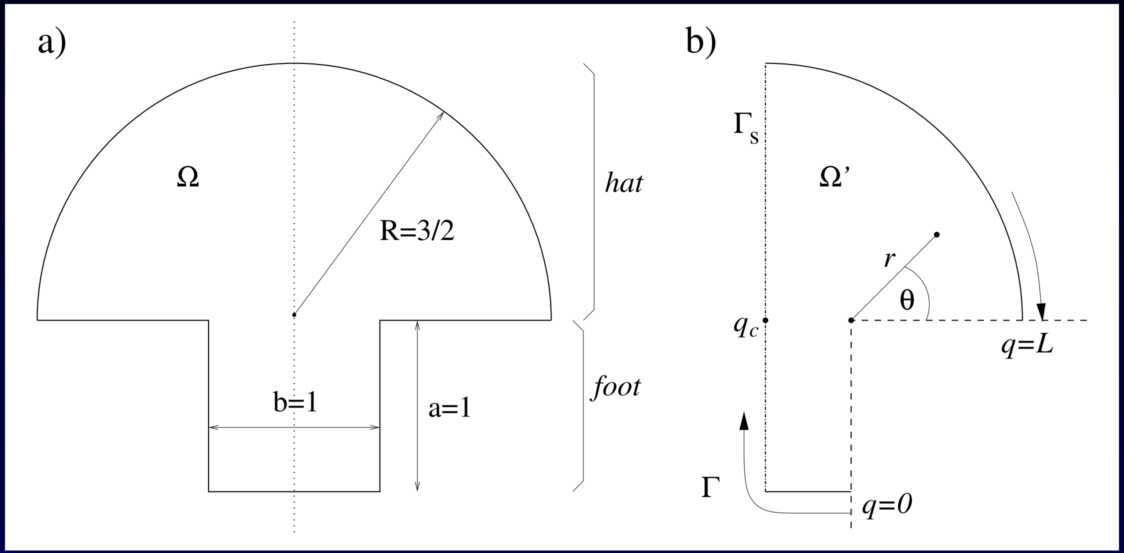
best fit $\gamma = 0.48 \pm 0.01$

(FP Conj. $\gamma = 1/2$)

- large numbers of modes $\longrightarrow$ unprecedented accuracy ($< 1\%$)
- asymptotic regime seen for first time (but more data needed!)
- consistent with FP Conj., convergence very slow: 7% off at $j = 10^5$

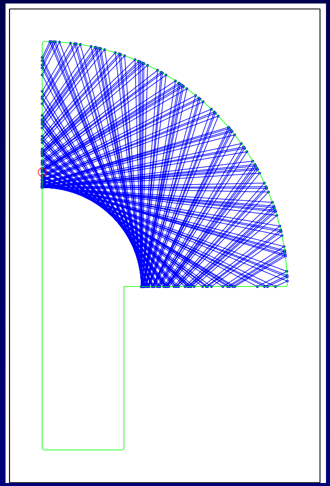
II. New type of ‘moving scar’

Mushroom billiard

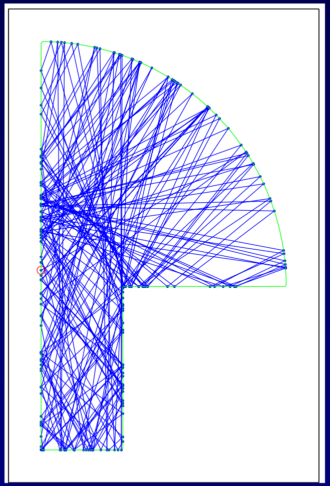


Divided phase space, free from usual KAM hierarchy (Bunimovich '01)

regular:



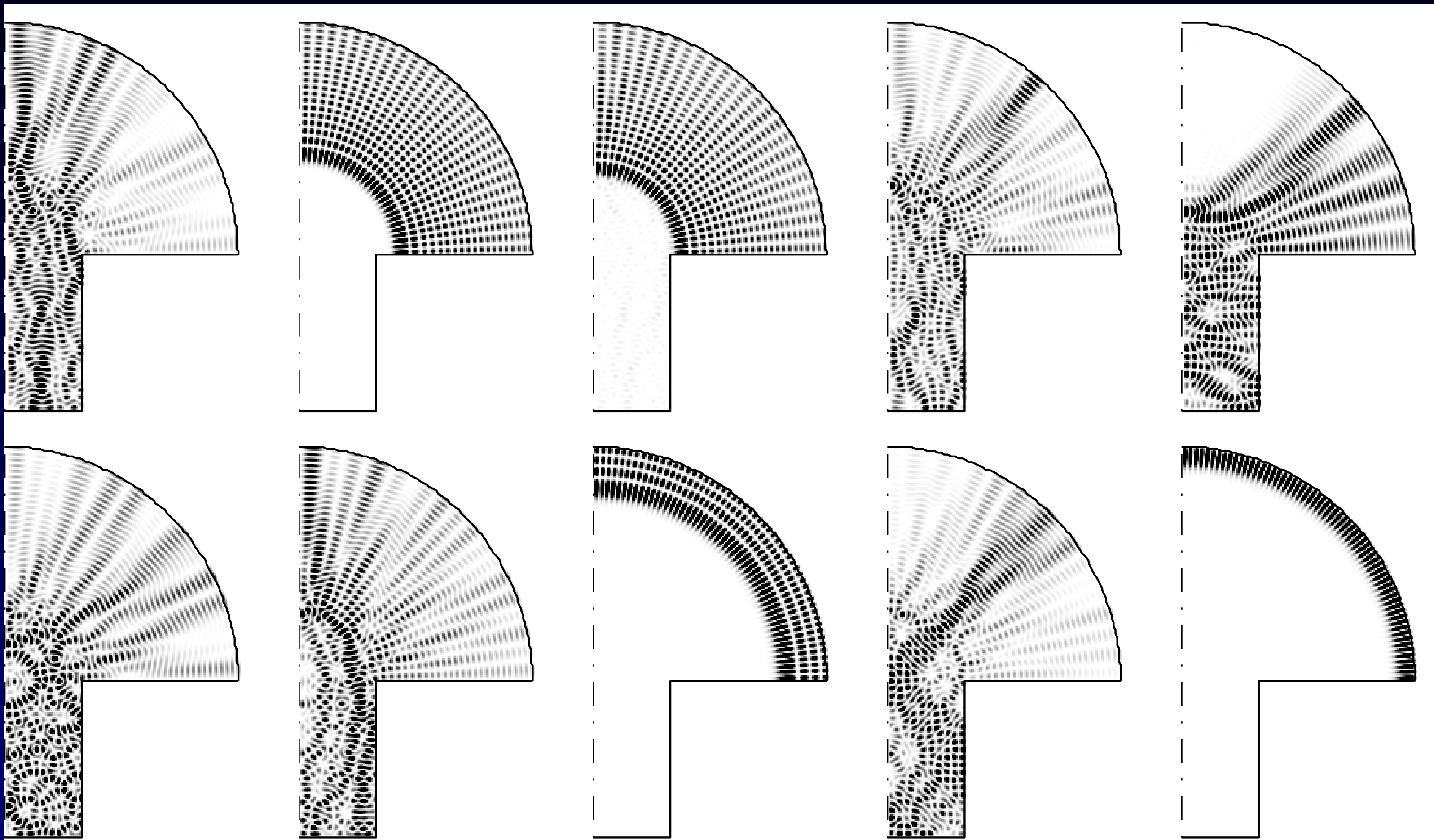
ergodic:



Eigenmodes have not been computed before now. . .

High freq. mushroom modes

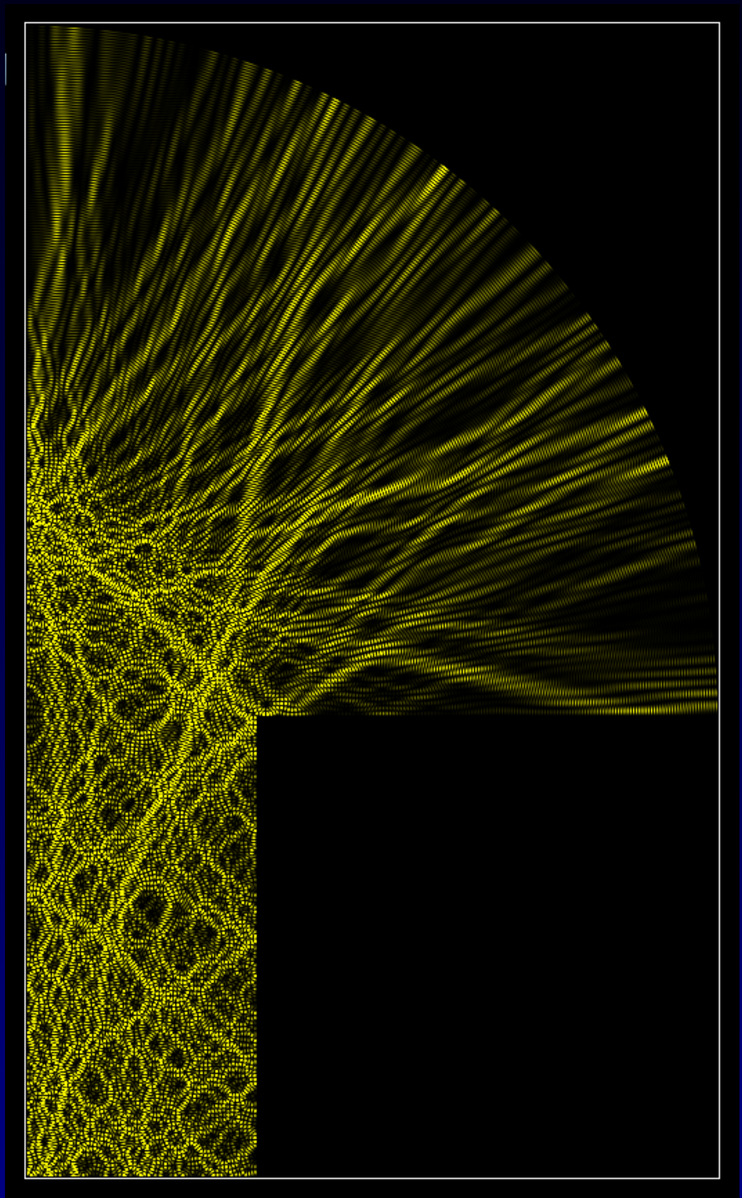
(B-Betcke, sub. to Chaos)



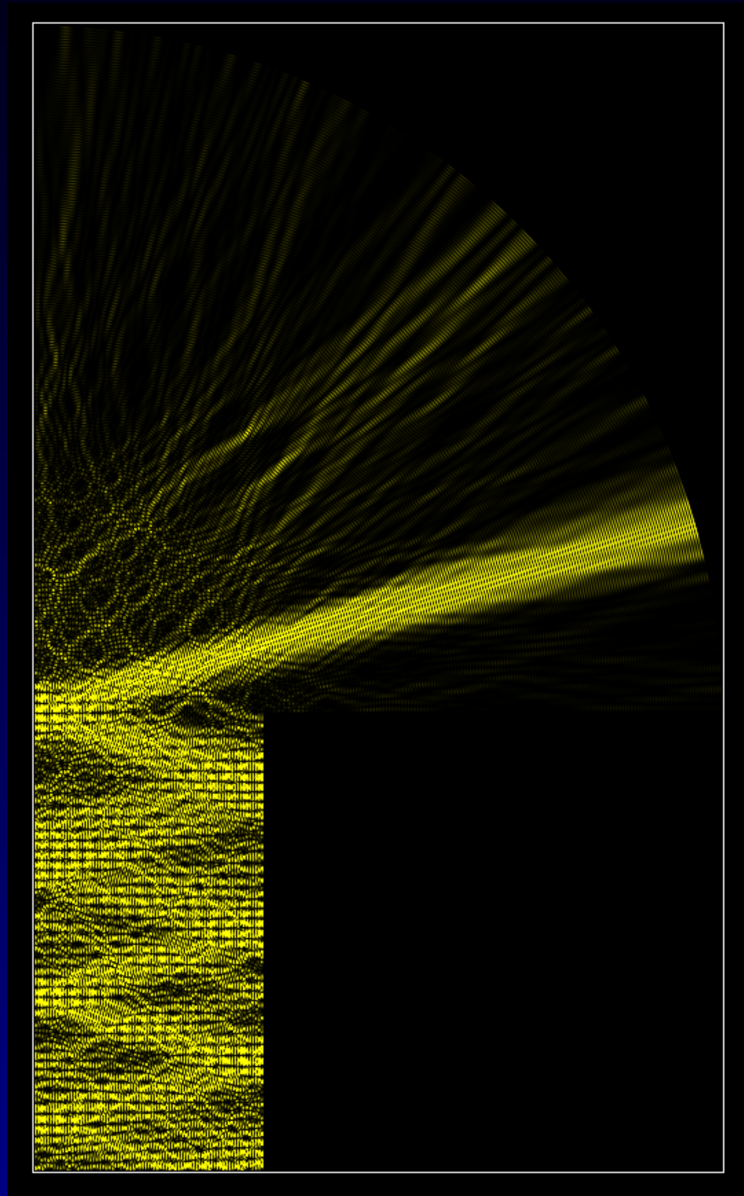
$k = 100$
$j \approx 2000$

- Percival's conjecture verified:
  modes localize to either regular or chaotic region

Very high freq. mushroom modes



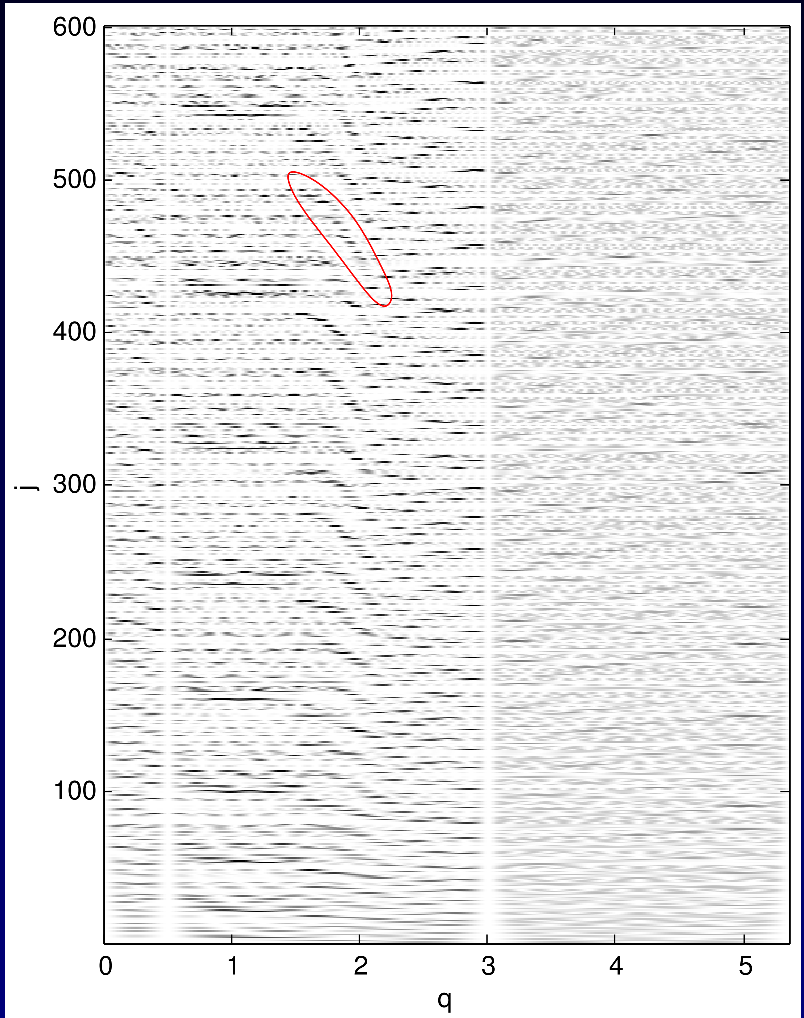
ergodic, equidistributed



ergodic, strongly scarred

Moving scar in boundary functions

$|\partial_n \phi_j(q)|^2$, boundary location q:



- sloping streak effect

MODES SMOOTHED

Moving scar in boundary functions

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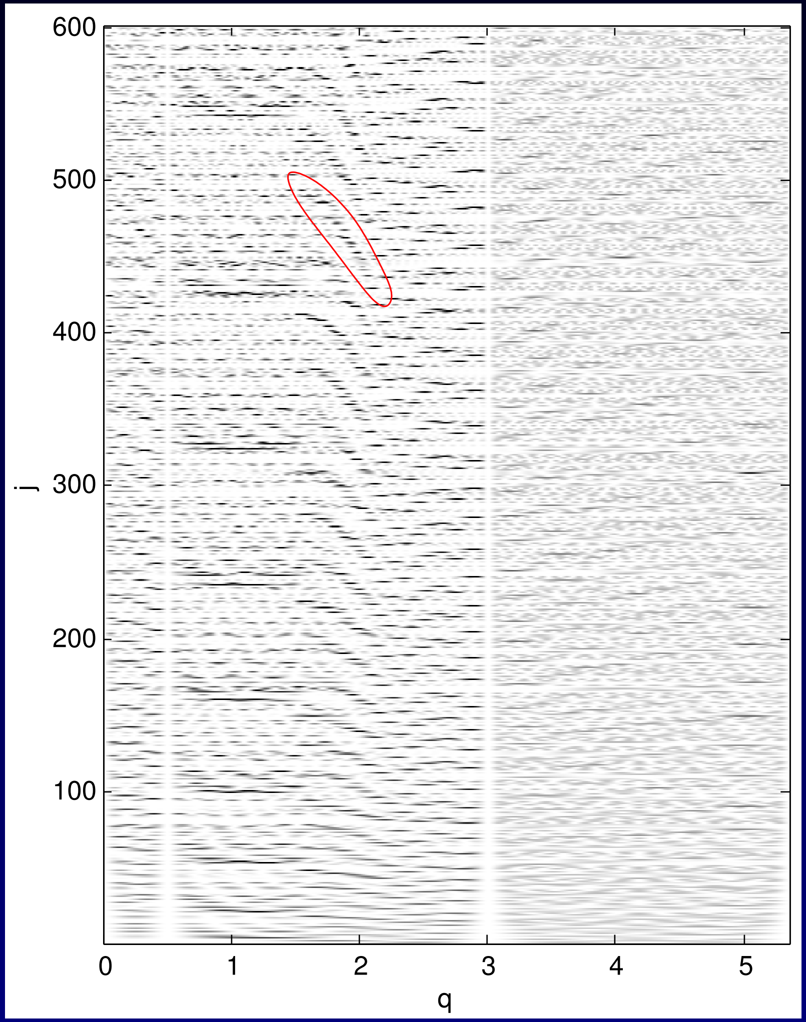
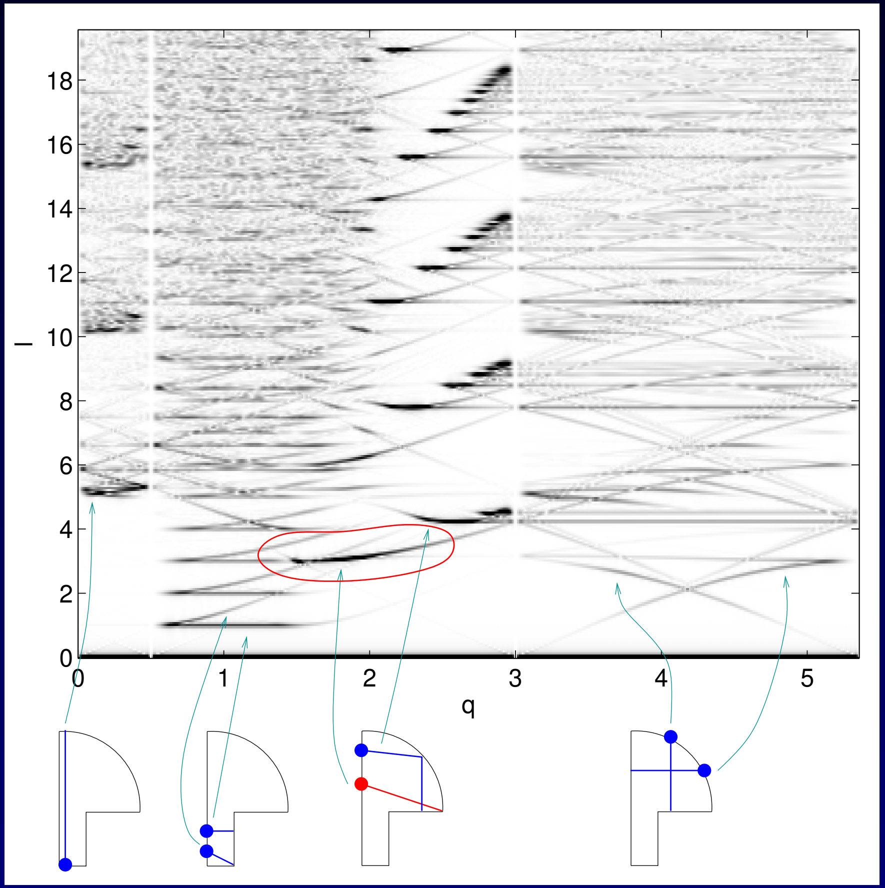


- sloping streak effect

MODES SMOOTHED

take FT along k axis, gives: wave autocorrelation in time



- refocused returning orbits
- return length varies with q

EVOLVE

III. Numerics (sketch)

Method of Particular Solutions

Given trial energy parameter $E > 0$:

- choose basis function set $\{\xi_i(E;\mathbf{x})\}_{i=1\cdots N}$ with $-\Delta\xi_i = E\xi_i$ in Ω

  global Helmholtz solutions with wrong BCs

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

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- if can find coeff vector $\mathbf{a} \in \mathbb{R}^N$ 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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Rayleigh quotient $$t(E)^2 := \min_u \frac{\int_{\partial\Omega} u^2\, ds}{\int_\Omega u^2\, d\mathbf{x}} = \min_{\mathbf{a}\neq\mathbf{0}} \frac{\mathbf{a}^T F_E \mathbf{a}}{\mathbf{a}^T G_E \mathbf{a}} = \lambda_1(E)$$

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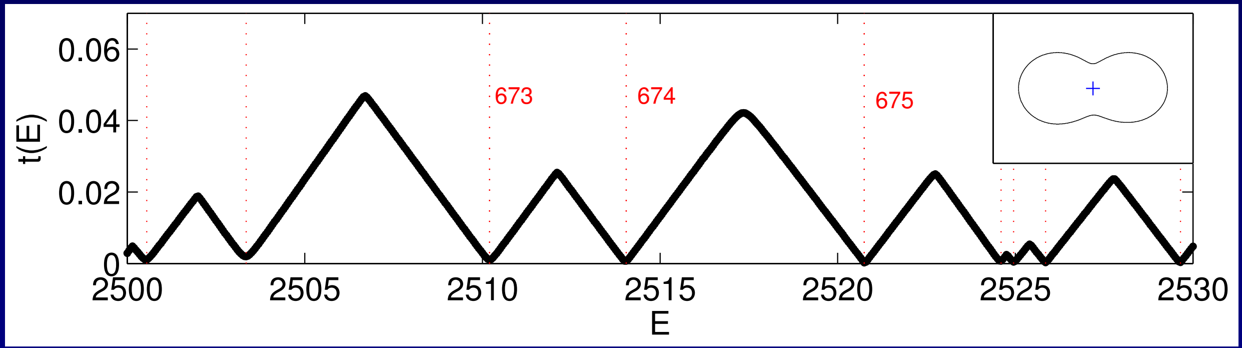
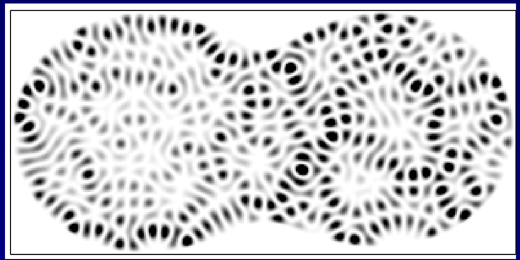


$\Omega =$ peanut, $j \approx 700$



- Each E_j found at a $t(E)$ minimum

Basis functions

Each basis func $\xi_i(E; \mathbf{x})$ is a *global* Helmholtz soln at energy E …

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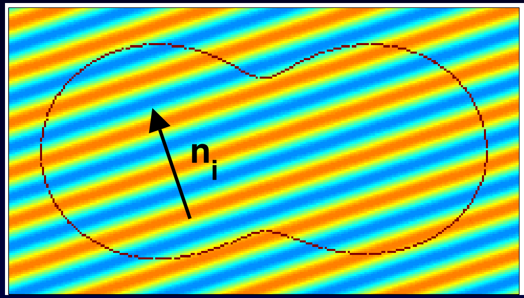

$$\begin{cases} \text{Plane waves} & \sin(k\mathbf{n}_i \cdot \mathbf{x}), \qquad k^2{=}E \\ \text{Fourier-Bessel} & J_l(kr)\sin(l\theta) \end{cases}$$

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

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

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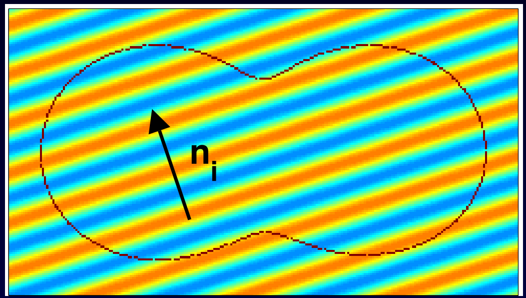

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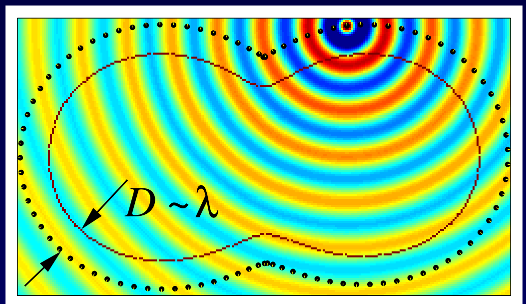

Fundamental solutions

$Y_0(k|\mathbf{x} - \mathbf{x}_i|)$ with $\{\mathbf{x}_i\}$ on outer boundary

Practice: excellent, also w/ non-reentrant corners (B ’06)

Ongoing analysis of coeff sizes (w/ Timo Betcke)

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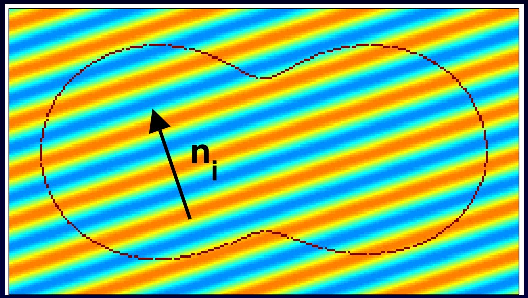

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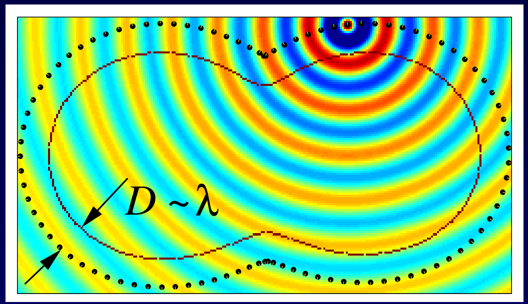

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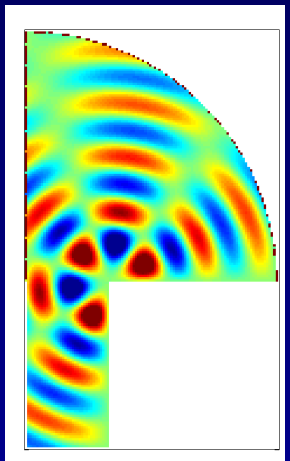

Corner-adapted Fourier-Bessel:

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

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

Scaling method

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

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

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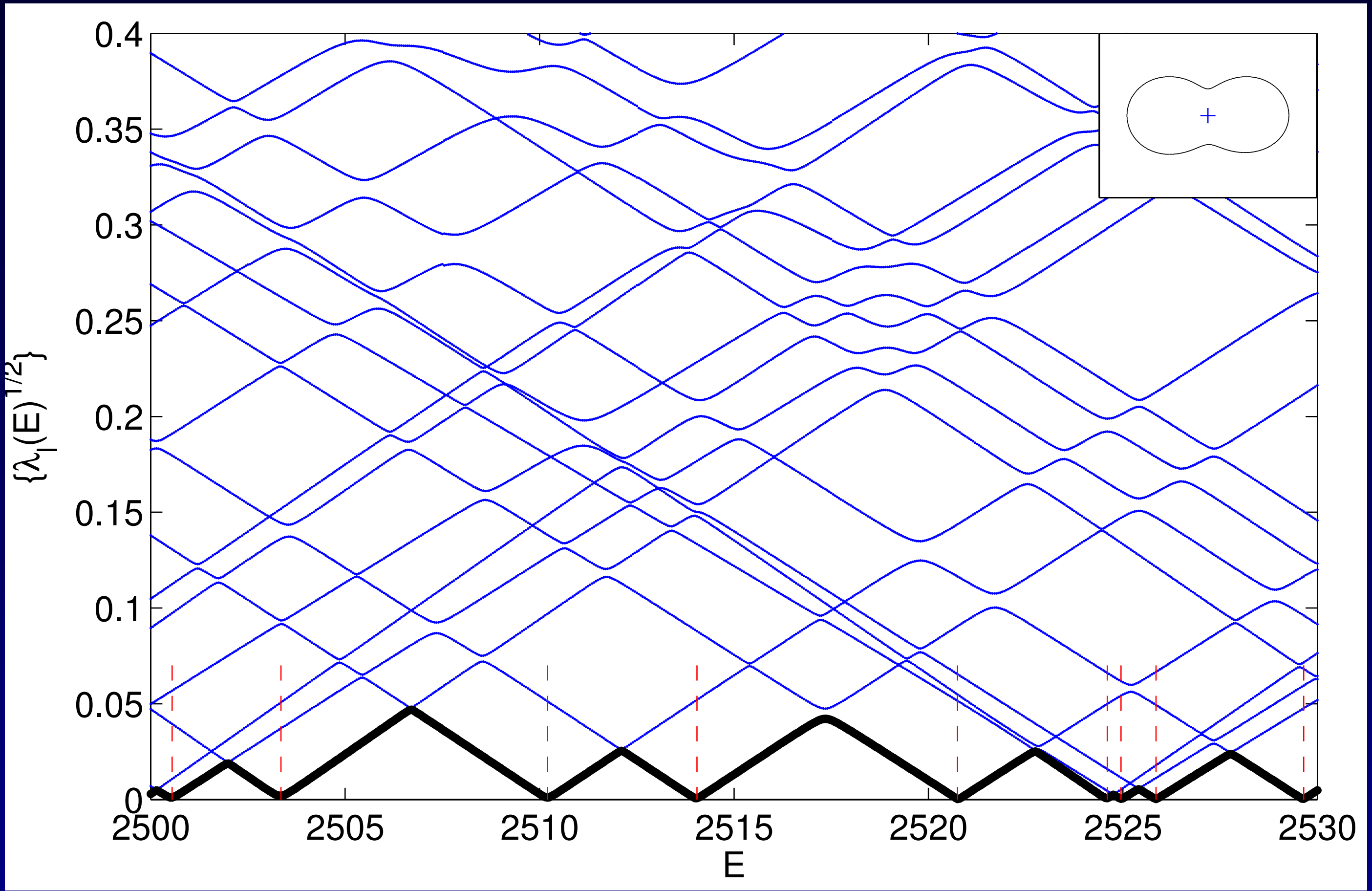
Include higher generalized eigenvalues…



- 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: $\int_{\partial\Omega}(\mathbf{x}\cdot\mathbf{n})^{-1}|u|^2 ds \big/ \int_{\partial\Omega}(\mathbf{x}\cdot\mathbf{n})^{-1} u\mathbf{x}\cdot\nabla u\, ds$

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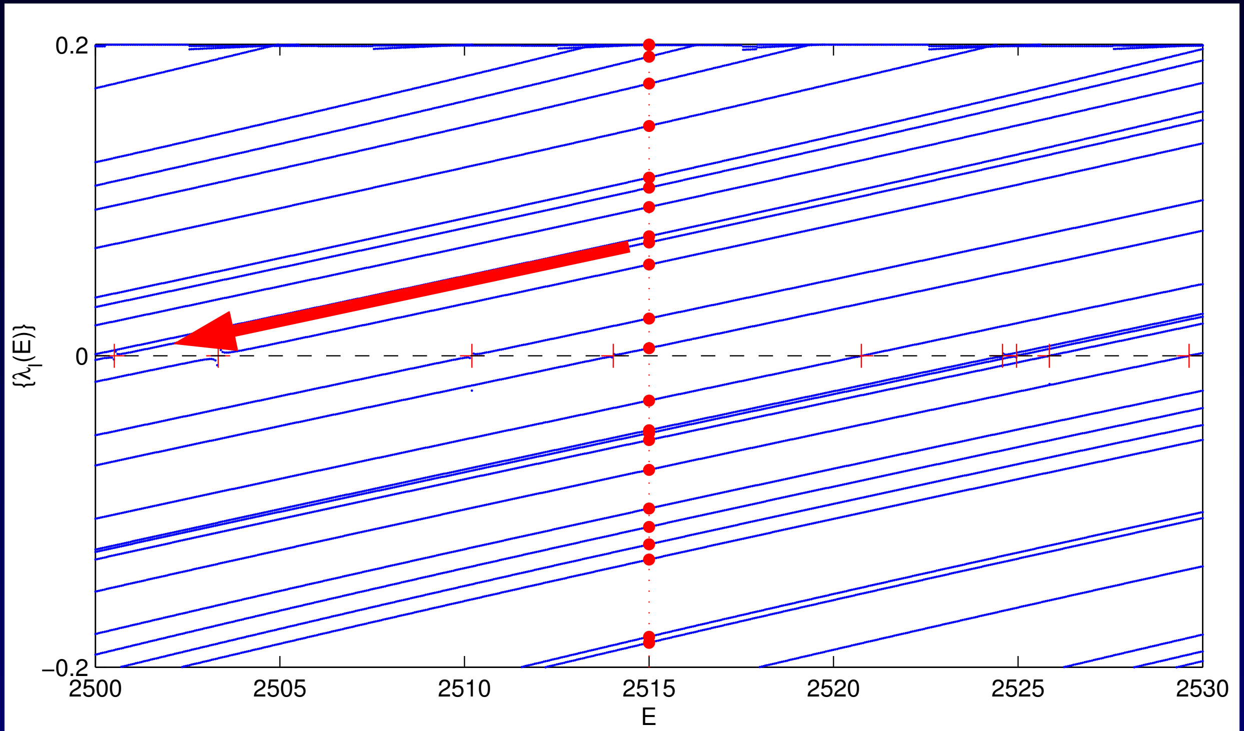
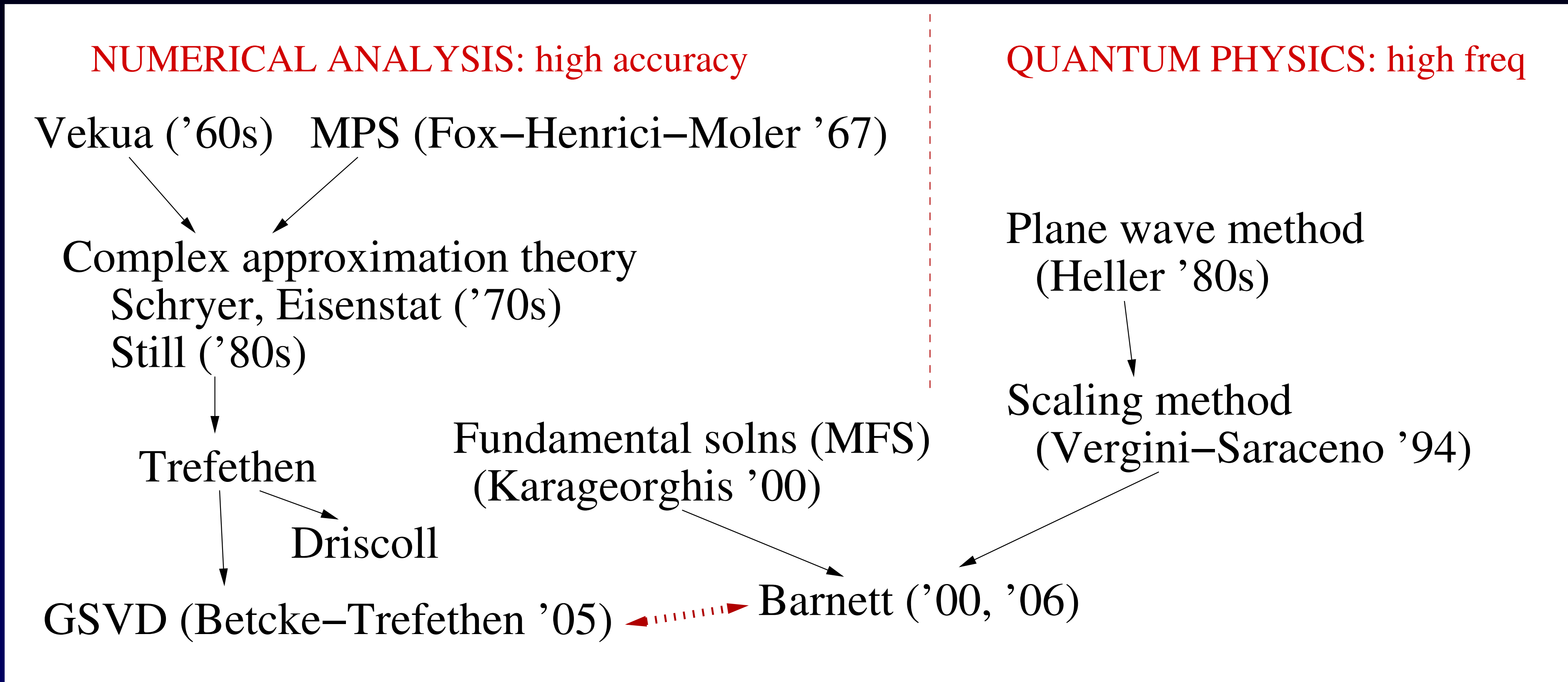
New Rayleigh quotient: $\int_{\partial\Omega}(\mathbf{x}\cdot\mathbf{n})^{-1}|u|^2 ds / \int_{\partial\Omega}(\mathbf{x}\cdot\mathbf{n})^{-1} u\mathbf{x}\cdot\nabla u\, ds$

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



- solving $F_E\mathbf{a} = \lambda G_E\mathbf{a}$ at single E value gives *all* nearest $O(k)$ modes
- no root search, no missing levels, speed gain $O(k) \sim 10^3$ 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)

Bifurcated genealogy



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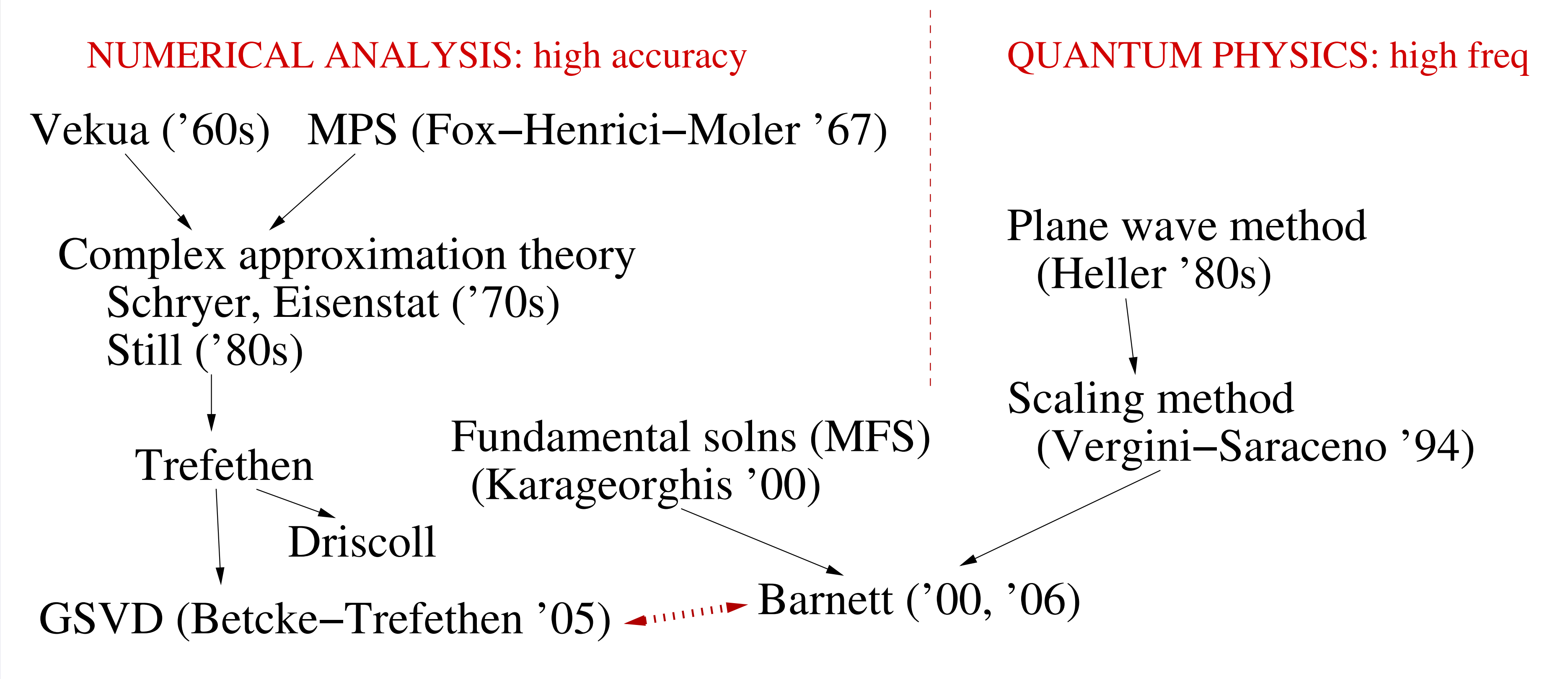


Researchers using my code: M. Porter (Caltech), P. Doyle (Dartmouth), M. Wright (ISVR, UK), J. Belmonte (UCLM, Spain), H. Mosadegh (Isfahan, Iran), Vinayak (Nehru U., India) …

Conclusion

Dirichlet eigenproblem: a paradigm linear wave resonance problem

Verified numerically in high-frequency regime…

- asymptotic decay $E^{-1/4}$ of fluctuations in chaotic modes
- found in mushroom: new moving scar fringe effect at focal points

Numerics: global basis methods excel at high frequency $E \gg 1$:

- scaling method $O(E^{1/2})$ (typ. 10^3) faster than any known method
- working on: basis choice; errors; dielectric resonator problem…

Thanks: T. Betcke (Manchester)
P. Sarnak (Princeton)
L. N. Trefethen (Oxford)
S. Zelditch (JHU)
P. Deift (NYU)

Funding: NSF (DMS-0507614)

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

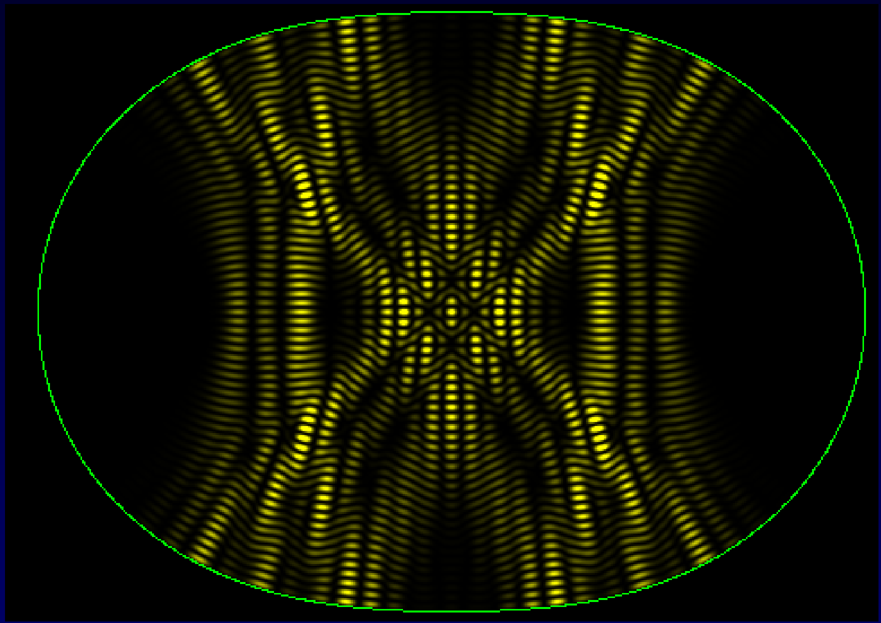
made with: Linux, LaTeX, `Prosper`

Laser modes

In reality the laser modes leak out into free space (they radiate)

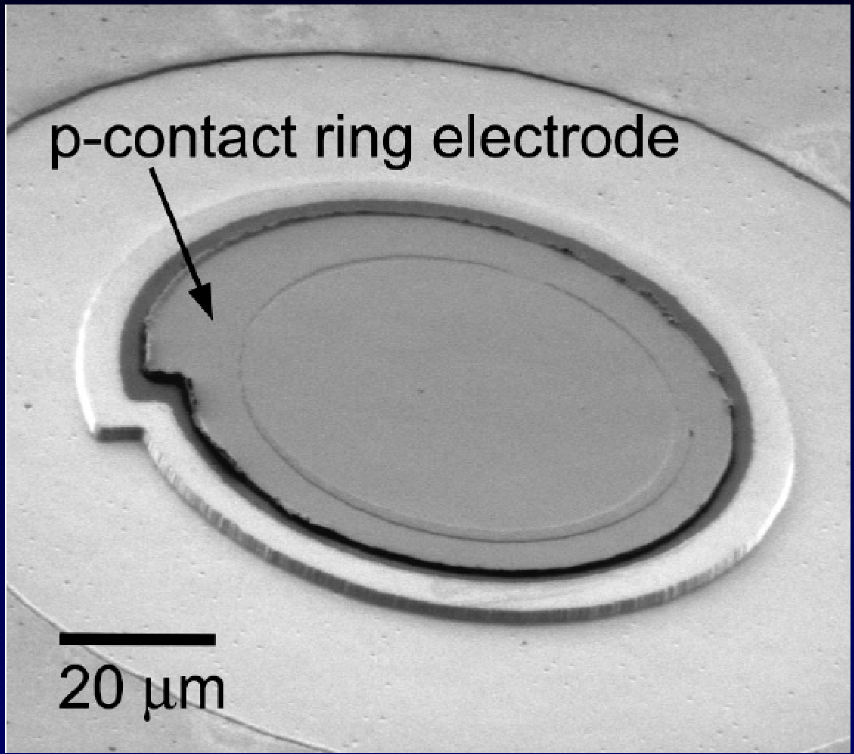
Let's approximate by close cavity (Dirichlet BC):

$E = 16417.2$ MODES

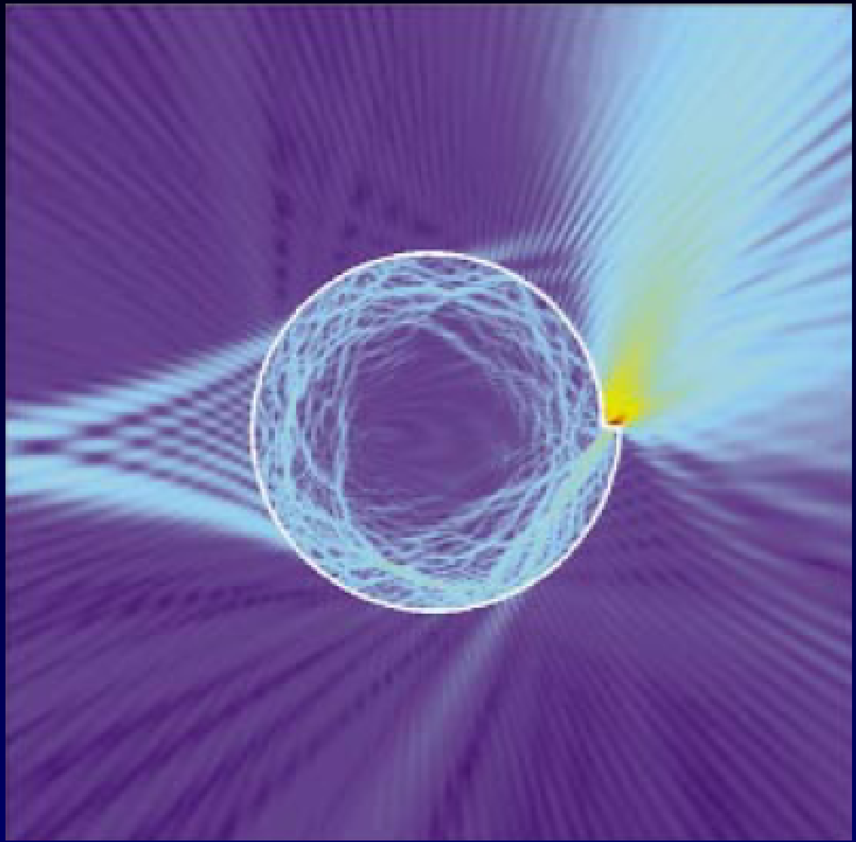


CPU / mode	method
60 s	MPS, root search
10 s	scaling, ϕ_j across Ω
0.6 s	scaling, ϕ_j bdry only

Bizarre laser shapes: spiral cavity



micrograph (Kneissl *et al.* '04)



numerics (Chern *et al.* '03)

- what is optimal shape/pumping?
- hard numerical calculations

Random plane waves

Conjecture (Berry '77): statistical model of eigenmodes

$$\phi_n \sim \lim_{N\to\infty} \frac{1}{\sqrt{N}} \sum_{j=1}^{N} a_j \sin(\mathbf{k}_j \cdot \mathbf{r} + \alpha_j)$$

iid amplitudes $a_j \in \mathbb{R}$
iid phases $\alpha_j \in [0, 2\pi)$

Wavevectors $\mathbf{k}_j$, spaced uniformly in direction, $|\mathbf{k}_j| = k$.

- Ray analogue of classical ergodicity.
- uniform measure as $E = k^2 \to \infty$