Eigenfunctions of the Laplacian: quantum ergodicity, chaos, and fast numerical methods

October 12, 2004

Alex Barnett

Courant Institute, NYU

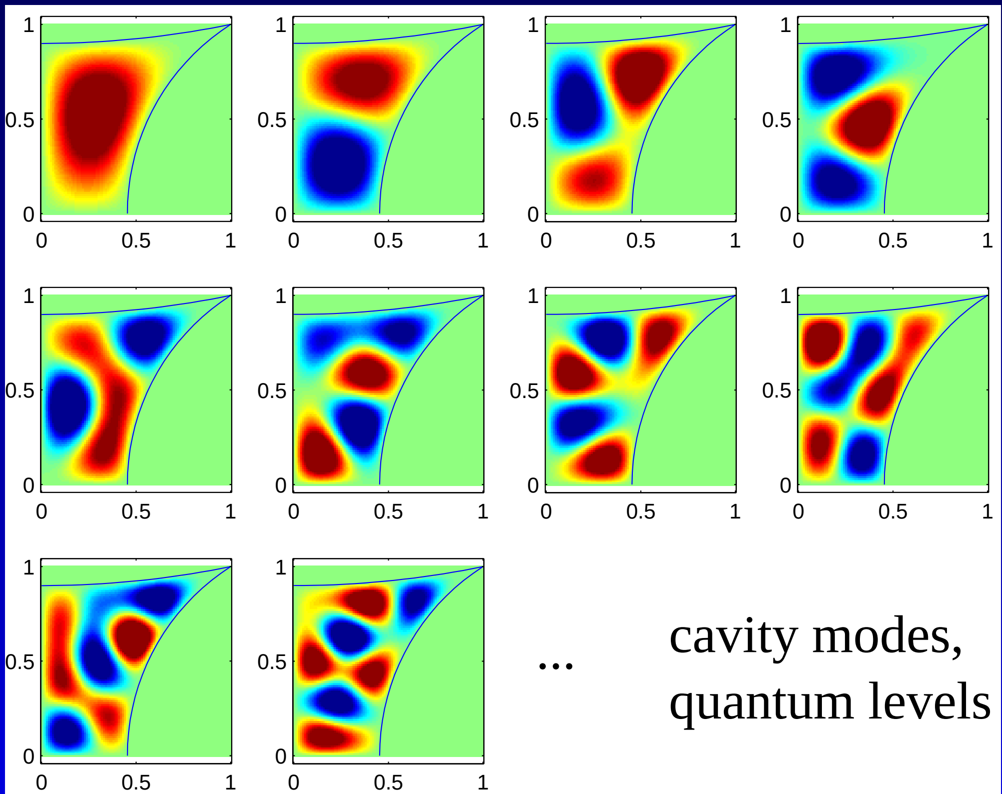
Thanks to Peter Sarnak, Percy Deift, Jonathan Goodman. . .

Dirichlet eigenproblem

Normal modes of elastic membrane or ‘drum’ (150 yr old)

Eigenfunctions ϕ_j of Laplacian in bounded domain $\Omega \subset \mathbb{R}^2$

$$-\Delta\phi_j = E_j\phi_j, \qquad \phi_j|_{\partial\Omega} = 0 \qquad \langle \phi_i, \phi_j \rangle = \delta_{ij}$$



‘level’ $j = 1 \cdots \infty$

‘energy’ eigenvalue E_j

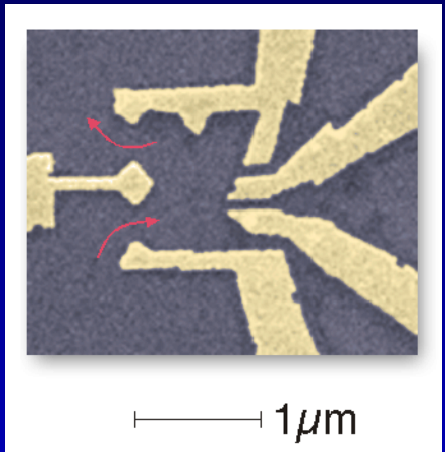
wavelength $= 2\pi / E_j^{1/2}$

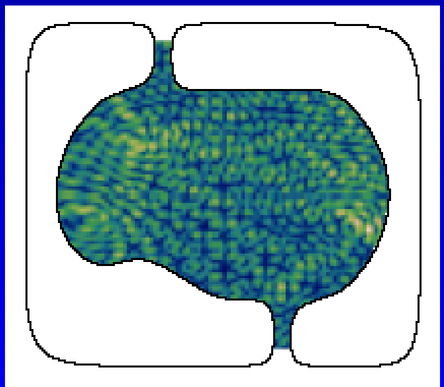
$\boxed{\text{MOVIE } j \approx 3000}$

- What happens to ϕ_j in the $E_j \to \infty$ (short wavelength) limit?
- How best to numerically calculate many modes efficiently?

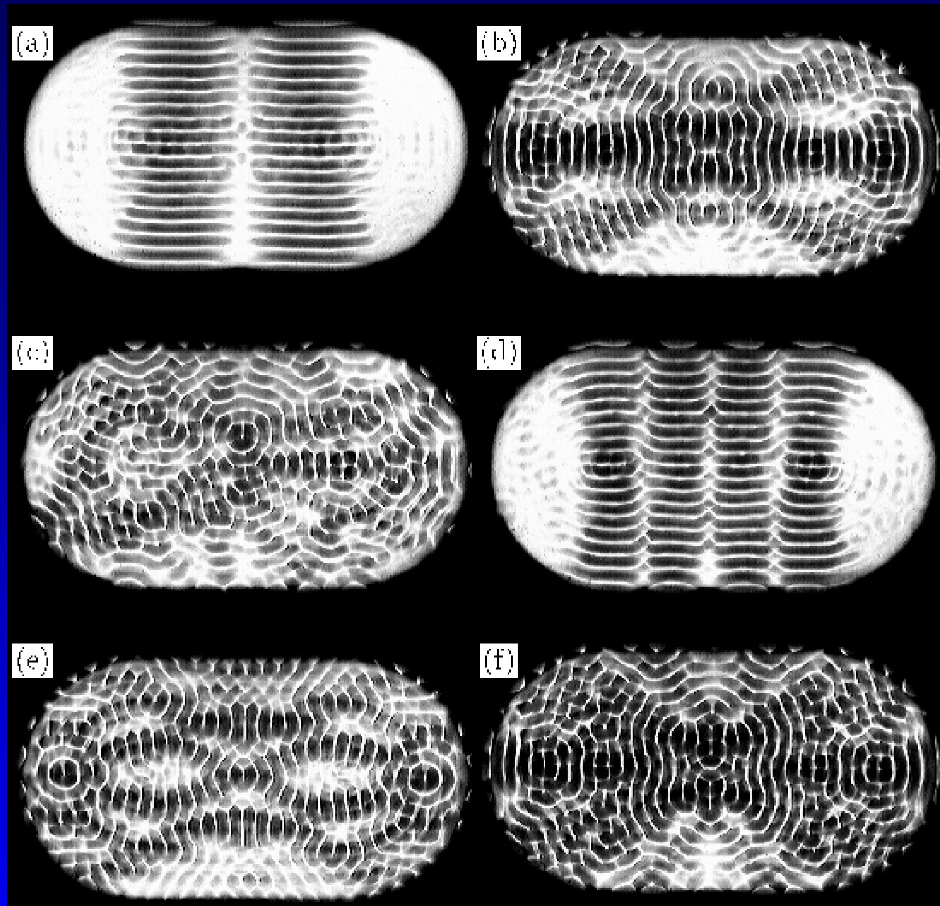
Modern applications

- electromagnetic modes of waveguide ($\partial\Omega$ = metallic wall)
- acoustic resonances and duct transmission (Neumann BCs)
- spectral geometry *e.g.* Kac's drum problem, Riemann surfaces
- physics *e.g.* model cold electrons in 'quantum dots'





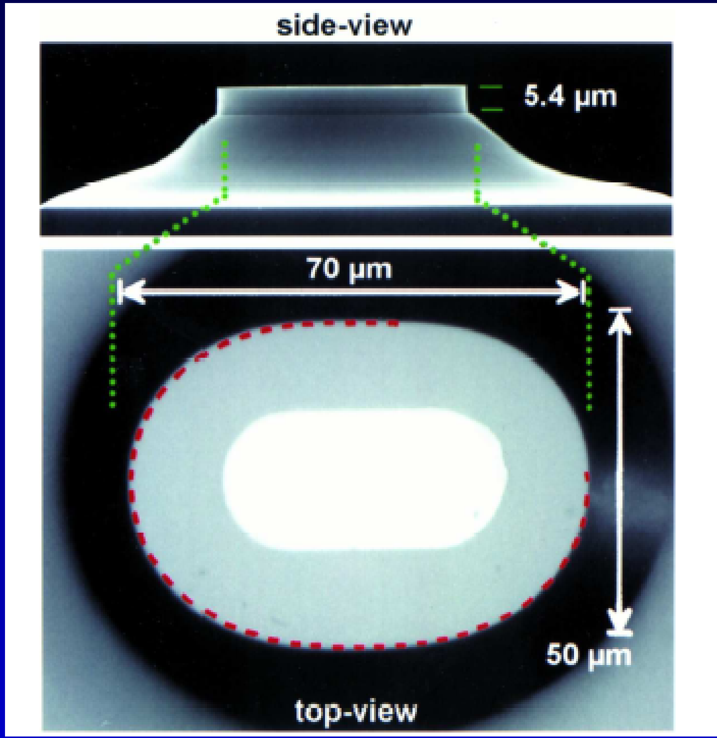
quantum dots (Marcus)



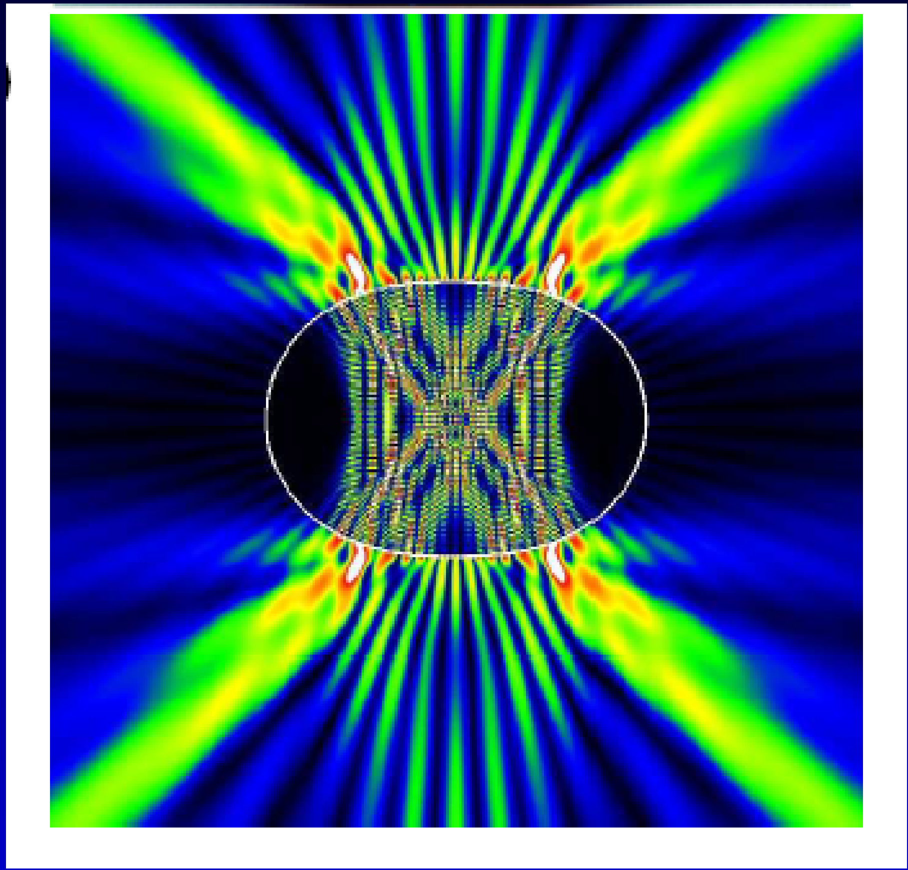
resonant liquid surfaces (Kudrolli)

Dielectric micro-cavity lasers

quantum-cascade laser



mode and emission pattern

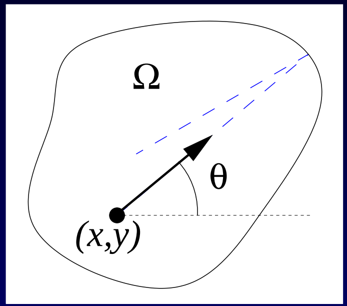


- 2D confinement due to total internal reflection, asymmetric cavity
- ‘scarred’ modes give power output $\times 10^3$ (Gmachl *et al* ’98)
- design & modeling: need compute many cavity modes (Tureci ’03)

Outline

- Background: ‘billiards’ and ‘quantum chaos’
- Quantum ergodicity
- Numerical results on quantum ergodicity
- Numerics: analysis of the ‘Method of Particular Solutions’
- Accelerated ‘scaling method’

Connection to dynamical systems



Drum problem is *quantized* equivalent of ‘billiards’

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

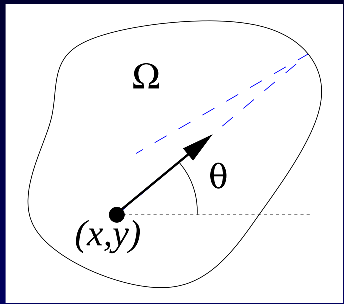
phase space $= (x, y, \theta)$

Connection to dynamical systems

Drum problem is *quantized* equivalent of ‘billiards’

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

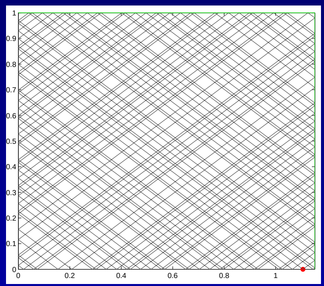
phase space $= (x, y, \theta)$

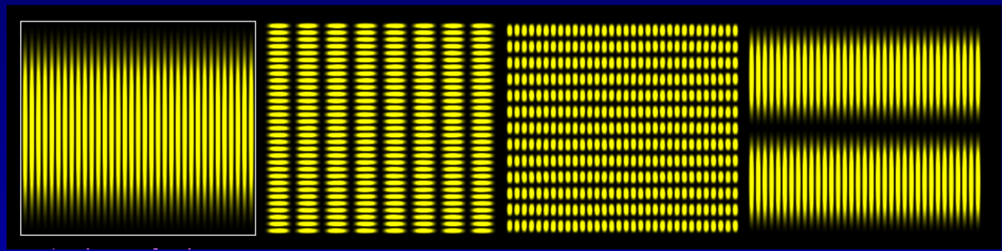


classical eigenfunctions ϕ_j: ‘quantum’

Integrable:

conserved quantities

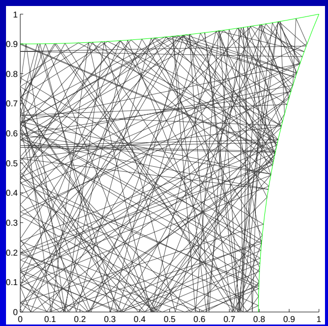


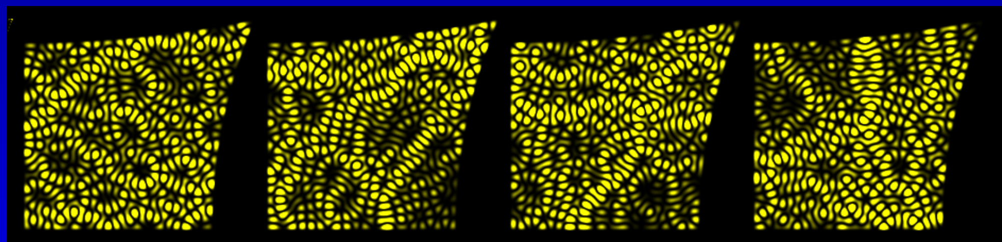


localization (tori in phase space: EBK)

Ergodic:

covers all phase space





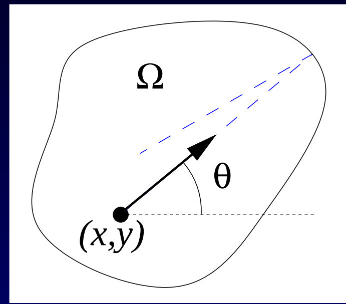
‘quantum chaos’ (Einstein 1917 realised!)

Connection to dynamical systems

Drum problem is *quantized* equivalent of ‘billiards’

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

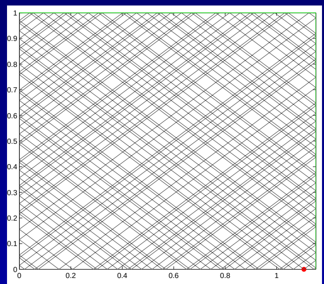
phase space $= (x, y, \theta)$

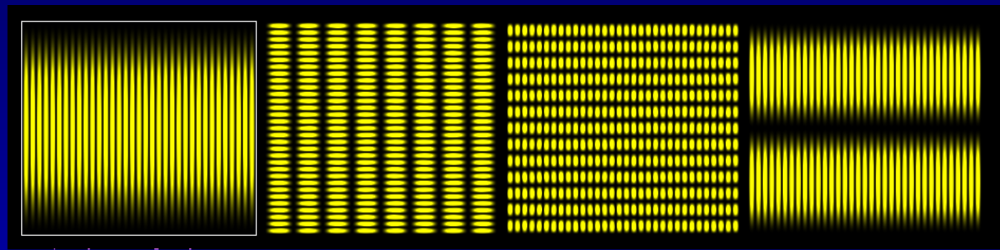


classical   eigenfunctions ϕ_j: ‘quantum’

Integrable:

conserved quantities

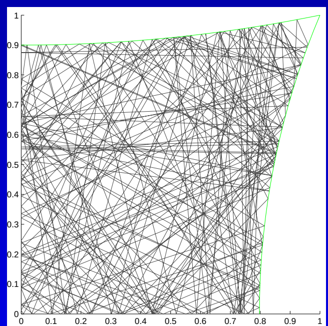


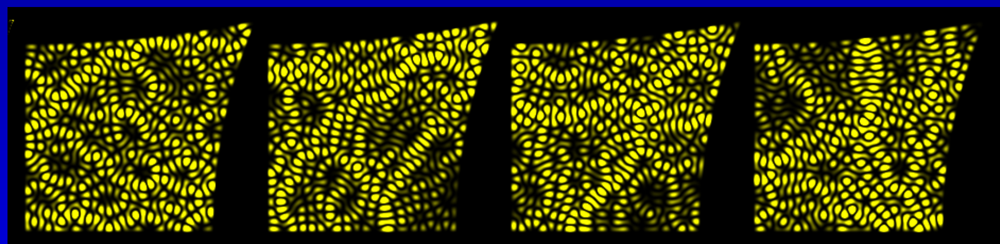


localization (tori in phase space: EBK)

Ergodic:

covers all phase space





‘quantum chaos’ (Einstein 1917 realised!)

- So, shape of domain Ω is crucial to behaviour in $E \to \infty$ limit

Quantum ergodicity

If the domain Ω is ergodic, does the intensity ϕ_j^2 become *equidistributed* (uniform across space) as $E_j \to \infty$?

Quantum ergodicity

If the domain Ω is ergodic, does the intensity ϕ_j^2 become *equidistributed* (uniform across space) as $E_j \to \infty$?

More precisely, pick any test function $A = A(\mathbf{r}),\ \mathbf{r} \in \Omega$

- classical phase space average $\overline{A} = \dfrac{1}{\mathrm{vol}(\Omega)} \displaystyle\int_\Omega A(\mathbf{r}) d\mathbf{r}$
- quantum intensity average

$$\int_\Omega A(\mathbf{r})\phi_j(\mathbf{r})^2 d\mathbf{r} \ := \ \langle \phi_j, \hat{A}\phi_j \rangle$$

diagonal matrix element of $\hat{A}$, operator multiplying by $A(\mathbf{r})$

Quantum ergodicity

If the domain Ω is ergodic, does the intensity ϕ_j^2 become *equidistributed* (uniform across space) as $E_j \to \infty$?

More precisely, pick any test function $A = A(\mathbf{r}), \;\; \mathbf{r} \in \Omega$

- classical phase space average $\overline{A} = \dfrac{1}{\mathrm{vol}(\Omega)} \displaystyle\int_\Omega A(\mathbf{r}) d\mathbf{r}$
- quantum intensity average

$$\int_\Omega A(\mathbf{r})\phi_j(\mathbf{r})^2 d\mathbf{r} \;\; := \;\; \langle \phi_j, \hat{A}\phi_j \rangle$$

diagonal matrix element of $\hat{A}$, operator multiplying by $A(\mathbf{r})$

Quantum Ergodicity Theorem (QET): "almost all levels equidistribute"

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

For ergodic domain Ω and all well-behaved A,

$$\lim_{E_j \to \infty} \langle \phi_j, \hat{A}\phi_j \rangle - \overline{A} \;=\; 0$$

holds for a subset of levels with density $\to 1$ as $E_j \to \infty$

- exceptional subset *can persist*, but must have vanishing density

Questions to investigate

1. *How* dense is exceptional set?
2. What is *rate* of convergence of $\langle \phi_j, \hat{A}\phi_j \rangle$ to $\overline{A}$?

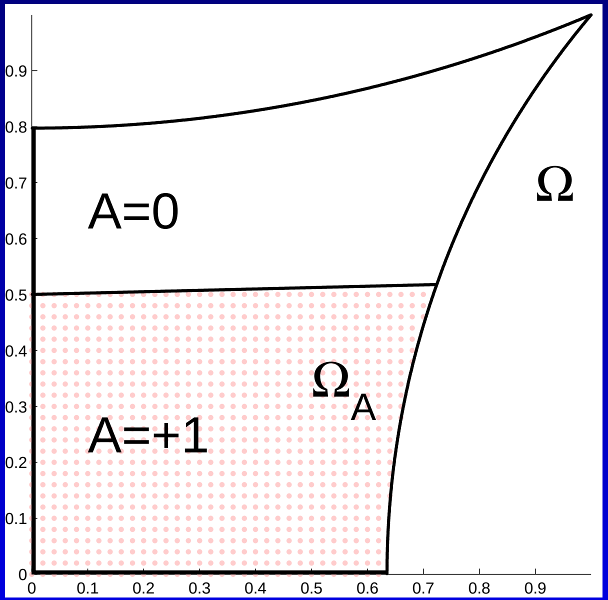
Determines *practical* applicability of QET:

How high in E do you have to go to get the "Correspondence Principle"?

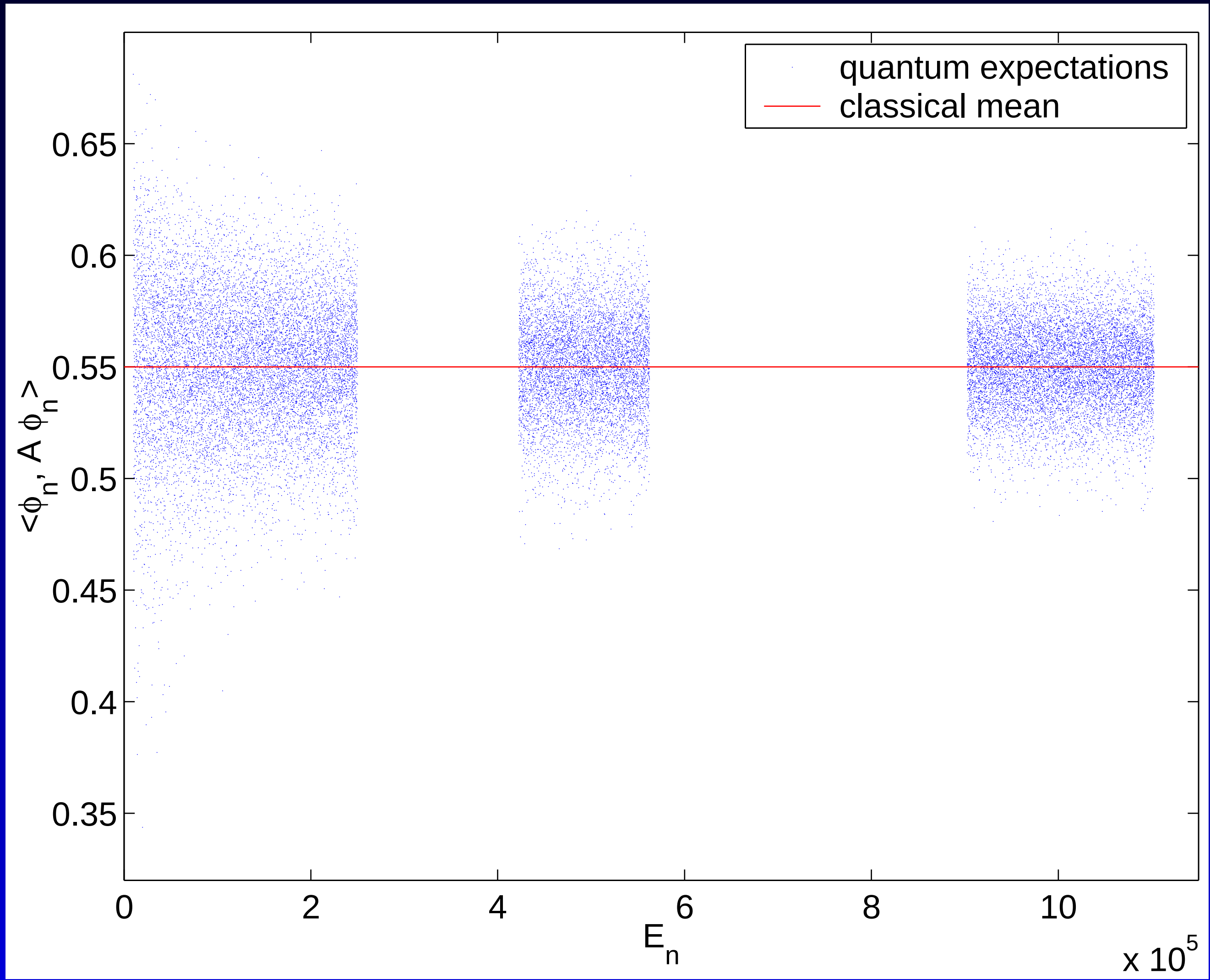
Examine numerically for…

Sinai-type domain (proven uniformly hyperbolic)
Piecewise constant A (numerically convenient)
Up to very high level numbers $j \sim 10^6$
Collect as many levels as you can!

(B '04)



Results: Diagonal matrix elements



25000 levels
of first 50000

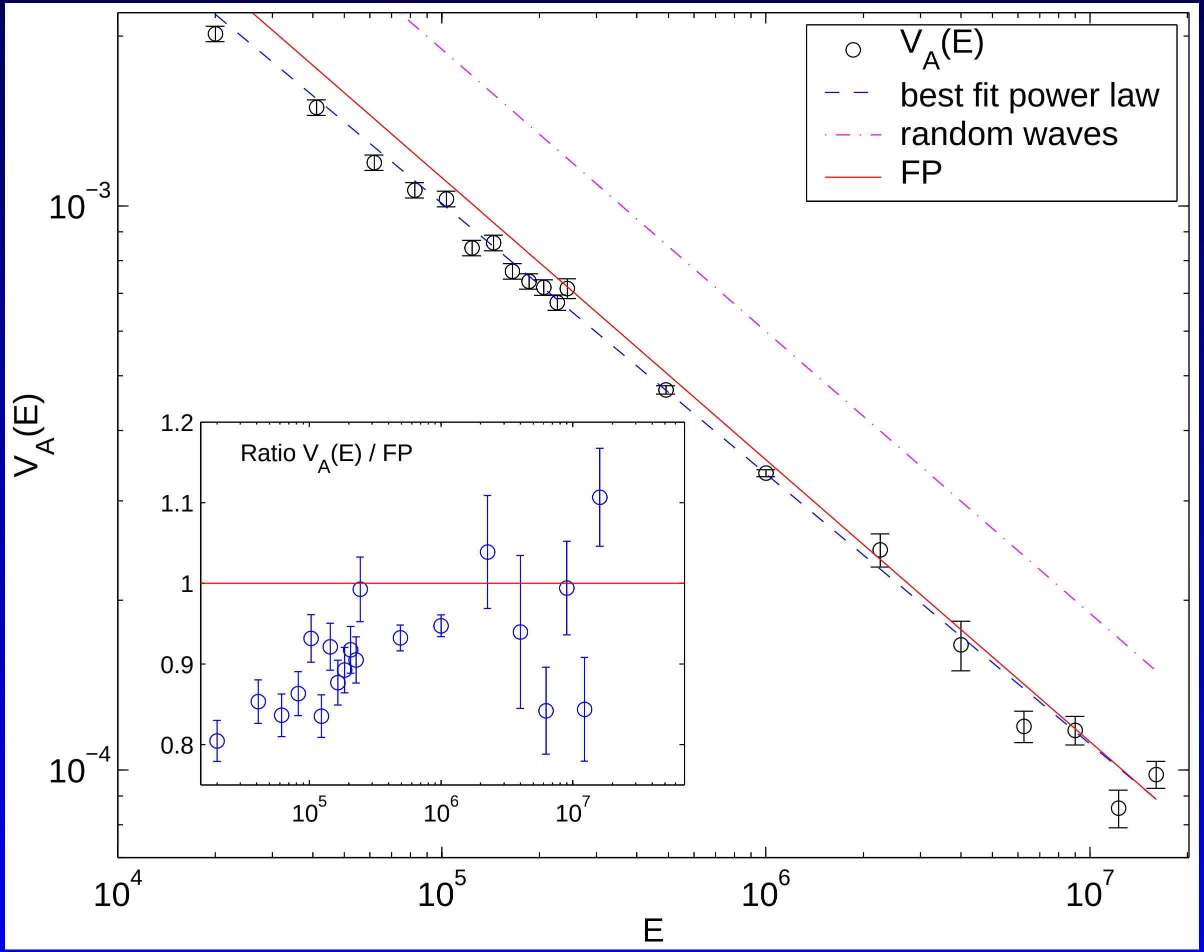
mean
$\langle \phi_j, \hat{A}\phi_j \rangle \rightarrow \overline{A}$

- No exceptional levels! (or their density $\lesssim 3 \times 10^{-5}$)
- Variance slowly decreasing, but how?

Results: Rate of variance decay with E

Local variance $$V_A(E) := \frac{1}{m} \sum_{E_n \approx E}^{N \le n < N+m} \left| \langle \phi_j, \hat{A}\phi_j \rangle - \overline{A} \right|^2$$

- Hard to measure *e.g.* 1% needs $m \sim 2 \times 10^4$ indep samples!



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

fit $\gamma = 0.48 \pm 0.01$

Discussion

- Previous studies: $j < 6000$, found various $\gamma \approx 0.3$–0.5 (Bäcker '98)

  ...we go 100 times higher in j: true asymptotic regime

Discussion

- Previous studies: $j < 6000$, found various $\gamma \approx 0.3$–0.5 (Bäcker '98)

  ...we go 100 times higher in j: true asymptotic regime

- $\gamma = 1/2$ consistent with RANDOM WAVES model:

  $$\phi_j \text{ statistically similar to } \lim_{N\to\infty} N^{-1/2} \sum_{i=1}^{N} \sin(k\mathbf{n}_i \cdot \mathbf{r}) \qquad \text{(Berry '77)}$$

  all directions $\mathbf{n}_i$, wavenumber $k = E^{1/2}$

  However prefactor *not* consistent with this model: 80% error

Discussion

- Previous studies: $j < 6000$, found various $\gamma \approx 0.3$–0.5 (Bäcker '98)

  ... we go 100 times higher in j: true asymptotic regime

- $\gamma = 1/2$ consistent with RANDOM WAVES model:

  $$\phi_j \text{ statistically similar to } \lim_{N\to\infty} N^{-1/2} \sum_{i=1}^{N} \sin(k\mathbf{n}_i \cdot \mathbf{r})$$ (Berry '77)

  all directions $\mathbf{n}_i$, wavenumber $k = E^{1/2}$

  However prefactor *not* consistent with this model: 80% error

- To understand prefactor: need semiclassical theory (Feingold-Peres '86)

  variance of off-diag matrix els $\langle \phi_i, \hat{A}\phi_j \rangle \leftrightarrow$ classical auto-correlation func of A

  But find convergence surprisingly slow: 7% error at $E \sim 10^6$

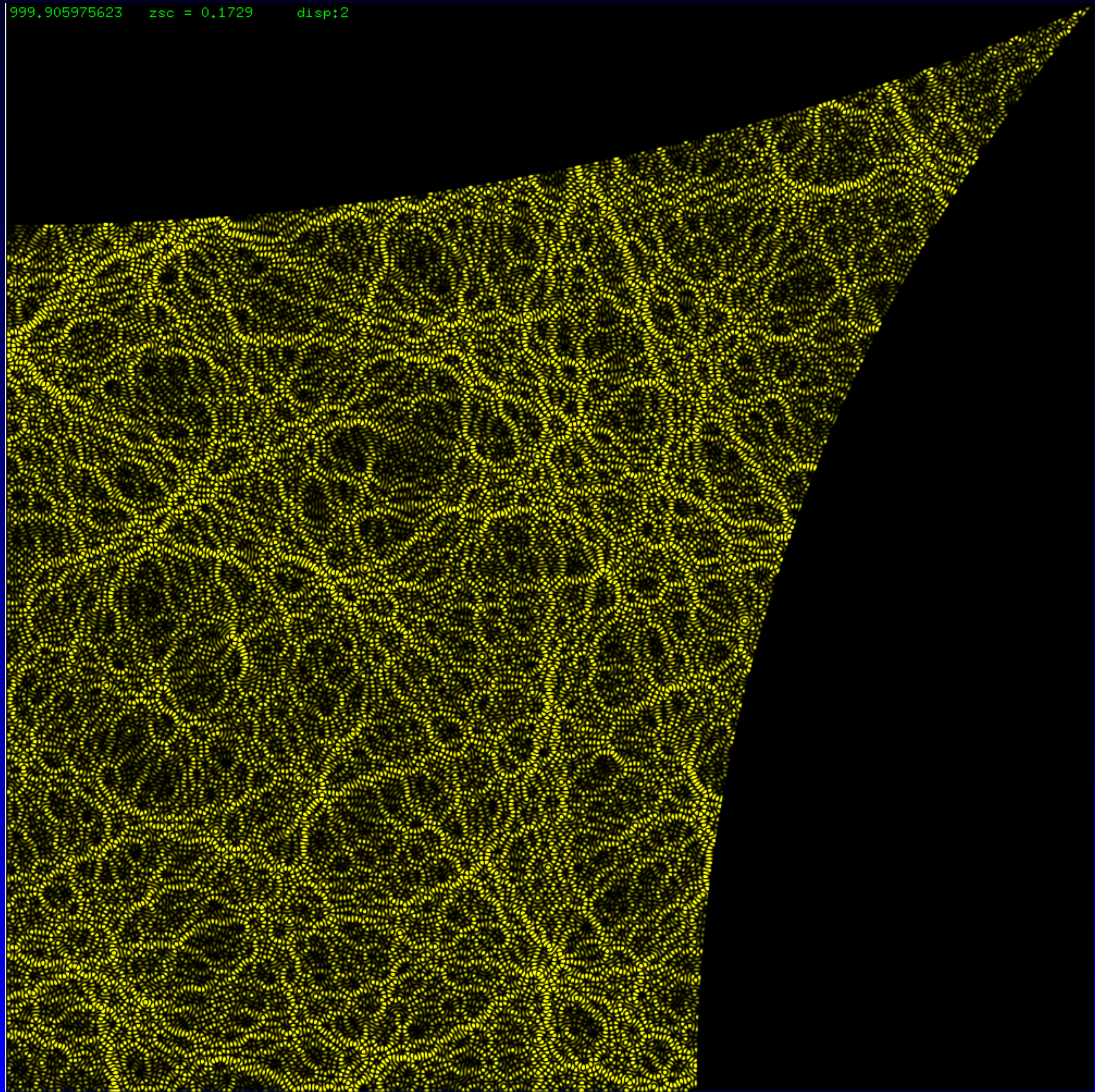
High-energy eigenfunction ϕ_n

$E \approx 10^6$

wavenumber
$k \approx 10^3$

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

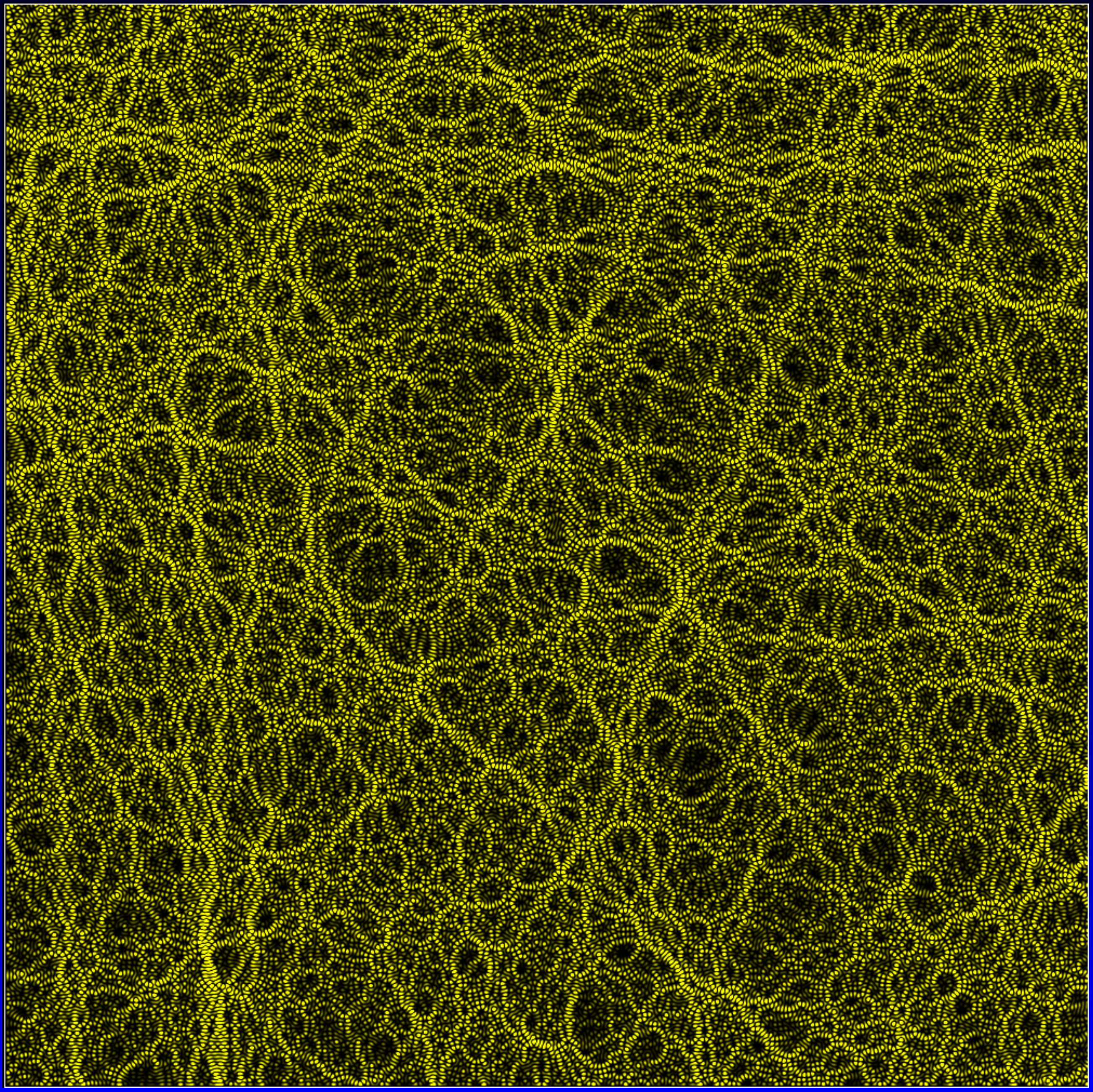
Compare to…



Random plane waves

interesting stringy ridge structures appear due to $|\mathbf{k}| = \text{const.}$

…not ‘scars’ (O’Connor-Heller ’86)



Quantum Unique Ergodicity & ‘scars’

QUE Conjecture (Rudnick-Sarnak ’94): *there are no exceptional levels*

…made in context of negatively-curved manifolds

- Found strong evidence for QUE in ergodic domain
- Number theorists care about this (*e.g.* automorphic forms)

Quantum Unique Ergodicity & ‘scars’

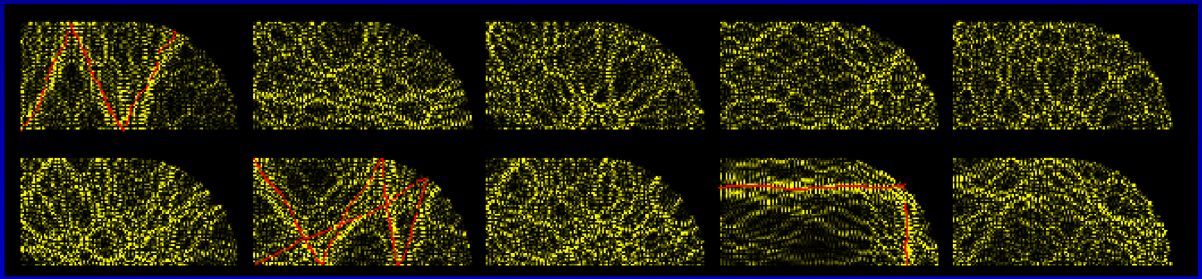
QUE Conjecture (Rudnick-Sarnak ’94): *there are no exceptional levels*

…made in context of negatively-curved manifolds

- Found strong evidence for QUE in ergodic domain
- Number theorists care about this (*e.g.* automorphic forms)

SCARS: enhanced intensity ϕ_j^2 along *unstable* periodic orbits

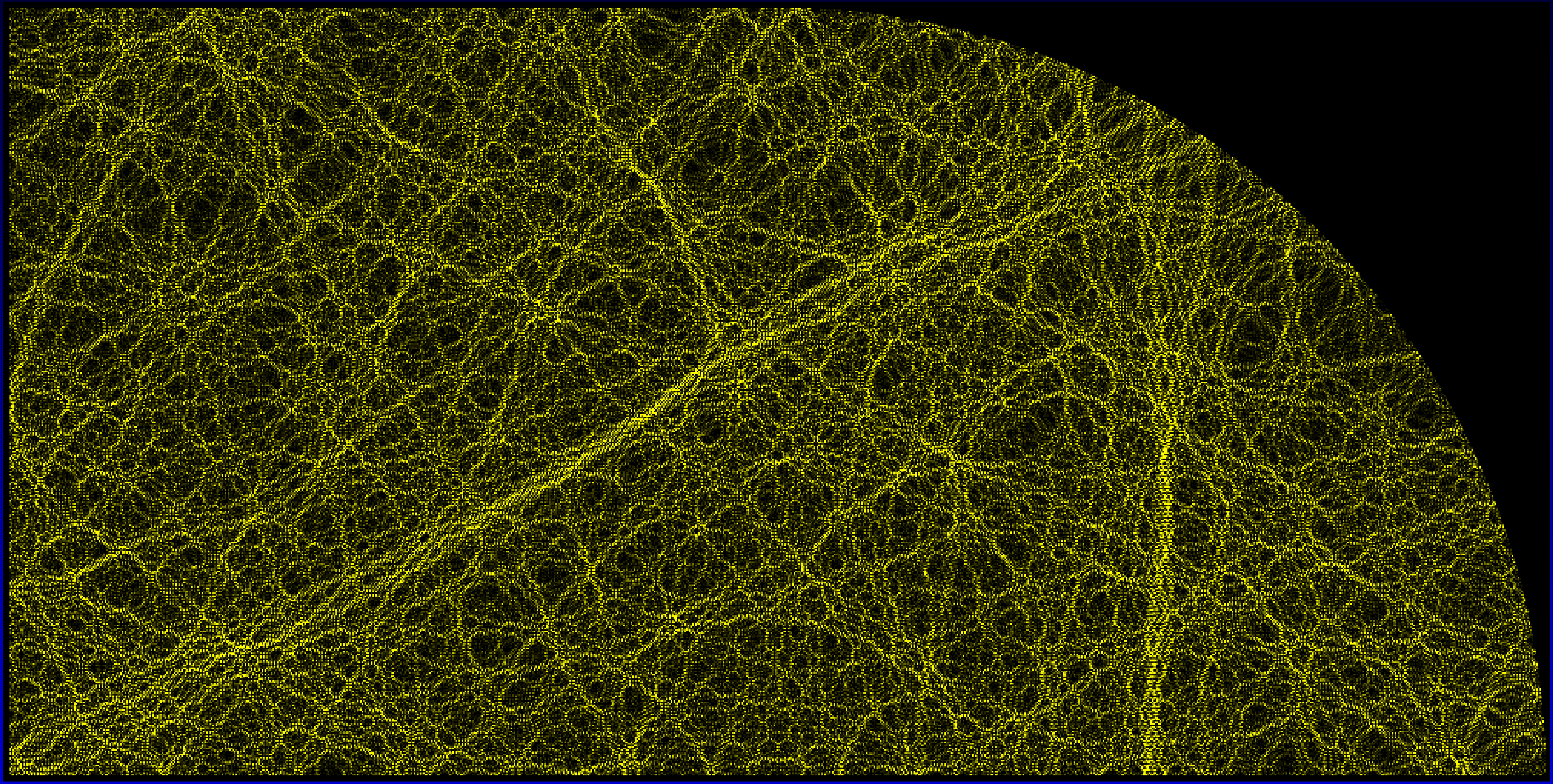
- surprise numerical discovery by physicist (Heller ’84)



- QUE $\Rightarrow$ effect of scars dies out
- variance decay $\sim E^{-1/2}$ consistent with expected narrowing of scars

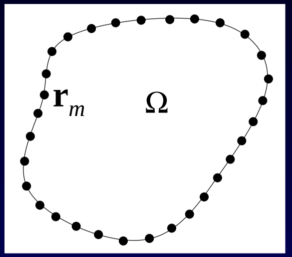
Scarred eigenfunction at high E

Ω = stadium (ergodic)



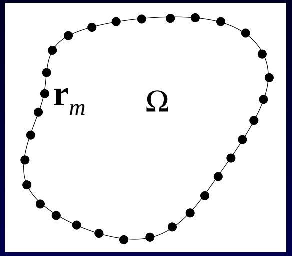
~ 300 wavelengths across, $E \sim 10^6$

Numerical method for eigenproblem



10^2-10^3 wavelengths across system: Direct discretization (finite elements, etc) *extremely inefficient*—need boundary method

Numerical method for eigenproblem



10^2-10^3 wavelengths across system: Direct discretization (finite elements, etc) *extremely inefficient*—need boundary method

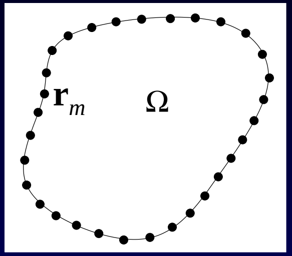
Method of Particular Solutions (MPS): (Fox '67, etc)

1. Guess energy parameter E.
2. Choose basis set $\{\xi_i\}$ obeying Helmholtz eqn: $-\Delta\xi_i = E\xi_i$

   e.g. Bessels $J_i(kr)\sin l\theta$, plane waves $\sin(k\mathbf{n}_i \cdot \mathbf{r})$
3. Trial function $u = \sum_{i=1}^{N} x_i\xi_i$ coeff vector $\mathbf{x} \in \mathbb{R}^N$
4. Find $t(E) = \min_{|\mathbf{x}|=1} ||u||_{\partial\Omega}$ lowest 'boundary condition error'

   use M quadrature points $\mathbf{r}_m$, $t(E)$ is min sing val of $B_{mi} := \xi_i(\mathbf{r}_m)$
5. Repeat & root search: levels E_j are where $t(E) \to 0$ (or v. small)

Numerical method for eigenproblem



10^2-10^3 wavelengths across system: Direct discretization (finite elements, etc) *extremely inefficient*—need boundary method

Method of Particular Solutions (MPS): (Fox '67, etc)

1. Guess energy parameter E.
2. Choose basis set $\{\xi_i\}$ obeying Helmholtz eqn: $-\Delta\xi_i = E\xi_i$
   e.g. Bessels $J_i(kr)\sin l\theta$, plane waves $\sin(k\mathbf{n}_i \cdot \mathbf{r})$
3. Trial function $u = \sum_{i=1}^{N} x_i\xi_i$ coeff vector $\mathbf{x} \in \mathbb{R}^N$
4. Find $t(E) = \min_{|\mathbf{x}|=1} ||u||_{\partial\Omega}$ lowest 'boundary condition error'
   use M quadrature points $\mathbf{r}_m$, $t(E)$ is min sing val of $B_{mi} := \xi_i(\mathbf{r}_m)$
5. Repeat & root search: levels E_j are where $t(E) \to 0$ (or v. small)

MPS largely abandoned by numerical analysts in 70's ... Why?

- increase N: *many* vanishing sing vals at *all* E! $\longrightarrow$ useless

Domain norm vs boundary norm

Easy to fix: use Rayleigh quotient $\lambda_1(E) = \min_{u \neq 0} \frac{||u||^2_{\partial\Omega}}{||u||^2_{\Omega}}$ (B '00)

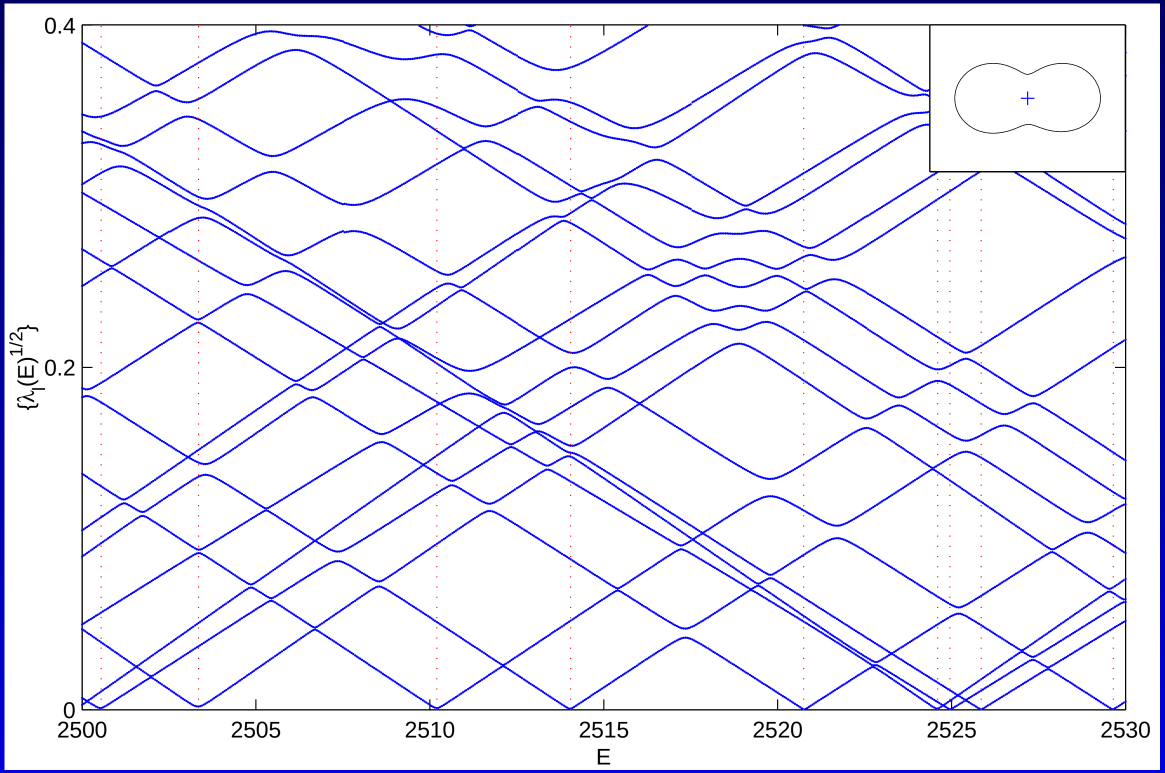
min eigenvalue of (singular) generalized matrix eigenproblem

Domain norm vs boundary norm

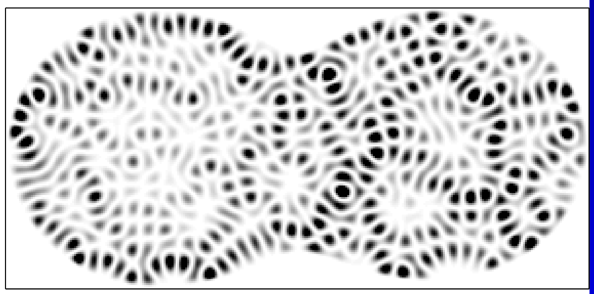
Easy to fix: use Rayleigh quotient $\lambda_1(E) = \min_{u \neq 0} \frac{||u||^2_{\partial\Omega}}{||u||^2_{\Omega}}$ (B '00)

min eigenvalue of (singular) generalized matrix eigenproblem

Look at E-dependent spectrum $\{\lambda_l(E)^{1/2}\}$:



around level $j \sim 700$

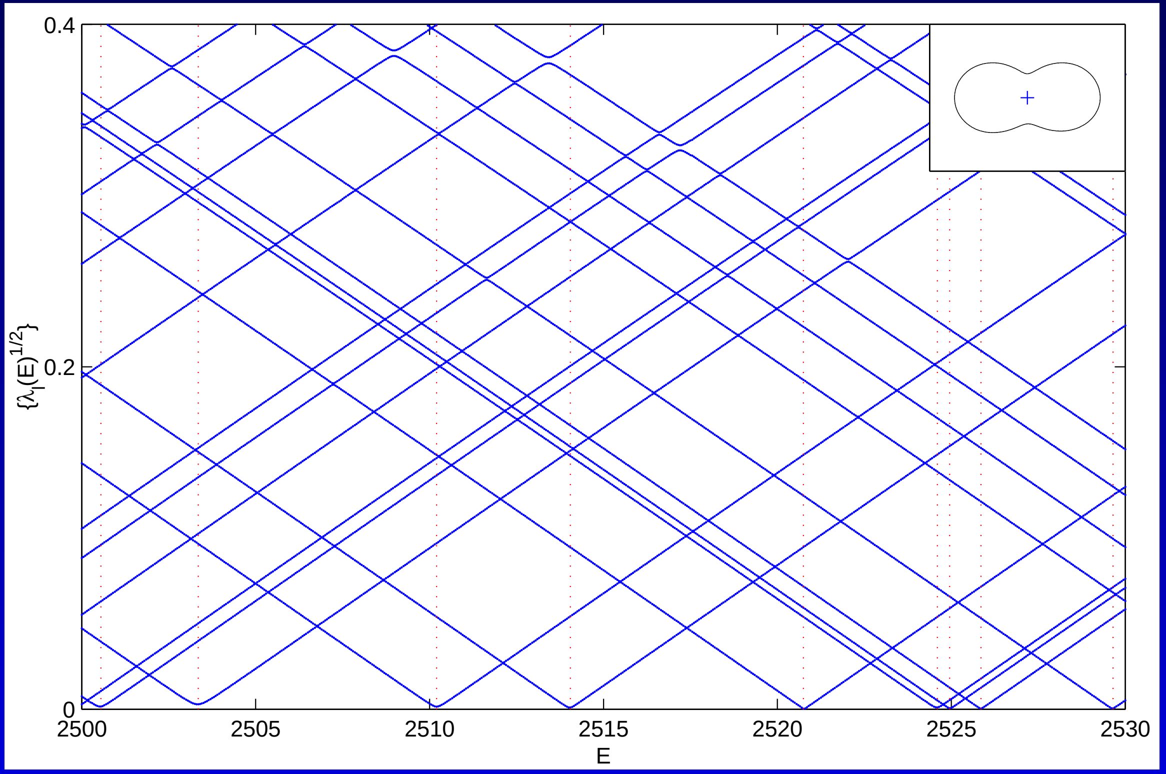


- λ_1 seems quadratic in $(E - E_j)$, but coefficients (slopes) differ
- higher eigenvalue structure!

Special boundary weighting

What if replace $||u||^2_{\partial\Omega}$ by $||u||^2_{w,\partial\Omega} := \int_{\partial\Omega} w(s)\, u(s)^2 ds$?

Choose weight $w(s) = [\mathbf{r}(s) \cdot \mathbf{n}(s)]^{-1}$ . . . requires Ω star-shaped



- special: all coeffs (slopes) equal $\rightarrow$ predictive power!
- much reduced *avoided crossings* between eigenvalues

WHY?

Analysis of spectrum $\{\lambda_l(E)\}$ – sketch

Basis set $\{\xi_i\}$ approx spans $\mathcal{H}_\Omega(E) := \{u : -\Delta u = Eu \text{ in } \Omega\}$

Analysis of spectrum $\{\lambda_l(E)\}$ – sketch

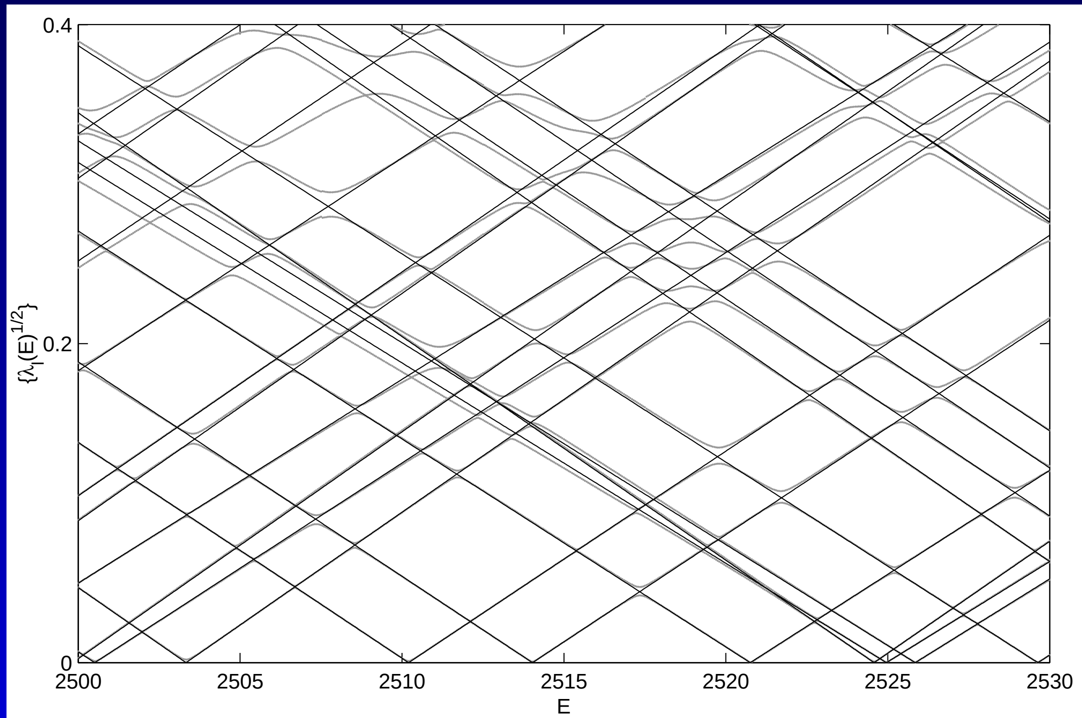
Basis set $\{\xi_i\}$ approx spans $\mathcal{H}_\Omega(E) := \{u : -\Delta u = Eu \text{ in } \Omega\}$

Via complete set $\{\partial_n \phi_j\}$ on boundary, show spectrum identical to that of $D\mathbf{v} = \lambda Q_w \mathbf{v}$ ∞-dim matrices: $D(E) = \text{diag }(E-E_j)^2$, Q_w = indep of E

Analysis of spectrum $\{\lambda_l(E)\}$ – sketch

Basis set $\{\xi_i\}$ approx spans $\mathcal{H}_\Omega(E) := \{u : -\Delta u = Eu \text{ in } \Omega\}$

Via complete set $\{\partial_n \phi_j\}$ on boundary, show spectrum identical to that of $D\mathbf{v} = \lambda Q_w \mathbf{v}$ ∞-dim matrices: $D(E) = \text{diag } (E - E_j)^2,\ Q_w = \text{indep of } E$



Perturbation theory of matrix problem yields:

$(\text{coeffs})^{-1} = \text{diag of } Q_w,$ avoided crossing sizes = off-diag of Q_w

The matrix Q_w: quasi-orthogonality

$$(Q_w)_{ij} := \int_{\partial\Omega} w^{-1}\, \partial_n\phi_i \partial_n\phi_j \, ds$$

Eigenfunction normal derivs $\partial_n\phi_j$ not orthogonal on $\partial\Omega$, but…

For special choice $w = (\mathbf{r}\cdot\mathbf{n})^{-1}$: $\quad (Q_w)_{ij} \;=\; 2\delta_{ij}E_j \;+\; c_{ij}$

- Conjecture (Vergini '94): off-diag error term growth $|c_{ij}| \sim |E_i - E_j|$
- Semiclassics (B-Cohen-Heller '00): for Ω ergodic, $|c_{ij}| \sim (E_i - E_j)^2$

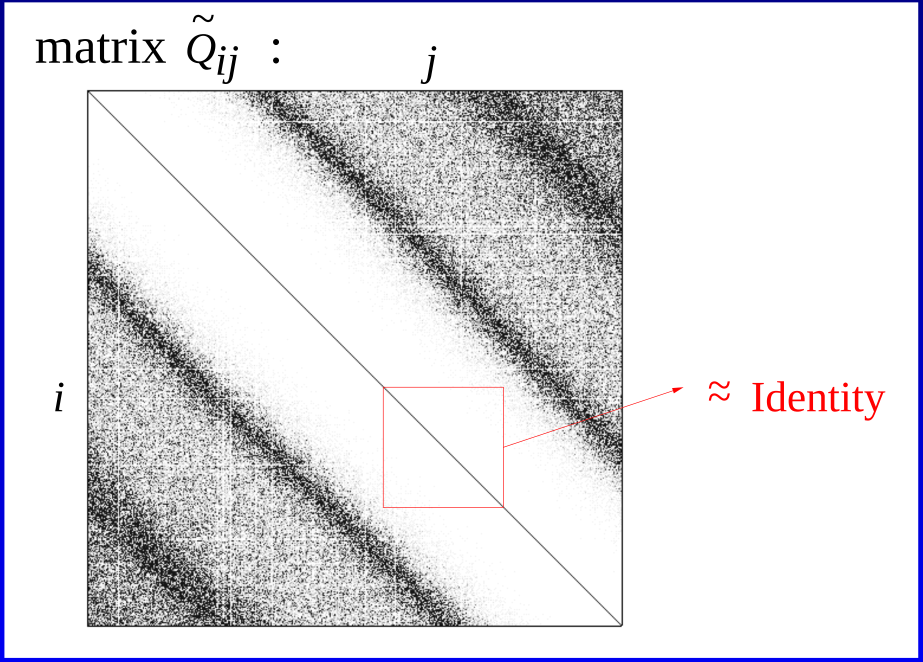
The matrix Q_w: quasi-orthogonality

$$(Q_w)_{ij} := \int_{\partial\Omega} w^{-1}\, \partial_n\phi_i \partial_n\phi_j \, ds$$

Eigenfunction normal derivs $\partial_n \phi_j$ not orthogonal on $\partial\Omega$, but…

For special choice $w = (\mathbf{r}\cdot\mathbf{n})^{-1}$: $\quad (Q_w)_{ij} \;=\; 2\delta_{ij}E_j \;+\; c_{ij}$

- Conjecture (Vergini '94): off-diag error term growth $|c_{ij}| \sim |E_i - E_j|$
- Semiclassics (B-Cohen-Heller '00): for Ω ergodic, $|c_{ij}| \sim (E_i - E_j)^2$
- Theorem (B '04): for *all* Ω, ergodic or not, $|c_{ij}| \le C_\Omega (E_i - E_j)^2$



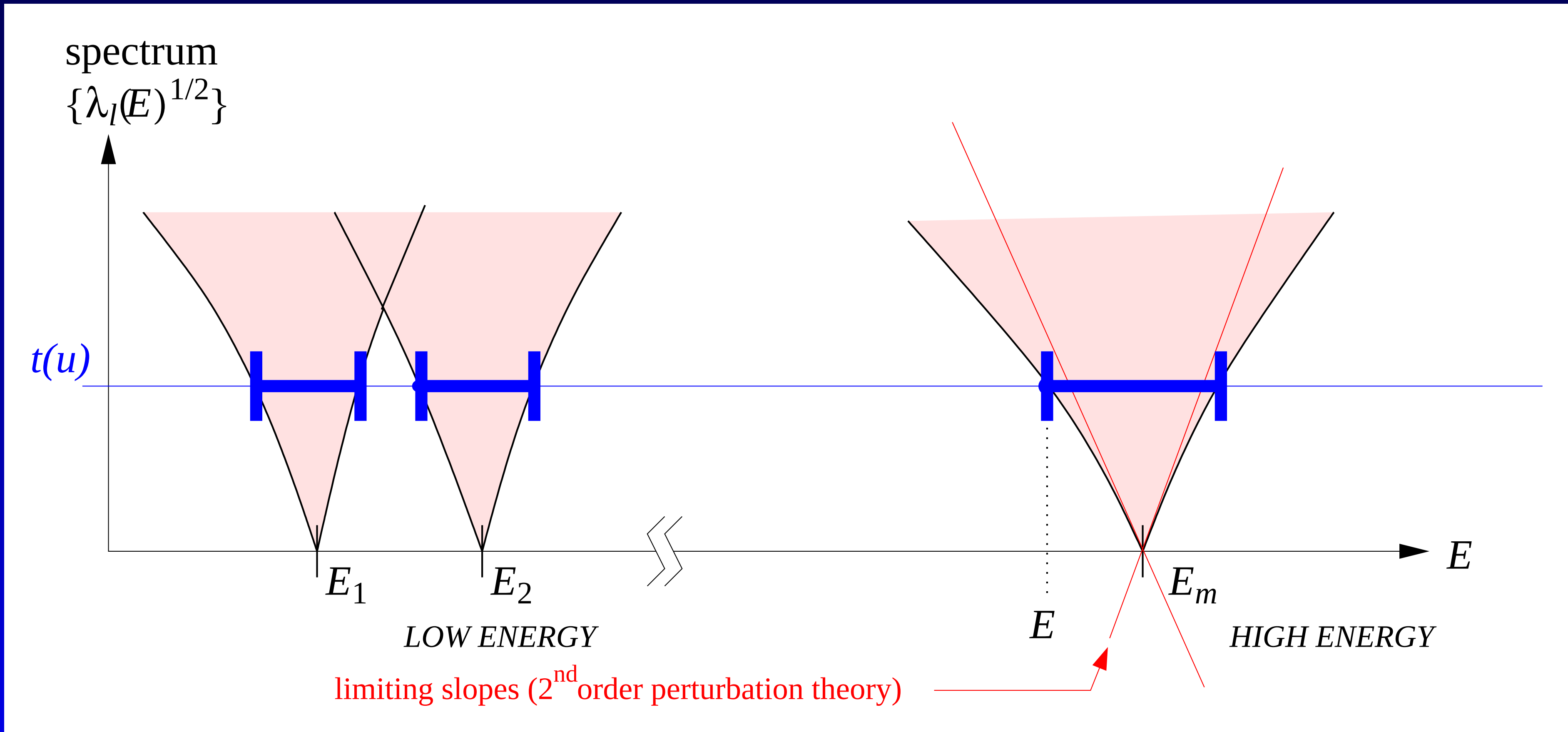
quasi-orthogonality:
locally, $Q_w \longrightarrow$ Identity
as $E_i, E_j \longrightarrow \infty$

explains coeffs, and
small avoided crossings

Result 1: Improved inclusion bounds

In practise $t(u) = ||u||_{w,\partial\Omega}/||u||_\Omega$ never reaches zero.

But we can bound the distance to nearest level $\frac{|E-E_j|}{E_j^{1/2}} \le C_\Omega t(u)$

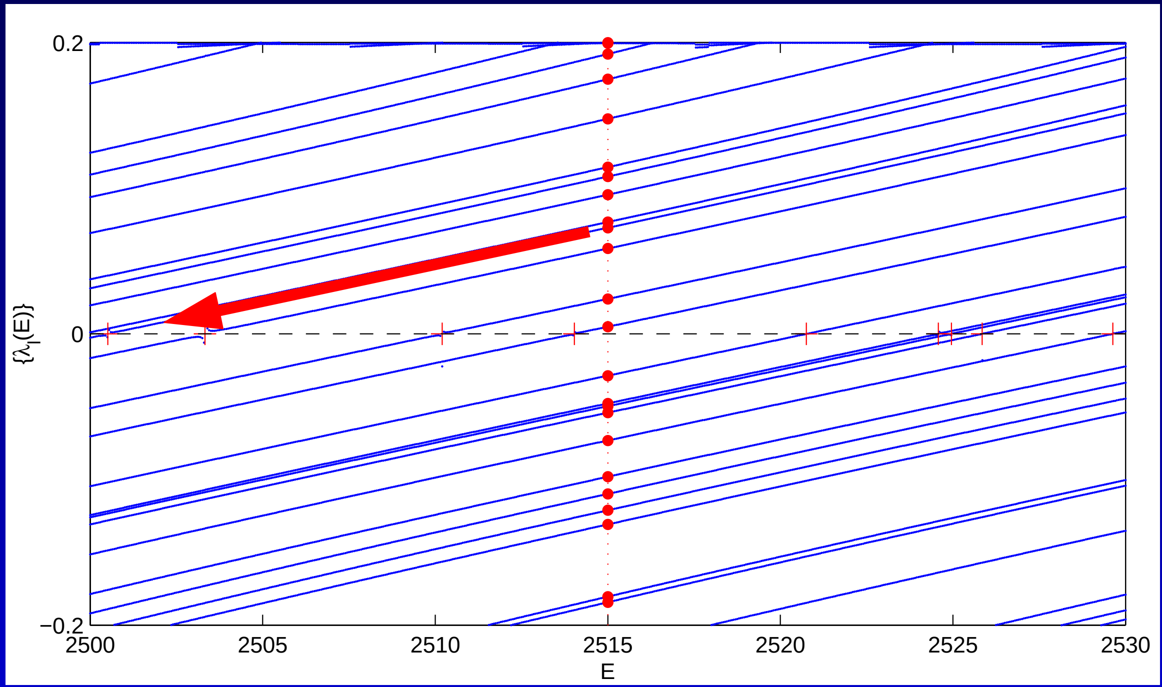


- $O(E^{1/2})$ tighter than classical bounds (Kuttler-Sigillito '84)

Result 2: scaling method (Vergini ’94, explained by B ’00, ’04)

Replace norm $||u||^2_\Omega$ in Rayleigh quotient by $\displaystyle\int_{\partial\Omega} (\mathbf{r}\cdot\mathbf{n})^{-1} u\mathbf{r}\cdot\nabla u\, ds$

Then E-dependent spectrum allows accurate prediction at high E:



- Many levels (E_j and ϕ_j) result from single matrix eigenproblem
- Speed gain (vs all known methods, incl integral eqns): $O(E^{1/2})$, can be 10^3
- Whole calculation $\sim 10^4$ levels at $j \sim 10^5$ takes only few CPU days

Basis set for $\mathcal{H}_\Omega(E)$ (B '02)

Plane waves

$\xi_l(\mathbf{r}) = e^{i\mathbf{k}_l \cdot \mathbf{r}}$

- inaccurate *e.g.* $\Omega =$ stadium
- fail as $E \to \infty$ if Ω nonconvex

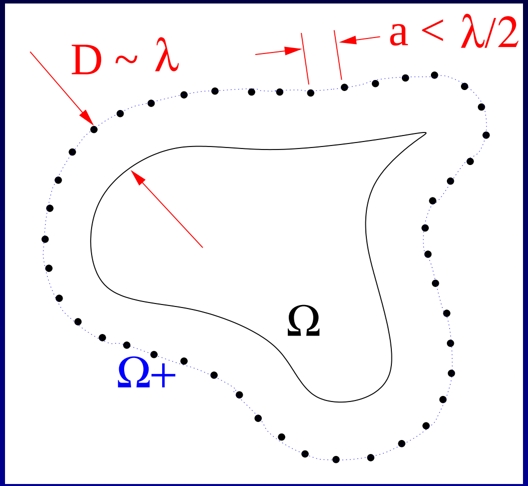
Basis set for $\mathcal{H}_\Omega(E)$ **(B '02)**

Plane waves
$\xi_l(\mathbf{r}) = e^{i\mathbf{k}_l\cdot\mathbf{r}}$

- inaccurate *e.g.* $\Omega =$ stadium
- fail as $E \to \infty$ if Ω nonconvex

Neumann functions
$\xi_l(\mathbf{r}) = Y_0(k|\mathbf{r} - \mathbf{x}_l|)$

good for nonconvex



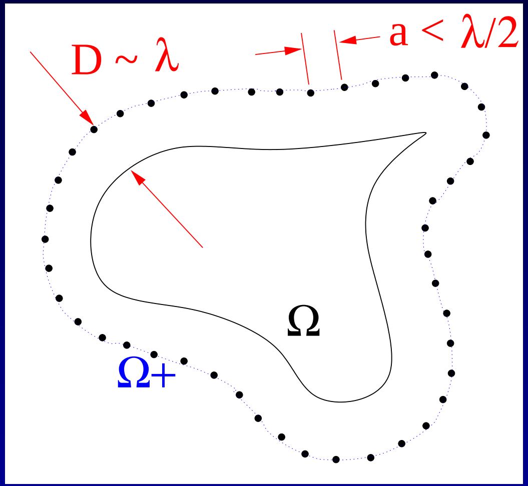
Why?

- $\partial\Omega^+$ layer potential complete in $\mathcal{H}_{\Omega^+}(E)$, for $k \neq$ Dir. eigenvalue of Ω^+
- $\mathcal{H}_{\Omega^+}(E)$ dense $\subset$ $\mathcal{H}_\Omega(E)$ (Lax '56, Runge approx)

Basis set for $\mathcal{H}_\Omega(E)$ **(B '02)**

Plane waves
$\xi_l(\mathbf{r}) = e^{i\mathbf{k}_l\cdot\mathbf{r}}$

- inaccurate *e.g.* $\Omega =$ stadium
- fail as $E \to \infty$ if Ω nonconvex



Neumann functions
$\xi_l(\mathbf{r}) = Y_0(k|\mathbf{r} - \mathbf{x}_l|)$

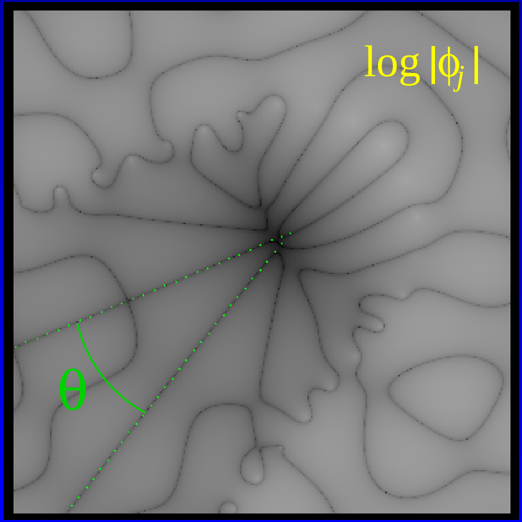
good for nonconvex

Why?

- $\partial\Omega^+$ layer potential complete in $\mathcal{H}_{\Omega^+}(E)$, for $k \neq$ Dir. eigenvalue of Ω^+
- $\mathcal{H}_{\Omega^+}(E)$ dense $\subset$ $\mathcal{H}_\Omega(E)$ (Lax '56, Runge approx)

If no analytic continuation of
ϕ_j outside Ω ? (Eckmann-Pillet '95)

e.g. corner, $\theta \neq \dfrac{\pi}{n}$



Empirical: errors small! MOVIE

Conclusions

Dirichlet eigenproblem –

- Applications: technology, to physics, to number theory…

At high energy, wealth of interesting phenomena –

- Equidistribution of modes: unprecedented numerical tests
- Accelerated ($\times 10^3$) computational tools: analyzed and developed

Conclusions

Dirichlet eigenproblem –

- Applications: technology, to physics, to number theory…

At high energy, wealth of interesting phenomena –

- Equidistribution of modes: unprecedented numerical tests
- Accelerated ($\times 10^3$) computational tools: analyzed and developed

Many future directions:

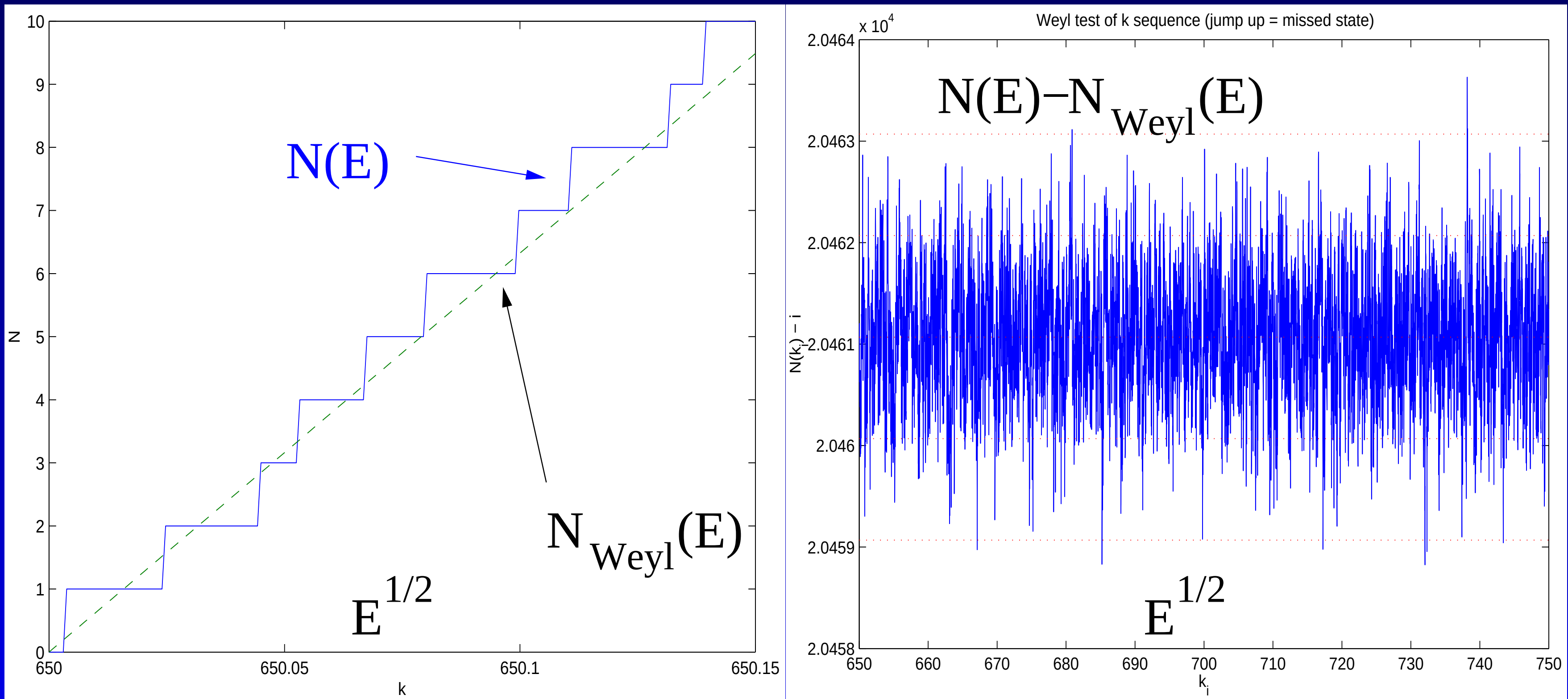
- Break the star-shaped restriction?
- Can similarly accelerate integral equation eigenmethods?
- Resonance, open (scattering) problems? *e.g.* laser cavity

Preprints/talks: `http://www.cims.nyu.edu/~barnett`

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