Plank's constant, time, and stationary states in quantum mechanics

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Overview of lectures

These lectures survey recent results on the 'semi-classical' asymptotics as $\lambda_j \to \infty$ of eigenfunctions of the Laplacian

$$\Delta \varphi_j = -\lambda_j^2 \varphi_j$$

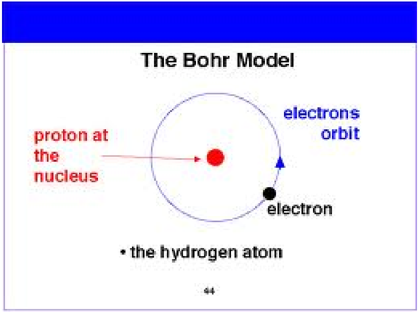
on a Riemannian manifold (M, g) of dimension m.

The main point is to relate nodal sets, L^p norms, or matrix elements $\langle A\varphi_j, \varphi_j \rangle$ to dynamics of the geodesic flow.

This line of research is basic in quantum mechanics and its relation to classical mechanics. Let us recall the early history.

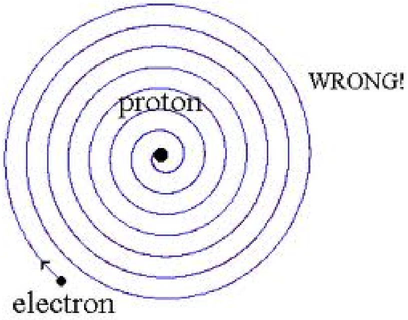
Visualizing an atom

Quantum mechanics resolves a puzzle about stability of atoms. Just before quantum mechanics, a hydrogen atom was roughly pictured as a 2-body planetary system, i.e. in terms of the classical Hamiltonian $H(x, \xi) = \frac{1}{2}|\xi|^2 + V(x)$ with $V = -\frac{1}{|x|}$.



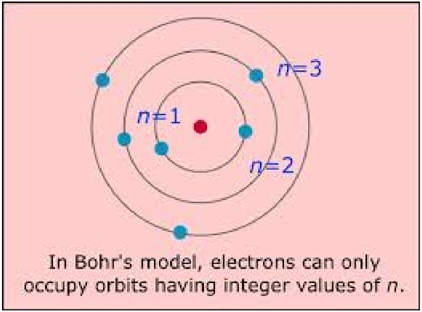
Visualizing an atom

But that can't be right: the electron would radiate energy and spiral into the nucleus.



So Bohr proposed that the electron can only occupy special stable orbits whose 'actions' were integral.

Bohr-Sommerfeld quantizable orbits



The 'energy levels' are a discrete set of periodic orbits γ whose actions $\int_\gamma pdq$ satisfy the Bohr-Sommerfeld quantization condition.

Bohr-Sommerfeld quantizable orbits

The Bohr theory is semi-classical: the energy levels are determined by classical orbits satisfying a quantization condition.

But this cannot be used for Helium, much less more complex atoms: bound orbits of Hydrogen are all periodic but very few Helium orbits are periodic and it is next to impossible to find them.

A completely different approach was developed by Heisenberg, Schrödinger, Dirac etc.

Schrödinger equation

Schrödinger (Zurich, 1926) proposed the accepted theory:

Quantisierung als Eigenwertproblem, Annalen der Physik (1926)

The energy states of the electron are modelled as eigenfunctions of the Schrödinger operator:

$$\hat{H}\varphi_j := (-\frac{\hbar^2}{2}\Delta + V)\varphi_j = E_j(\hbar)\varphi_j,$$

where $\Delta = \sum_j \frac{\partial^2}{\partial x_j^2}$ is the Laplacian and V is the potential, a multiplication operator on L^2. Here $\hbar$ is Planck's constant. We let $\{\varphi_j\}$ denote an orthonormal basis (ONB) of eigenfunctions.

Stationary states

Quantum mechanics replaces classical mechanics with linear algebra (an eigenvalue problem). The time evolution of an energy state is given by

$$U_\hbar(t)\varphi_j = e^{-i\frac{t}{\hbar}(-\frac{\hbar^2}{2}\Delta+V)}\varphi_j = e^{-i\frac{tE_j(\hbar)}{\hbar}}\varphi_j.$$

The only *observable quantities* are the the modulus square $|\varphi_j(x)|^2dx$ (the probability density of finding the particle at x) and matrix elements

$$\langle A\varphi_j, \varphi_j\rangle$$

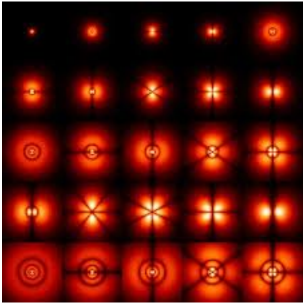
of observables (A is a self adjoint operator). The factors of $e^{-i\frac{tE_j(\hbar)}{\hbar}}$ cancel and so the particle evolves as if "stationary".

How do eigenstates relate to classical mechanics?

Quantum mechanics resolved the puzzle of how the electron can be moving and stationary at the same time. But it also replaced the geometric (classical mecahnical) Bohr model of classical orbits with eigenfunctions

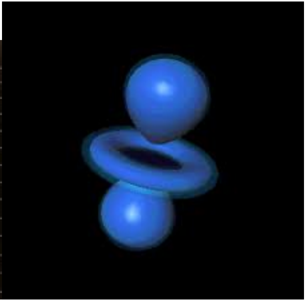
$$\hat{H}\varphi_j := (-\frac{\hbar^2}{2}\Delta + V)\varphi_j = E_j(\hbar)\varphi_j.$$

How does the semi-classical Bohr theory connect to the Schrödinger theory? How do we relate eigenfunctions to classical mechanics?



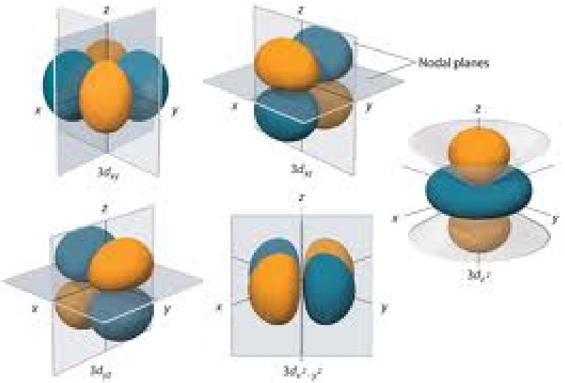
Intensity plots and excursion sets

The goal is to understand the size and shapes of eigenfunctions of Schrödinger operators and how they relate to classical mechanics. The modulus square $|\varphi_j(x)|^2 dx =$ the probability density of finding the particle at x. Below are graphed the *intensity plots* which darken in the regions where $|\varphi_j(x)|^2$ is large (most probable locations).

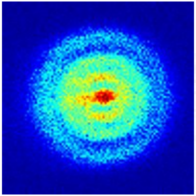
Nodal plots

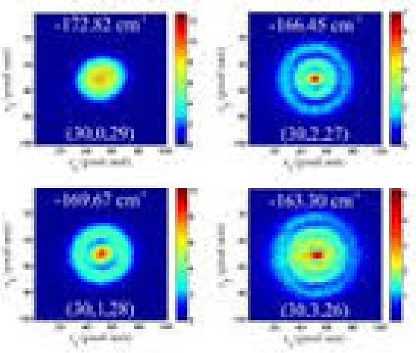
At the opposite are plots of the nodal hypersurfaces: the zero set $\mathcal{N}_j = \{x : \varphi_j(x, \hbar) = 0\}$.



These are the (windowpane) points where the probability (density) of the particle's position vanishes.

Experimental view of nodal sets of hydrogen: Stodoina





Vibrating string

Nodal sets were originally studied for vibrating strings, drums, membranes...the nodal set consists of the points where a vibrating membrane is stationary. In dimension 1 we are dealing with eigenfunctions $\varphi'' = -\lambda\varphi$ with $\varphi(0) = \varphi(L) = 0$, i.e. $\varphi(x) = \sin\frac{n\pi x}{L}$. The zeros are called nodes. Anti-nodes are the local maxima and minima. The nth eigenfunction has $n-1$ nodes.

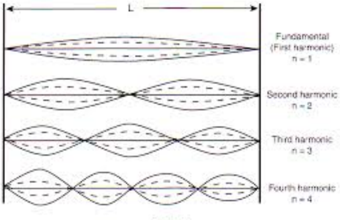
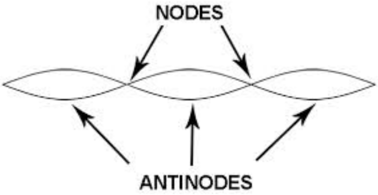


Figure 5

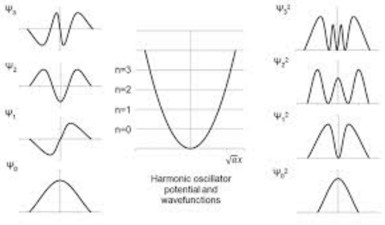


Sturm Liouville

More generally, one may study the real or complex zeros of one-dimensional Sturm-Liouville equations

$$(-\hbar^2 \frac{d^2}{dx^2} + V(x))\psi(x) = E(\hbar)\psi(x), \quad x \in \mathbb{R},$$

on all of $\mathbb{R}$ or on a finite interval. Below are graphics of Harmonic oscillator eigenfunctions, $V = x^2$. The nth eigenfunction has n nodes.



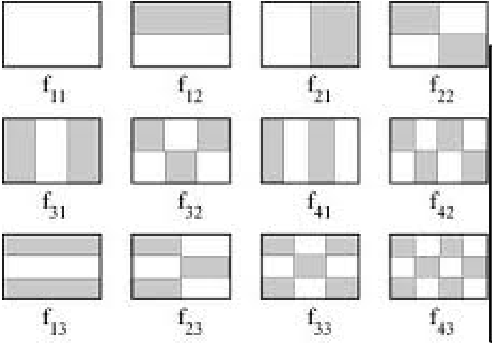
Naive higher dimensional generalization

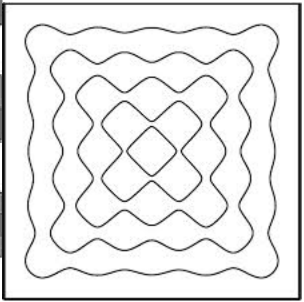
A naive idea is that in dimension 2, the nth eigenfunction might have n nodal domains, n^2 critical points (anti-nodes).

This turns out to be completely wrong in general. Even on the standard sphere or square, there are sequences of eigenfunctions with eigenvalue tending to infinity with just two or three nodal domains and just 10 critical points.

Higher dimensions; separation of variables

The only simple case where the 1D picture generalizes is when one can separate variables and write eigenfunctions as products, $\psi(x, y) = f(x)g(y)$ of 1-dimensional functions. The system is then *completely integrable* , and the nodal sets form checkerboard patterns. If one take linear combinations, the checkerboard breaks up.





The main questions

Relate asymptotics of nodal sets, L^p norms etc. as the 'energy' or eigenvalue λ increases to the dynamics of the geodesic flow.

We survey some recent results on:

- Nodal sets and domains: Numbers of nodal domains when the geodesic flow of (M, g) is ergodic; Volume of nodal sets in the real and complex domains; equidistribution of complex nodal sets in the ergodic case;

- L^p norms: Eigenfunctions which have extremal sup norms, i.e. which are extremal for $\frac{||\varphi_\lambda||_{L^\infty}}{||\varphi||_{L^2}}$, and the (M, g) which carry them;

Notation

Let (M, g) be a compact Riemannian manifold and let

$$\Delta_g = \frac{1}{\sqrt{g}} \sum_{i,j=1}^{n} \frac{\partial}{\partial x_i} \left(g^{ij} \sqrt{g} \frac{\partial}{\partial x_j} \right).$$

be its Laplace operator.
Let $\{\varphi_j\}$ be an orthonormal basis of eigenfunctions

$$\Delta \varphi_j = -\lambda_j^2 \, \varphi_j, \quad \langle \varphi_j, \varphi_k \rangle = \delta_{jk}$$

The NODAL SET of φ_j is its zero set:

$$\mathcal{N}_{\varphi_j} = \{x : \varphi_j(x) = 0\}.$$

Polynomials versus eigenfunctions

Let $\Delta \varphi_j = -\lambda_j^2 \varphi_j$.

- λ_j is known as the frequency, $\frac{1}{\lambda_j}$ as the wave length. φ_j oscillates on the scale $\frac{1}{\lambda_j}$.

- λ_j is analogous to the degree of a polynomial. For spherical harmonics on S^d, eigenfunctions of eigenvalue $\sim N^2$ are restrictions to S^d of harmonic homogeneous polynomials of degree N on $\mathbb{R}^{d+1}$.

- Nodal sets are analogous to real algebraic varieties of degree λ_j. But eigenfunctions have more zeros than a typical polynomial:φ_j **has a zero in every ball of radius** $\frac{a}{\lambda_j}$ **for** $a > 0$ **dependingly only on** (M, g)**.**

Elliptic versus hyperbolic

The eigenvalue equation $(\Delta + \lambda_j^2)\,\varphi_j = 0$ appears to be elliptic. But the correct notion of elliptic takes λ_j^2 as part of the symbol: the symbol is $|\xi|_g^2 - \lambda^2$ on T^*M where $|\xi_j|^2 = g^{ij}\xi_i\xi_j$. It vanishes on the 'energy surface' $\lambda_j S^*M$

The equation should be viewed as

- Elliptic on the scale $r = \frac{\epsilon}{\lambda_j}$ for small ϵ. I.e. on balls $B_r(p)$ of this radius, mean value inequalities, maximum principle etc are valid; they are not valid on larger balls containing more than one wave length.

- Hyperbolic on larger scales, e.g. r independent of λ. Natural tool on such scales is the wave equation. The relation to classical mechanics is only visible on this scale.

What is known about nodal sets, nodal domains and L^p norms

As in complex analysis, we would like to relate growth of eigenfunctions to growth of zero sets.

Growth is measured by L^p norms of L^2-normalized eigenfunctions:

$$||\varphi_\lambda||_{L^p}^p = \int_M \varphi_\lambda^p dV_g.$$

The NODAL SET of φ_λ is its zero set:

$$\mathcal{N}_{\varphi_\lambda} = \{x : \varphi_\lambda(x) = 0\}.$$

A NODAL DOMAIN is a connected component of $M \backslash \mathcal{N}_{\varphi_\lambda}$.

Nodal domains

The nodal domains partition M into disjoint open sets:

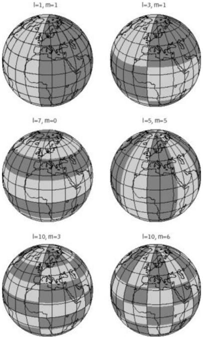
$$M \backslash \mathcal{N}_{\varphi_\lambda} = \bigcup_{j=1}^{N(\varphi_\lambda)} \Omega_j.$$

When 0 is a regular value of φ_λ the level sets are smooth hypersurfaces. In 2D, if 0 is a singular value, the singular set has Hausdorff codimension 1 in the nodal set (2 in M).

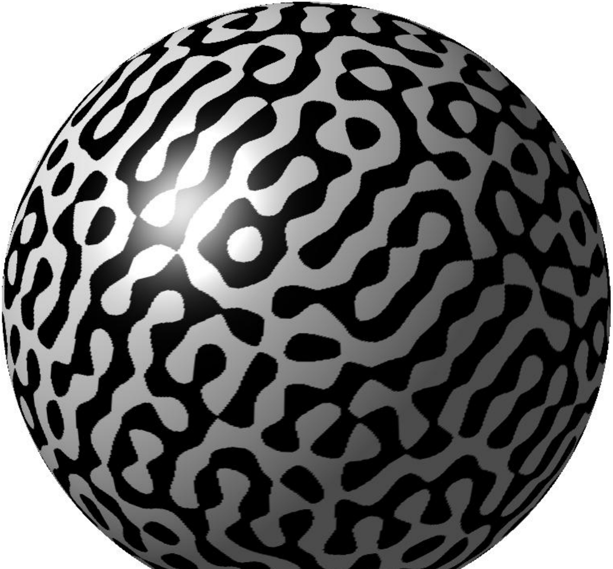
Courant theorem: $N(\varphi_{\lambda_n}) \leq n$. Improvements: Pleijel, Bourgain.

Not known How $N(\varphi_\lambda)$ grows with λ– even if it does.

Nodal domains for $\Re Y_m^\ell$ spherical harmonics: geodesic flow integrable: Eigenfunctions coming from separation of variables



Degree 40 spherical harmonic



Volume of nodal hypersurfaces

$\Delta\varphi_\lambda = -\lambda^2\varphi_\lambda.$

CONJECTURE

(Yau, 1978) For any C^∞ metric,

$$c_1\lambda \leq \mathcal{H}^{n-1}(\mathcal{N}_{\varphi_\lambda}) \leq C_2\lambda.$$

Lower bound proved in dimension 2: Brüning ('78).
Best upper bound to date in C^∞ case: (Hardt-Simon (1987)): $\mathcal{H}^{n-1}(\mathcal{N}_{\varphi_\lambda}) \leq C_2\lambda^\lambda$.

THEOREM

(Donnelly-Fefferman, 1988) Suppose that (M, g) is real analytic and $\Delta\varphi_\lambda = \lambda^2\varphi_\lambda$. Then

$$c_1\lambda \leq \mathcal{H}^{n-1}(\mathcal{N}_{\varphi_\lambda}) \leq C_2\lambda.$$

Some known results and conjectures

(1) Length in dimension 2 (Brüning, Yau, Donelly-Fefferman, Dong, 80's):

$C_g\sqrt{\lambda} \leq |\mathcal{N}_{\varphi_\lambda}| \leq C_b\lambda^{3/4}$.

- There exist (M, g) and sequences $\varphi_{\lambda_{j_k}}, \lambda_{j_k} \to \infty$, with a uniformly bounded number of nodal domains: $N(\varphi_{\lambda_{j_k}}) \leq 3$ on the standard sphere (Hans Lewy), and ≤ 10 for some metrics on the 2-torus (Jakobson-Nadirashvili). Hence, $N(\varphi_{\lambda_{j_k}})$ does not have to grow to infinity.
- Conjecture: for any g there exists some sequence of eigenfunctions such that $N(\varphi_{\lambda_{j_k}}) \to \infty$.

Recent lower bounds on volumes of nodal hypersurfaces: C^∞ case

Recently (2012) (by very different methods):

- (Colding-Minicozzi; Sogge-Z) $\mathcal{H}^{n-1}(\mathcal{N}_{\varphi_\lambda}) \geq \lambda^{\frac{3-n}{2}}$;
- (Hezari-Sogge) $\mathcal{H}^{n-1}(\mathcal{N}_{\varphi_\lambda}) \geq \lambda \, ||\varphi_\lambda||_{L^1}^2$, which would prove Yau conjecture for sequences with $||\varphi_\lambda||_{L^1} \geq C > 0$.

Distribution of nodal hypersurfaces

How do nodal hypersurfaces wind around on M.?
We put the natural Riemannian hyper-surface measure $d\mathcal{H}^{n-1}$ to consider the nodal set as a *current of integration* $\mathcal{N}_{\varphi_j}]$: for $f \in C(M)$ we put

$$\langle[\mathcal{N}_{\varphi_j}], f\rangle = \int_{\mathcal{N}_{\varphi_j}} f(x) d\mathcal{H}^{n-1}.$$

Problems:

- How does $\langle[\mathcal{N}_{\varphi_j}], f\rangle$ behave as $\lambda_j \to \infty$.
- If $U \subset M$ is a nice open set, find the total hypersurface volume $\mathcal{H}^{n-1}(\mathcal{N}_{\varphi_j} \cap U)$ as $\lambda_j \to \infty$.
- How does it reflect dynamics of the geodesic flow?

Physics conjecture on real nodal hypersurface: ergodic case

CONJECTURE

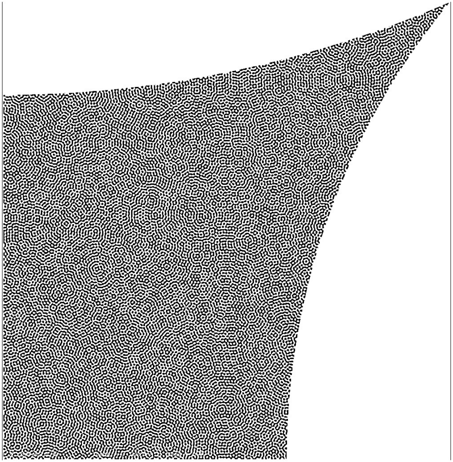
Let (M, g) be a real analytic Riemannian manifold with ergodic geodesic flow, and let $\{\varphi_j\}$ be the density one sequence of ergodic eigenfunctions. Then,

$$\frac{1}{\lambda_j}\langle[\mathcal{N}_{\varphi_j}], f\rangle \sim \frac{1}{Vol(M,g)}\int_M f dVol_g.$$

Evidence: it follows from the "random wave model", i.e. the conjecture that eigenfunctions in the ergodic case resemble Gaussian random waves of fixed frequency.

Ergodic billiards

We expect the dynamics of the geodesic flow to have an important impact on the number of nodal domains. In the case of chaotic geodesic flow, we expect nodal domains to be random.



Classical and Quantum ergodicity

- Classical ergodicity: G^t preserves the unit cosphere bundle $S^*_g M$. Ergodic = almost all geodesics are uniformly dense in $S^*_g M$.

- Quantum ergodicity: eigenfunctions become uniformly distributed in phase space (Shnirelman; Z, Colin de Verdière, Zworski-Z) . E.g. in configuration space M,

$$\int_E \varphi_j^2 dV_g \to \frac{Vol(E)}{Vol(M)}, \quad \forall E \subset M : Vol(\partial E) = 0.$$

- Ergodicity forces eigenfunctions to oscillation maximally in all directions, causing many zeros.

Over-view of new results

- (i) Counting nodal domains: on a surface of negative curvature (hence with ergodic geodesic flow) and with a concave boundary, the number of nodal domains tends to infinity (2014, J. Jung-Z). This is based on:
- (ii) Counting intersections of nodal lines and geodesics: upper and lower bounds (Jung-Z, Z, Toth-Z 2013). This is based on
- Improving L^∞ estimates of eigenfunctions and on "quantum ergodic restriction theorems". Real analytic surfaces (M, g) carrying eigenfunctions φ_{j_k} of maximal L^∞ growth must have points p so that all geodesics through p are closed (Sogge-Z, 2014).
- Phase space distribution of nodal hypersurfaces: If (M, g) is real analytic, then the zero sets $\{\varphi_j^{\mathbb{C}} = 0\}$ in $M_{\mathbb{C}} \simeq T^*M =$ complexification of M become equidistributed in $M_{\mathbb{C}}$ and on complex geodesics (Z, 2007, 2012).

New result of Z with Junehyuk Jung

There are two cases where we can prove that the number of nodal domains must tend to infinity along (almost the) entire sequence of eigenfunctions of an orthonormal basis $\{\varphi_j\}$:

- When (M, g) is a non-positively curved surface with concave boundary ("Sinai billiard");
- When (M, J, σ, g) is a Riemann surface surface with anti-holomorphic involution σ and with Fix(σ) a separating set = complexification of a real algebraic curve that divides its complexification. g is any negatively curved metric on M.

Number of nodal domains of Dirichlet/Neumann eigenfunctions of Sinai billiards tends to infinity

$$N(\varphi_\lambda) = \#\text{nodaldomainsof } \varphi_\lambda$$

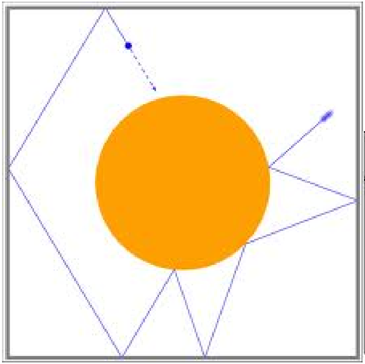
$$\Delta\varphi_j = -\lambda_j^2\varphi_j, \;\; \langle \varphi_j, \varphi_k \rangle = \delta_{jk}.$$

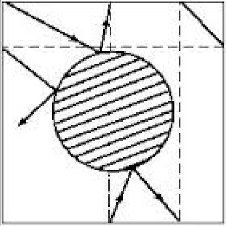
Theorem

Let (X, g) be a surface with curvature $k \leq 0$ and let D be a small disc in X. Remove one (or more non-overlapping) disc(s) to obtain a Sinai-Lorentz billiard $M = X \backslash D$. Then for any orthonormal eigenbasis $\{\varphi_j\}$ of eigenfunctions, one can find a density 1 subset A of $\mathbb{N}$ such that

$$\lim_{\substack{j \to \infty \\ j \in A}} N(\varphi_j) = \infty,$$

Sinai billiard: Ergodic, in fact hyperbolic





Number of domains tends to infinity for almost all even/odd eigenfunctions of a real Riemann surface of negative curvature

Theorem

Let (M, g) be a compact negatively curved C^∞ surface with an orientation-reversing isometric involution $\sigma : M \to M$ with $Fix(\sigma)$ separating. Then for any orthonormal eigenbasis $\{\varphi_j\}$ of $L^2_{even}(Y)$, resp. $\{\psi_j\}$ of $L^2_{odd}(M)$, one can find a density 1 subset A of $\mathbb{N}$ such that

$$\lim_{\substack{j\to\infty \\ j\in A}} N(\varphi_j) = \infty,$$

resp.

$$\lim_{\substack{j\to\infty \\ j\in A}} N(\psi_j) = \infty,$$

For odd eigenfunctions, the conclusion holds as long as $Fix(\sigma) \neq \emptyset$.

Remarks

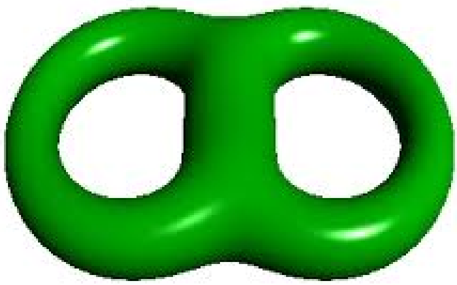
For a generic σ-invariant metric, the eigenvalues have multiplicity 1. Hence all eigenfunctions are either even or odd, and the parity restriction is not actually a restriction.

A density one subset $A \subset \mathbf{N}$ is one for which

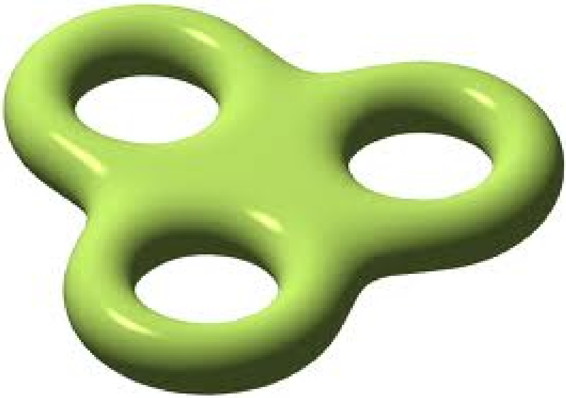
$$\frac{1}{N}\#\{j \in A, j \leq N\} \to 1, \quad N \to \infty.$$

Hyperelliptic Riemann surface $g = 2$: Involution: top-bottom

As this picture indicates, the surfaces in question are complexifications of real algebraic curves. $Fix(\sigma)$ is the underlying real curve.



Hyperelliptic Riemann surface $g = 3$ top-bottom



Ghosh-Reznikov-Sarnak (2013)

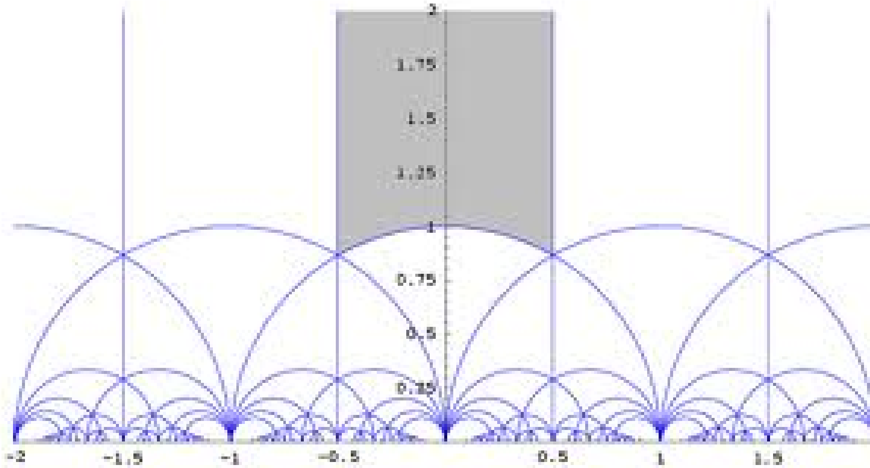
They give a power law lower bound for special eigenfunctions on a special (M, g) assuming the Lindelof hypothesis. The argument is the inspiration for our work:

Theorem

(GRS)
Let φ be an even Maass-Hecke L^2 eigenfunction on $\mathbb{X} = SL(2,\mathbb{Z})\backslash\mathbb{H}$. Denote the nodal domains which intersect a compact geodesic segment $\beta \subset \delta = \{iy \mid y > 0\}$ by $N^\beta(\varphi)$. Assume β is sufficiently long and assume the Lindelof Hypothesis for the Maass-Hecke L-functions. Then

$$N^\beta(\varphi) \gg_\epsilon \lambda_\varphi^{\frac{1}{24}-\epsilon}.$$

Modular surface and vertical geodesic



Equidistribution of nodal sets

The second result concerns the conjecture:

Conjecture

Let (M, g) be a real analytic Riemannian manifold with ergodic geodesic flow, and let $\{\varphi_j\}$ be the density one sequence of ergodic eigenfunctions. Then,

$$\frac{1}{\lambda_j}\langle[\mathcal{N}_{\varphi_j}], f\rangle \sim \frac{1}{Vol(M,g)}\int_M f dVol_g.$$

We cannot prove or disprove it. But we can prove a positive result for

ANALYTIC CONTINUATIONS of EIGENFUNCTIONS $\varphi_j^{\mathbb{C}}$ to the complexification $M_{\mathbb{C}} \simeq T^*M$ when the geodesic flow is ergodic.

Equi-distribution of complex nodal sets in the ergodic case

Theorem

(Z, 2007) Assume (M, g) is real analytic and that the geodesic flow of (M, g) is ergodic. Then for all but a sparse subsequence of λ_j,

$$\frac{1}{\lambda_j} \int_{\mathcal{N}_{\varphi^{\mathbb{C}}_{\lambda_j}}} f \omega_g^{m-1} \to \frac{i}{\pi} \int_{M_\epsilon} f \bar{\partial}\partial \sqrt{\rho} \wedge \omega_g^{m-1}$$

Moreover (Z, 2013) Let γ be a geodesic satisfying a certain generic assymetry condition (postponed). Then for all but a sparse subsequence of λ_j, the intersection points $\zeta_k(\lambda_j) = t_k + i\tau_k$ of $\gamma_{\mathbb{C}} \cap \mathcal{N}_{\varphi^{\mathbb{C}}_{\lambda_j}}$ satisfy:

$$\frac{1}{\lambda_j} \sum_k f(\zeta_k(\lambda_j)) \to \int_{\mathbb{R}} f(t) dt.$$

Thus, the complex zeros condense on the real points of the geodesic and are uniformly distributed along it.