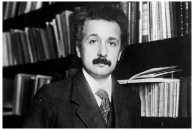
Delocalization of Schrödinger eigenfunctions

Nalini Anantharaman

Université de Strasbourg

I. Some history



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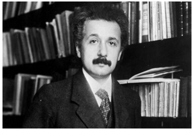

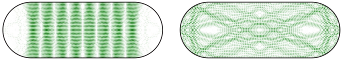

II. Quantum ergodicity

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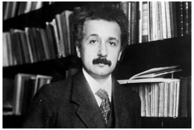
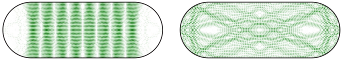
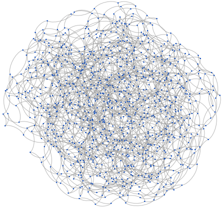




II. Quantum ergodicity

III. Toy model : discrete graphs



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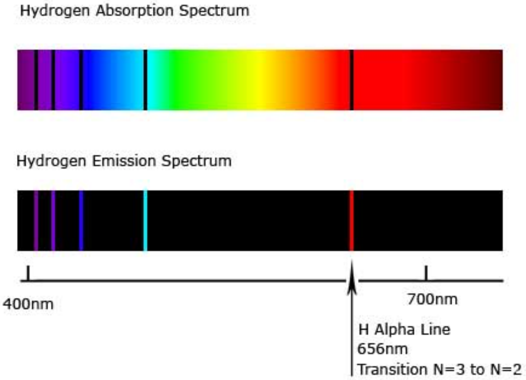
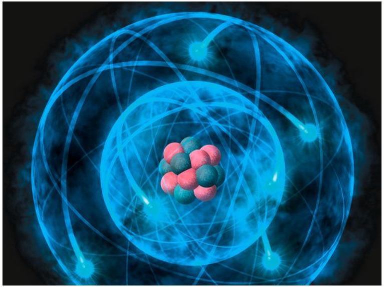
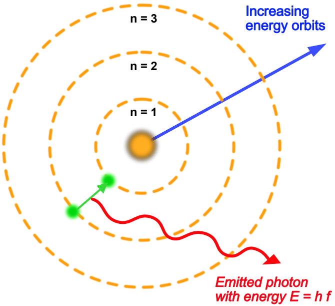


1913 : Bohr's model of the hydrogen atom





Kinetic momentum is "quantized" $J = nh$, where $n \in \mathbb{N}$.

1917 : A paper of Einstein

Zum Quantensatz von Sommerfeld und Epstein

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Zum Quantensatz von Sommerfeld und Epstein

Typus b): es treten unendlich viele p_i-Systeme an der betrachteten Stelle auf. In diesem Falle lassen sich die p_i nicht als Funktionen der q_i darstellen.

Man bemerkt sogleich, daß der Typus b) die im § 2 formulierte Quantenbedingung 11) ausschließt. Andererseits bezieht sich die klassische statistische Mechanik im wesentlichen nur auf den Typus b); denn nur in diesem Falle ist die mikrokanonische Gesamtheit der auf ein System sich beziehenden Zeitgesamtheit äquivalent[1]).

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[1]) In der mikrokanonischen Gesamtheit sind Systeme vorhanden, welche bei gegebenen q_i beliebig gegebene (mit dem Energiewert vereinbare) p_i besitzen.

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Type b): There are infinitely many p_i-systems at the location under consideration. In this case the p_i *cannot* be represented as functions of the q_i.

One notices immediately that type b) excludes the quantum condition we formulated in §2. On the other hand, classical statistical mechanics deals essentially *only* with type b); because only in this case is the microcanonic ensemble of *one* system equivalent to the time ensemble.[3]

In summarizing we can say: The application of the quantum condition (11) demands that there exist orbits such that a *single* orbit determines the p_i-field for which a potential J^* exists.

1925 : operators / wave mechanics

- Heisenberg : physical observables are operators (matrices) obeying certain commutation rules
$$[\,\widehat{p}\,,\,\widehat{q}\,] = i\hbar I.$$
The "spectrum" is obtained by computing eigenvalues of the energy operator $\widehat{H}$.

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- De Broglie (1923) : wave particle duality.
- Schrödinger (1925) : wave mechanics
$$i\hbar\,\frac{\mathrm{d}\psi}{\mathrm{d}t} = \Big(-\frac{\hbar^2}{2m}\Delta + V\Big)\psi$$
$\psi(x, y, z, t)$ is the wave function.

1925 : operators / wave mechanics

In Heisenberg's picture the spectrum is computed by diagonalizing the operator $\widehat{H}$.

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The two theories are mathematically equivalent : Schrödinger's picture corresponds to a representation of the Heisenberg algebra on the Hilbert space $L^2(\mathbb{R}^3)$.

But not physically equivalent !

Wigner 1950' Random Matrix model for heavy nuclei

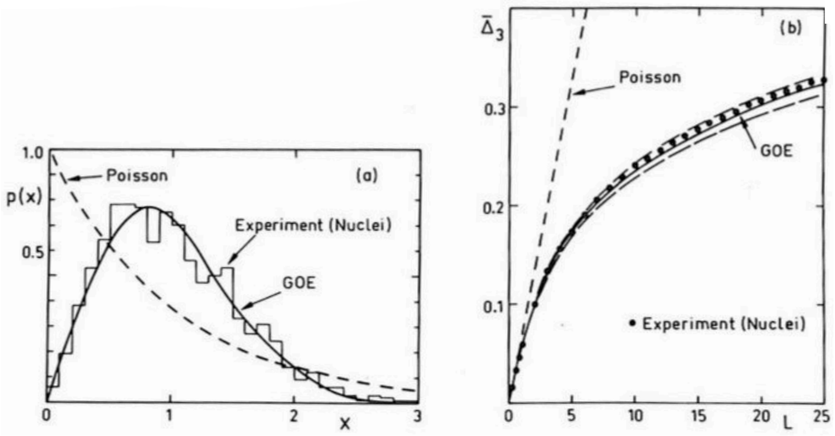

Figure: Left : nearest neighbour spacing histogram for nuclear data ensemble (NDE). Right : Dyon-Mehta statistic $\overline{\Delta}$ for NDE. Source O. Bohigas

Spectral statistics for hydrogen atom in strong magnetic field

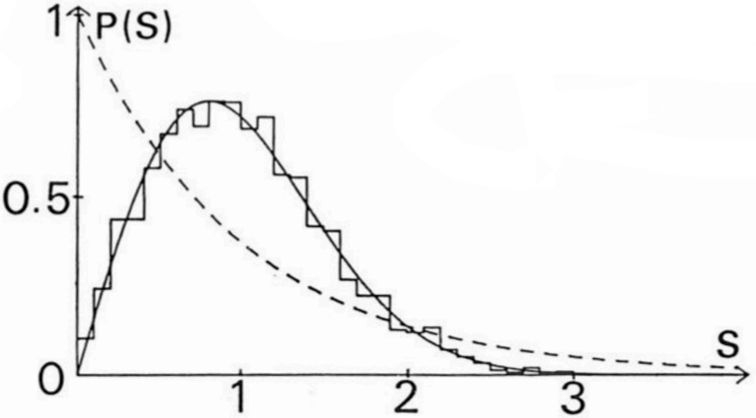

Figure: Source Delande.

Billiard tables

In classical mechanics, billiard flow $\phi^t : (x,\xi) \mapsto (x + t\xi, \xi)$.

In quantum mechanics, $i\hbar \dfrac{d\psi}{dt} = \left(-\dfrac{\hbar^2}{2m}\Delta + 0 \right)\psi$.

Spectral statistics for several billiard tables

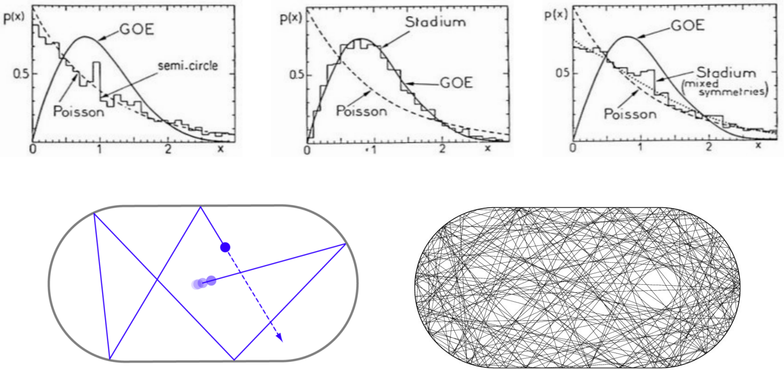

Figure: Random matrices and chaotic dynamics

A list of questions and conjectures

For classically ergodic / chaotic systems,

- show that the spectrum of the quantum system resembles that of large random matrices (Bohigas-Giannoni-Schmit conjecture);

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- study the probability density $|\psi(x)|^2$, where $\psi(x)$ is a solution to the Schrödinger equation (Quantum Unique Ergodicity conjecture);
- show that $\psi(x)$ resembles a gaussian process ($x \in B(x_0, R\hbar), R \gg 1$) (Berry conjecture).

A list of questions and conjectures

This is meant in the limit $\hbar \to 0$ (small wavelength).

$$\Big(-\frac{\hbar^2}{2m}\Delta + V \Big)\psi = E\psi \implies \|\nabla\psi\| \sim \frac{\sqrt{2mE}}{\hbar}$$

II. Quantum ergodicity

M a billiard table / compact Riemannian manifold, of dimension d.

In classical mechanics, billiard flow $\phi^t : (x, \xi) \mapsto (x + t\xi, \xi)$
(or more generally, the geodesic flow = motion with zero acceleration).

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In quantum mechanics :

$$i\hbar \frac{d\psi}{dt} = \Big(-\frac{\hbar^2}{2m}\Delta + 0 \Big)\psi$$
$$-\frac{\hbar^2}{2m}\Delta\psi = E\psi,$$

in the limit of small wavelengths.

Disk

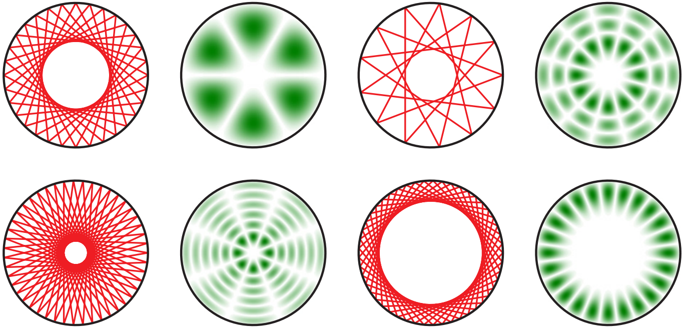


Figure: Billiard trajectories and eigenfunctions in a disk. Source A. Bäcker.

Sphere

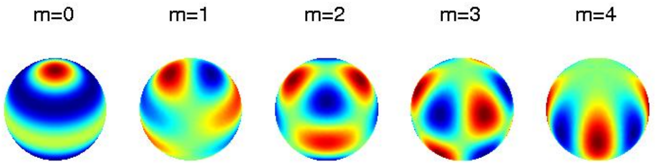


Figure: Spherical harmonics

Square / torus

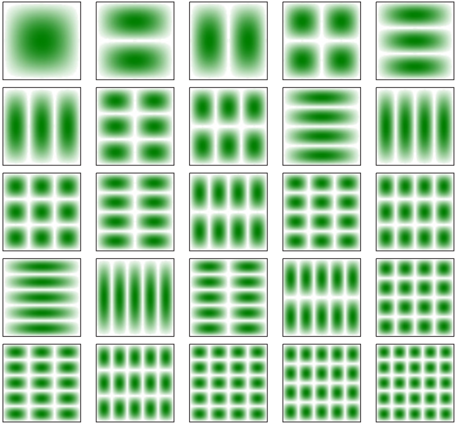


Figure: Eigenfunctions in a square. Source A. Bäcker.

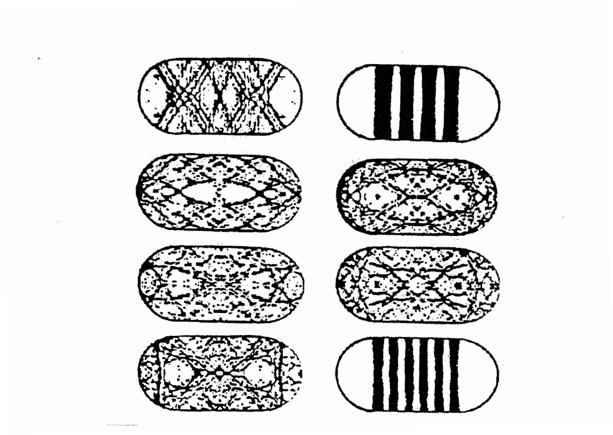


Figure: A few eigenfunctions of the Bunimovich billiard (Heller, 89).

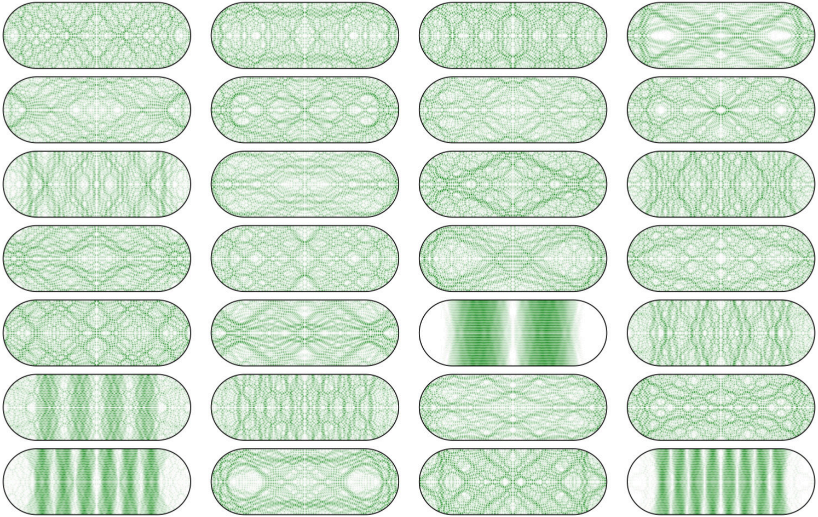
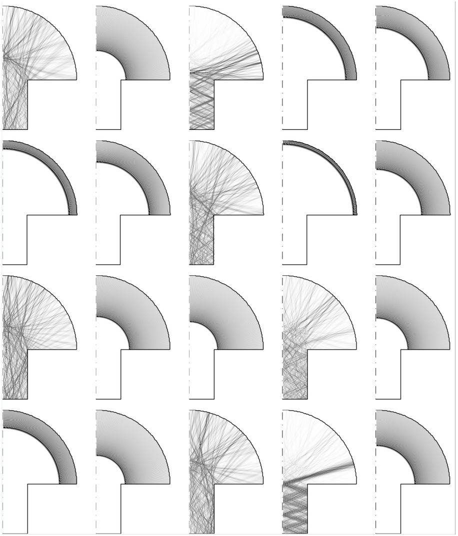


Figure: Source A. Bäcker

Eigenfunctions in a mushroom-shaped billiard. Source A. Bäcker



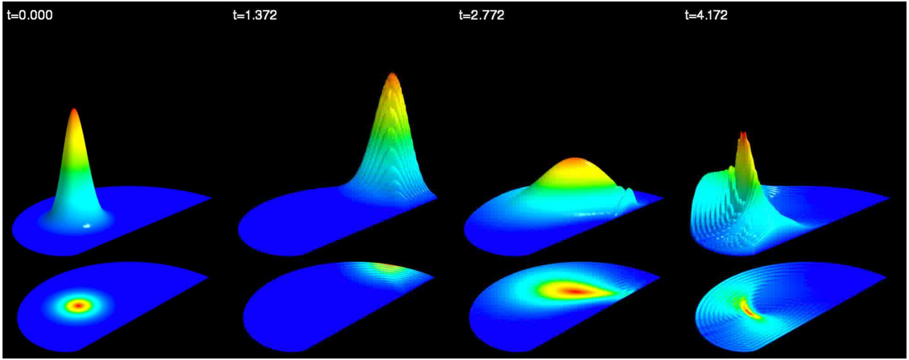
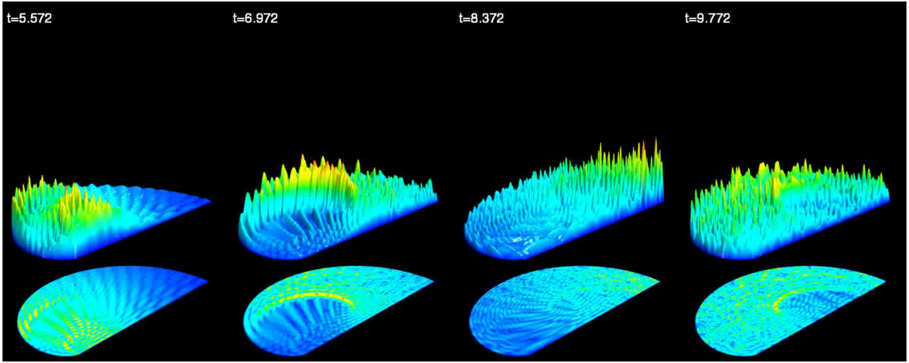


Figure: Propagation of a gaussian wave packet in a cardioid. Source A. Bäcker.



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Eigenfunctions in the high frequency limit

M a billiard table / compact Riemannian manifold, of dimension d.

$$\Delta\psi_k = -\lambda_k\psi_k \quad \text{or} \quad -\frac{\hbar^2}{2m}\Delta\psi = E\psi,$$

$$\|\psi_k\|_{L^2(M)} = 1,$$

in the limit $\lambda_k \longrightarrow +\infty$.

We study the weak limits of the probability measures on M,

$$\left|\psi_k(x)\right|^2 \mathrm{d}\,\mathrm{Vol}(x).$$

Let $(\psi_k)_{k\in\mathbb{N}}$ be an orthonormal basis of $L^2(M)$, with

$$-\Delta\psi_k = \lambda_k\psi_k, \qquad \lambda_k \leqslant \lambda_{k+1}.$$

QE Theorem (simplified): Shnirelman 74, Zelditch 85, Colin de Verdière 85

Assume that the action of the geodesic flow is **ergodic** for the Liouville measure. Let $a \in C^0(M)$. Then

$$\frac{1}{N(\lambda)}\sum_{\lambda_k\leqslant\lambda}\left|\int_M a(x)|\psi_k(x)|^2 \,\mathrm{d}\,\mathrm{Vol}(x) - \int_M a(x)\,\mathrm{d}\,\mathrm{Vol}(x)\right| \xrightarrow[\lambda\to\infty]{} 0.$$

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Equivalently, there exists a subset $\mathcal{S} \subset \mathbb{N}$ of density 1, such that

$$\int_M a(x) \left|\psi_k(x)\right|^2 \mathrm{d}\,\mathrm{Vol}(x) \xrightarrow[\substack{k \longrightarrow +\infty \\ k \in \mathcal{S}}]{} \int_M a(x)\, \mathrm{d}\,\mathrm{Vol}(x).$$

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Equivalently,

$$\left|\psi_k(x)\right|^2 \mathrm{Vol}(x) \xrightarrow[\substack{k \longrightarrow +\infty \\ k \in \mathcal{S}}]{} \mathrm{d}\,\mathrm{Vol}(x)$$

in the weak topology.

The full statement uses analysis on phase space, i.e.

$$T^*M = \left\{(x,\xi), x \in M, \xi \in T^*_x M\right\}.$$

For $a = a(x,\xi)$ a "reasonable" function on phase space, we can define an operator on $L^2(M)$,

$$a(x, D_x) \quad \left(D_x = \frac{1}{i}\partial_x\right).$$

On $M = \mathbb{R}^d$, we identify the momentum ξ with the Fourier variable, and put

$$a(x, D_x)f(x) = \frac{1}{(2\pi)^d} \int_{\mathbb{R}^d} a(x, \xi)\, \widehat{f}(\xi)\, \mathrm{e}^{i\xi\cdot x}\, \mathrm{d}\xi.$$

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for a a "reasonable" function.

Say $a \in \mathcal{S}^0(T^*M)$ if a is smooth and 0-homogeneous in ξ (i.e. a is a smooth function on the sphere bundle SM).

$$-\Delta\psi_k = \lambda_k\psi_k, \qquad \lambda_k \leqslant \lambda_{k+1}.$$

For $a \in \mathcal{S}^0(T^*M)$, we consider

$$\langle \psi_k, a(x, D_x)\psi_k \rangle_{L^2(M)}.$$

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For $a \in \mathcal{S}^0(T^*M)$, we consider

$$\langle \psi_k, a(x, D_x)\psi_k \rangle_{L^2(M)}.$$

This amounts to $\int_M a(x)|\psi_k(x)|^2 \, \mathrm{d}\,\mathrm{Vol}(x)$ if $a = a(x)$.

Let $(\psi_k)_{k\in\mathbb{N}}$ be an orthonormal basis of $L^2(M)$, with

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QE Theorem (Shnirelman, Zelditch, Colin de Verdière)

Assume that the action of the geodesic flow is **ergodic** for the Liouville measure. Let $a(x,\xi) \in \mathcal{S}^0(T^*M)$. Then

$$\frac{1}{N(\lambda)} \sum_{\lambda_k \leqslant \lambda} \left| \left\langle \psi_k, a(x, D_x)\psi_k \right\rangle_{L^2(M)} - \int_{|\xi|=1} a(x,\xi)\, \mathrm{d}x\, \mathrm{d}\xi \right| \longrightarrow 0.$$

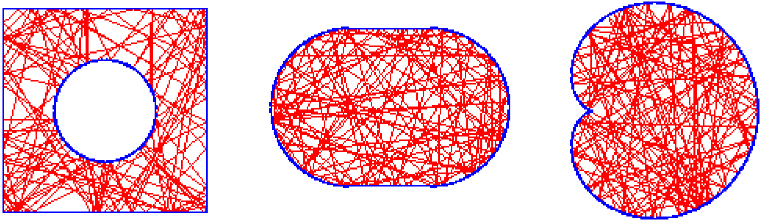
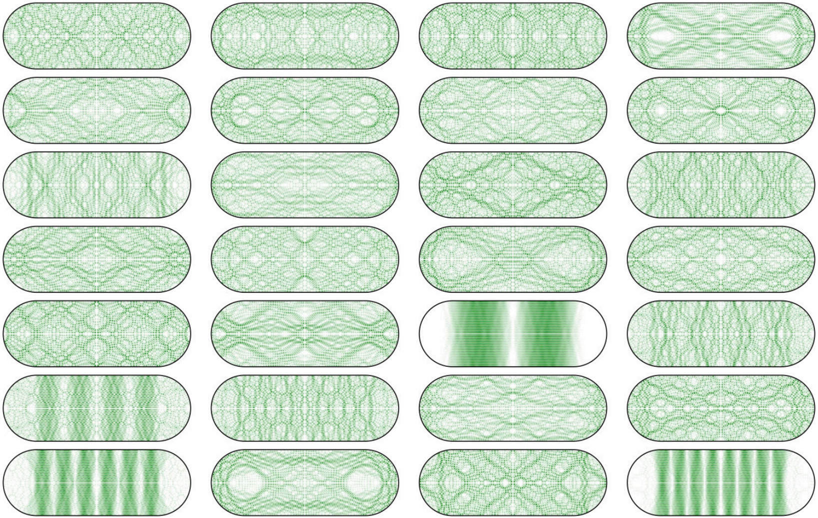


Figure: Ergodic billiards. Source A. Bäcker



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Why the geodesic flow ?

1. Define the "Quantum Variance"

$$Var_\lambda(K) = \frac{1}{N(\lambda)} \sum_{\lambda_k \leqslant \lambda} \left| \langle \psi_k, \qquad K \qquad \psi_k \rangle_{L^2(M)} \right| .$$

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   Invariance property under conjugacy by $e^{it\sqrt{\Delta}}$ (quantum dynamics).

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$$\limsup_{\lambda \longrightarrow \infty} \mathrm{Var}_\lambda\big(a(x, D_x)\big) = \limsup_{\lambda \longrightarrow \infty} \mathrm{Var}_\lambda\Big(\frac{1}{T}\int_0^T a \circ \phi^t(x, D_x) \, \mathrm{d}t\Big)$$

3 Control by the L^2-norm (Plancherel formula).

$$\limsup_{\lambda\to\infty} \mathrm{Var}_\lambda(a(x,D_x)) = \limsup_{\lambda\to\infty} \mathrm{Var}_\lambda\Big(\frac{1}{T}\int_0^T a\circ\phi^t(x,D_x)\,\mathrm{d}t\Big)$$

$$\leqslant \Big(\int_{x\in M,|\xi|=1}\Big|\frac{1}{T}\int_0^T a\circ\phi^t(x,\xi)\,\mathrm{d}t\Big|^2\mathrm{d}x\,\mathrm{d}\xi\Big)^{1/2}.$$

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4 Use the ergodicity of classical dynamics to conclude.
Ergodicity : if a has zero mean, then

$$\lim_{T\to+\infty}\frac{1}{T}\int_0^T a\circ\phi^t(x,\xi)\,\mathrm{d}t = 0$$

in $L^2(\mathrm{d}x\,\mathrm{d}\xi)$ and for almost every (x,ξ).

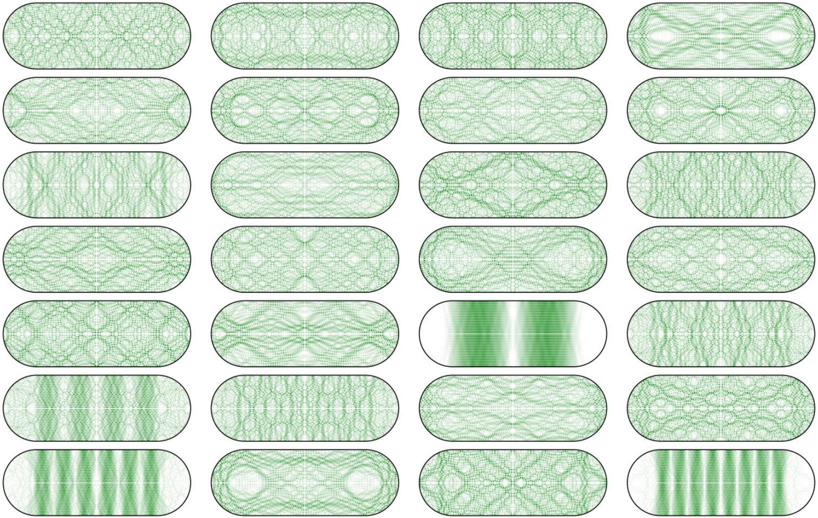

Figure: Source A. Bäcker

Quantum Unique Ergodicity conjecture : Rudnick, Sarnak 94

On a negatively curved manifold, we have convergence of the whole sequence :

$$\left\langle \psi_k , a(x, D_x)\psi_k \right\rangle_{L^2(M)} \longrightarrow \int_{(x,\xi)\in SM} a(x,\xi)\,\mathrm{d}x\,\mathrm{d}\xi.$$

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Proved by E. Lindenstrauss, in the special case of arithmetic congruence surfaces, for joint eigenfunctions of the Laplacian, and the Hecke operators.

Theorem

Let M have negative curvature and dimension d. Assume

$$\left\langle \psi_k , a(x, D_x)\psi_k \right\rangle_{L^2(M)} \longrightarrow \int_{(x,\xi)\in SM} a(x,\xi)\, \mathrm{d}\mu(x,\xi).$$

(1) [A-Nonnenmacher 2006] : μ must have positive (non vanishing) Kolmogorov-Sinai entropy.

For constant negative curvature, our result implies that the support of μ has dimension $\geqslant d = \dim M$.

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For constant negative curvature, our result implies that the support of μ has dimension $\geqslant d = \dim M$.

(2) [Dyatlov-Jin 2017] : $d = 2$, constant negative curvature, μ has full support.

III. Toy models

Toy models are “simple” models where either

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They often have a discrete character.
Instead of studying $\hbar \to 0$ one considers finite dimensional Hilbert spaces whose dimension $N \to +\infty$.

Regular graphs

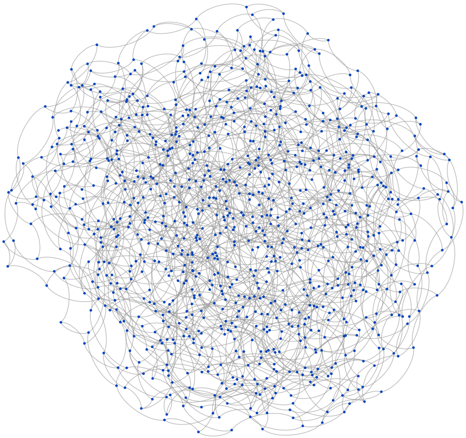

Figure: A (random) 3-regular graph. Source J. Salez.

Regular graphs

Let $G = (V, E)$ be a $(q+1)$-regular graph.

Discrete laplacian : $f : V \longrightarrow \mathbb{C}$,

$$\Delta f(x) = \sum_{y \sim x} \big(f(y) - f(x) \big) = \sum_{y \sim x} f(y) - (q+1) f(x).$$

$$\Delta = \mathcal{A} - (q+1) I$$

Why do they seem relevant ?

- They are locally modelled on the $(q+1)$- regular tree $\mathbb{T}_q$

.

- $\mathbb{T}_q$ may be considered to have curvature $-\infty$.
- Harmonic analysis on $\mathbb{T}_q$ is very similar to h.a. on $\mathbb{H}^n$.
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Why do they seem relevant ?

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- For $q = p$ a prime number, $\mathbb{T}_p$ is the symmetric space of the group $SL_2(\mathbb{Q}_p)$. $\mathbb{H}^2$ is the symmetric space of $SL_2(\mathbb{R})$.

A major difference

$$Sp(\mathcal{A}) \subset [-(q+1), q+1]$$

Let $|V| = N$. We look at the limit $N \to +\infty$.

Some advantages

- The adjacency matrix $\mathcal{A}$ is already an $N \times N$ matrix, so may be easier to compare with Wigner's random matrices.
- Regular graphs may be easily randomized : the $\mathcal{G}_{N,d}$ model.

A geometric assumption

We assume that G_N has "few" short loops ($=$ converges to a tree in the sense of Benjamini-Schramm).

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We assume that G_N has "few" short loops (= converges to a tree in the sense of Benjamini-Schramm).

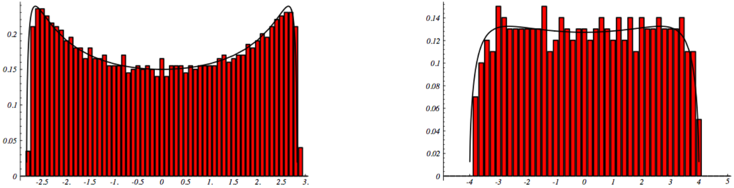
This implies convergence of the spectral measure (Kesten-McKay)

$$\frac{1}{N}\sharp\{i, \lambda_i \in I\} \xrightarrow[N\to+\infty]{} \int_I m(\lambda)\,\mathrm{d}\lambda$$

for any interval I.

The density m is completely explicit, supported in $(-2\sqrt{q}, 2\sqrt{q})$.

Numerical simulations on Random Regular Graphs (RRG)



(a) cubic graph on 2000 vertices; (b) 5-valent graph on 500 vertices.

Figure 1. Eigenvalue distributions of random graphs *vs* McKay's law

Figure: Source Jakobson-Miller-Rivin-Rudnick

Recent results : deterministic

A-Le Masson, 2013

Assume that G_N has "few" short loops and that it forms an **expander** family $=$ uniform spectral gap for $\mathcal{A}$.
Let $(\phi_i^{(N)})_{i=1}^N$ be an ONB of eigenfunctions of the laplacian on G_N.
Let $a = a_N : V_N \to \mathbb{R}$ be such that $|a(x)| \leqslant 1$ for all $x \in V_N$. Then

$$\lim_{N\to+\infty} \frac{1}{N} \sum_{i=1}^{N} \left| \sum_{x\in V_N} a(x) \left|\phi_i^{(N)}(x)\right|^2 - \langle a \rangle \right| = 0,$$

where

$$\langle a \rangle = \frac{1}{N} \sum_{x\in V_N} a(x).$$

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where

$$\langle a \rangle = \frac{1}{N} \sum_{x\in V_N} a(x).$$

For any $\epsilon > 0$,

$$\lim_{N\to+\infty} \frac{1}{N}\sharp\Big\{i, \Big|\sum_{x\in V_N} a(x)\left|\phi_i^{(N)}(x)\right|^2 - \langle a\rangle\Big| \geqslant \epsilon\Big\} = 0.$$

Recent results : deterministic

Brooks-Lindenstrauss, 2011

Assume that G_N has "few" loops of length $\leqslant c \log N$.
For $\epsilon > 0$, there exists $\delta > 0$ s.t. for every eigenfunction ϕ,

$$B \subset V_N, \quad \sum_{x \in B} \left|\phi(x)\right|^2 \geqslant \epsilon \implies |B| \geqslant N^\delta.$$

Proof also yields that $\|\phi\|_\infty \leqslant |\log N|^{-1/4}$.

Examples

Deterministic examples :

- the Ramanujan graphs of Lubotzky-Phillips-Sarnak 1988 (arithmetic quotients of the q-adic symmetric space $\mathsf{PGL}(2, \mathbb{Q}_q)/\mathsf{PGL}(2, \mathbb{Z}_q)$);

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- Cayley graphs of $SL_2(\mathbb{Z}/p\mathbb{Z})$, p ranges over the primes, (Bourgain-Gamburd, based on Helfgott 2005).

Recent results : random

Spectral statistics : Bauerschmidt, Huang, Knowles, Yau, 2016

Let $d = q + 1 \geqslant 10^{20}$.

For the $\mathcal{G}_{N,d}$ model, with large probability as $N \to +\infty$, the small scale Kesten-McKay law

$$\frac{1}{N} \sharp\{\, i, \lambda_i \in I \,\} \underset{N \longrightarrow +\infty}{\sim} \int_I m(\lambda)\, \mathrm{d}\lambda$$

holds for any interval I for $|I| \geqslant \log N^{\bullet}/N$, and

$$I \subset [-2\sqrt{q} + \epsilon, 2\sqrt{q} - \epsilon].$$

Recent results : random

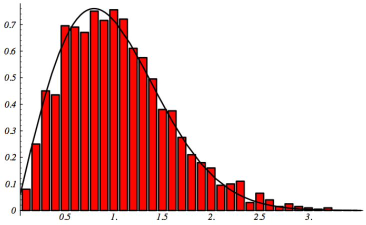

Figure 2. Level spacing distribution of a cubic graph on 2000 vertices *vs* GOE

Spectral statistics : Bauerschmidt, Huang, Knowles, Yau

Nearest neighbour spacing distribution coincides with Wigner matrices for

$$N^{\epsilon} < d(= q+1) < N^{2/3-\epsilon}.$$

Recent results : random

Delocalization : Bauerschmidt, Huang, Yau

Let $d = q + 1 \geqslant 10^{20}$.

For the $\mathcal{G}_{N,d}$ model,

- $\| \phi_i^{(N)} \|_{\ell^\infty} \leqslant \frac{\log N^\bullet}{\sqrt{N}}$ as soon as $\lambda_i^{(N)} \in [-2\sqrt{q} + \epsilon, 2\sqrt{q} - \epsilon]$;

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- *(see also Bourgade –Yau)* QUE : given $a : \{1, \ldots, N\} \longrightarrow \mathbb{R}$, for all $\lambda_i^{(N)} \in [-2\sqrt{q}+\epsilon, 2\sqrt{q}-\epsilon]$,

$$\sum_{x=1}^{N} a(x) \left|\phi_i^{(N)}(x)\right|^2 = \frac{1}{N} \sum_n a(x) + O\left(\frac{\log N^\bullet}{N}\right) \| a \|_{\ell^2}$$

with large probability as $N \to +\infty$.

Recent results : random

Gaussianity of eigenvectors, Backhausz-Szegedy 2016

Consider the $\mathcal{G}_{N,d}$ model.

With probability $1 - o(1)$ as $N \to \infty$, one has : for all eigenfunctions $\phi_i^{(N)}$, for all diameters $R > 0$, the distribution of

$$\phi_i^{(N)}{}_{|B(x,R)},$$

when x is chosen uniformly at random in $V(\mathcal{G}_{N,d})$, is close to a Gaussian process on $B_{\mathbb{T}_q}(o, R)$.

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Remaining open question : is this Gaussian non-degenerate ?

Open questions and suggestions

- QUE for deterministic regular graphs ?
- Stronger forms of QUE for Random Regular Graphs ?
- Non-regular graphs (joint work with M. Sabri).

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- QUE for deterministic regular graphs ?
- Stronger forms of QUE for Random Regular Graphs ?
- Non-regular graphs (joint work with M. Sabri).
- More systematic study of manifolds in the large-scale limit (cf. Le Masson-Sahlsten for hyperbolic surfaces, when genus $g \longrightarrow +\infty$).
- Random manifolds?

End

Thank you for your attention !

...and thanks to R. Séroul and all colleagues who provided pictures.