

Motivation

Periodic orbits in quantum mechanics

Unveiling heteroclinic motions in quantum mechanics

Unveiling homoclinic motions in quantum mechanics

Riemann zeta function

Classical Motions in Quantum Mechanics or Mr. Tompkins meets Poincaré

F. Borondo

Departamento de Química
Universidad Autónoma de Madrid

DDAYS06

October 18–21, 2006



Outline

- 1 Motivation
 - Who was Mr. Tompkins?
 - Poincaré as pioneer in classical chaos
 - What if Mr. Tompkins had met Poincaré?
- 2 Periodic orbits in quantum mechanics
 - Model
 - Primer in Quantum Mechanics
 - Scar functions: The Tool
- 3 Unveiling heteroclinic motions in quantum mechanics
 - Heteroclinic motion and cross-correlation function
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 - Homoclinic motion and eigenvalues
 - Homoclinic motion and wave functions
- 5 Riemann zeta function



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Who was Mr. Tompkins?

Poincaré as pioneer in classical chaos

What if Mr. Tompkins had met Poincaré?

Who was Mr. Tompkins?

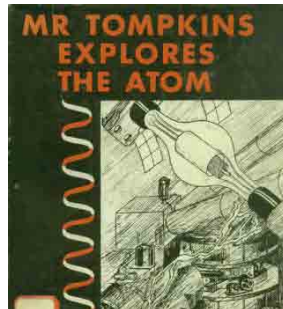
Main character in the books:

- *Mr. Tompkins in Wonderland* (1940)
- *Mr. Tompkins explores de atom* (1944)

written by the famous physicist of ukrainian origin Gamow.



F. Borondo



Mr. Tompkins meets Poincaré





The *G. Gamow*

George Gamow Memorial Lecture Series
 at the University of Colorado at Boulder

G. Gamow

- He played an important role in the development of quantum ideas: tunnel effect (also in astrophysics and cosmology)
- In his late years made a great job in popularizing science (UNESCO Kalinga prize)



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Poincaré as pioneer in classical chaos

What if Mr. Tompkins had met Poincaré?

In *Mr. Tompkins explores de atom* Gamow popularized the ideas of quantum mechanics



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Poincaré as pioneer in classical chaos



It all began with

...

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What if Mr. Tompkins had met Poincaré?

Mathematical competition in honor of King Oscar II sixtieth birthday



F. Borondo



Mr. Tompkins meets Poincaré

Announcement in Nature

Announcement of the Oscar Competition

Nature 30.7.1885

THE HIGHER MATHEMATICS

Prof. G. Mittag-Leffler, principal editor of the *Acta Mathematica*, forwards us the following communication, which will shortly appear in that journal:-

His Majesty Oscar II, wishing to give a fresh proof of his interest in the advancement of mathematical science, an interest already manifested by his graciously encouraging the publication of the journal *Acta Mathematica*, which is placed under his august protection, has resolved to award a prize, on January 21, 1889, the sixtieth anniversary of his birthday, to an important discovery in the field of higher mathematical analysis. This prize will consist of a gold medal of the eighteenth size bearing his Majesty's image and having a value of a thousand francs, together with a sum of two thousand five hundred crowns (1 crown = about 1 franc 4-centimes).

Announcement in Nature

(1) A system being given of a number whatever of particles attracting one another mutually according to Newton's law, it is proposed, on the assumption that there never takes place an impact of two particles to expand the coordinates of each particle in a series proceeding according to some known functions of time and converging uniformly for any space of time.

It seems that this problem, the solution of which will considerably enlarge our knowledge with regard to the system of the universe, might be solved by means of the analytical resources at our present disposition; this may at least be fairly supposed, because shortly before his death Lejeune-Dirichlet communicated to a friend of his, a mathematician, that he had discovered a method of integrating the differential equations of mechanics, and that he had succeeded, by applying this method, to demonstrate the stability of our planetary system in an absolutely strict

Motivation

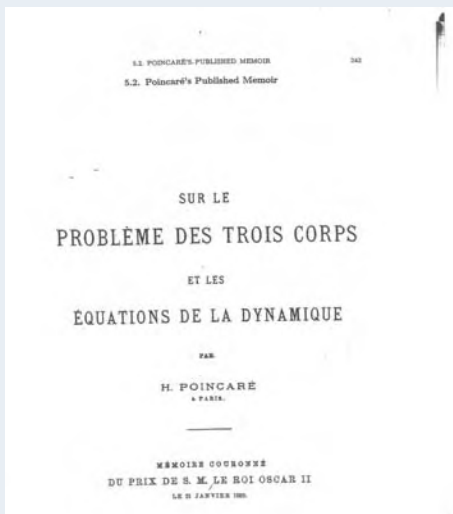
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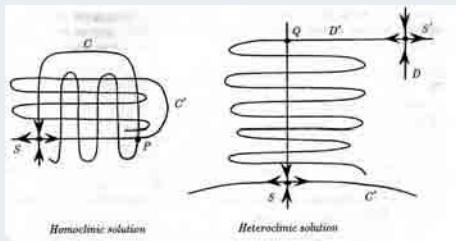
What if Mr. Tompkins had met Poincaré?

And the Oscar goes to ...



Poincaré results:

- Showed that the series used in Celestial Mechanics do not converge in general
 There is room for chaos
- Importance of:
 - Periodic orbits
 - Homoclinic solutions
 - Heteroclinic solutions



End of the story

- In the 1960's:
Birkhoff and Kolmogorov–Arnold–Moser



- In the 1990's:
Sussman&Wisdom and Laskar showing that **OUR** Solar System has some chaotic motions



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Poincaré as pioneer in classical chaos

What if Mr. Tompkins had met Poincaré?

What if Mr. Tompkins had met Poincaré?

If Mr. Tompkins had met Poincaré, Gamow would had written about homoclinic motion in his book!!!



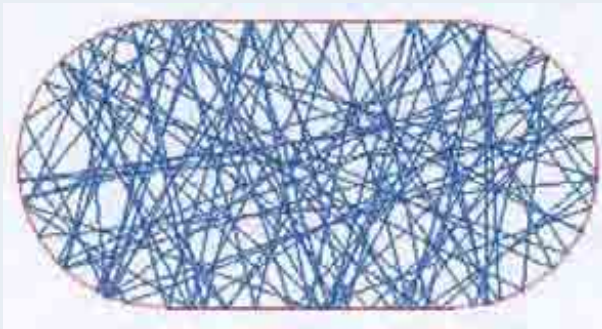
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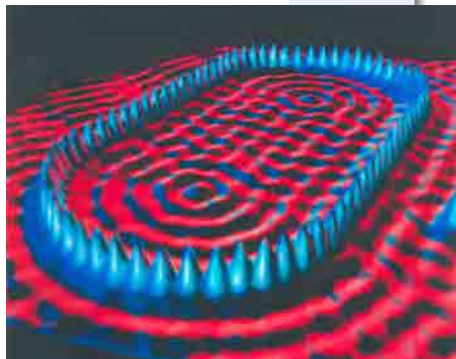
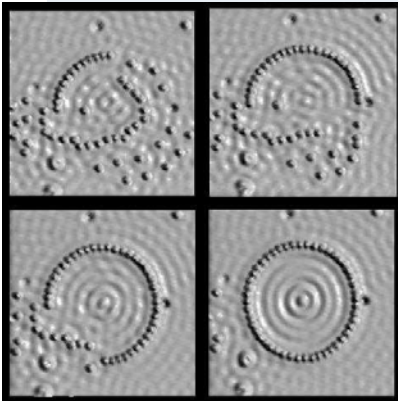


Model: Billiards

- Bunimovitch stadium billiard
- Hyperbolic dynamics
- Desymmetrized versions (1/4) of the stadium



Billiards: Models in Nanotechnology



Eigler

Billiards: Microwave Cavities

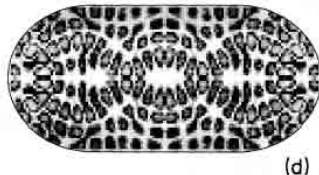
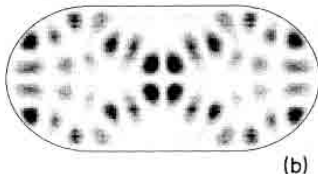
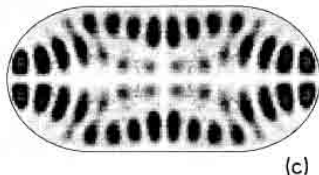
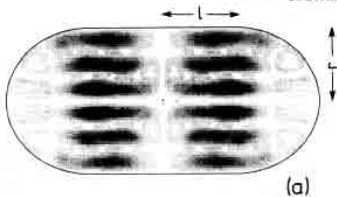
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PHYSICAL REVIEW LETTERS

11 MAY 1992

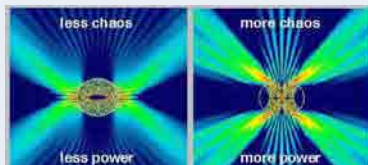
Experimental Determination of Billiard Wave Functions

J. Stein and H.-J. Stöckmann



Chaos in Optical Cavities

A. Douglas Stone, 1997



Billiards: Models in Acoustic

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VOLUME 53, NUMBER 1

JANUARY 1996

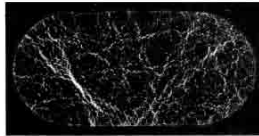
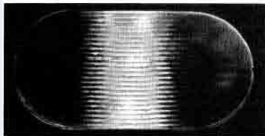
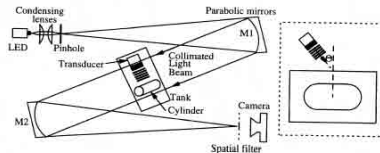
Experimental visualization of acoustic resonances within a stadium-shaped cavity

P. A. Chinnery and V. F. Humphrey

School of Physics, University of Bath, Bath BA2 7AY, United Kingdom.

(Received 15 September 1995)

Acoustic resonances of an insonified water-filled stadium-shaped cavity are located and visualized in a noninvasive manner using a schlieren technique. The chaotic nature of the geometry is seen to affect the form of the resonance patterns observed. Individual eigenstates of the cavity can be resolved at low frequencies; in particular, the "bouncing ball" modes. In the high-frequency (overlapping resonance) regime, nodal patterns are characterized by a network of ridges similar in form to those produced by a random superposition of plane waves.



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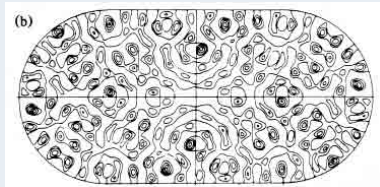


QM First Aid Kit

- De Broglie Hypothesis: $\lambda = \frac{h}{p} = \frac{2\pi\hbar}{P}$
- Wave function: $\psi(q, t)$, q =positions, t =time
- Interpretation: $|\psi|^2 = \psi^*\psi$ probability density
- Schrödinger equation: $i\hbar\frac{\partial\psi}{\partial t} = \hat{H}\psi$
- Stationary states: $\psi(q, t) = \phi_n(q) e^{-iE_n t/\hbar}$, with $\hat{H}\phi_n(q) = E_n\phi_n(q)$
- **Time evolution:** $\psi(q, t) = e^{i\hat{H}t/\hbar} \psi(q, 0)$
- Heisenberg Uncertainty Principle: $\Delta q \Delta p \geq \hbar/2$ and $\Delta E \tau \geq \hbar/2$

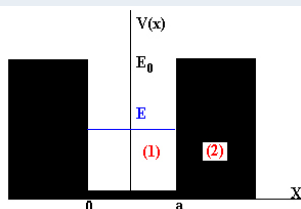


Example



- Helmholtz equation: $\nabla^2 \phi_n = k_n^2 \phi_n$
 $\phi_n(\text{boundary}) = 0$
- Dirac notation: $|n\rangle \equiv \phi_n$ $\langle n| \equiv \phi_n^*$
 scalar product $\equiv \langle n|m\rangle = \int \phi_n^* \phi_m \, d\tau$
- Time evolution:
 $|\psi(t)\rangle = e^{i\hat{H}t} |\psi(0)\rangle = e^{i\hat{H}t} \sum |n\rangle \langle n|\psi(0)\rangle =$
 $\sum |n\rangle \langle n|\psi(0)\rangle e^{-ik_n^2 t}$

Simpler example (even trivial)



- $-\frac{\hbar^2}{2m} \frac{d^2\psi}{dx^2} + V\psi = E\psi$
- $\frac{d^2\psi}{dx^2} + k^2\psi, \quad k = \frac{\sqrt{2mE}}{\hbar}$
- But, don't forget the dynamics:
 $k = \frac{P}{\hbar}$



Solution

- $\psi(x) = b \sin kx + c \cos kx$

- First boundary condition:

$$\psi(0) = 0 \longrightarrow c = 0 \longrightarrow \psi = b \sin kx$$

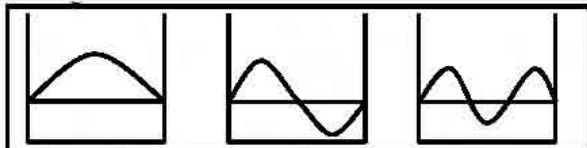
- Normalization condition:

$$\int_0^a |\psi|^2 dx = 1 \longrightarrow b = \sqrt{\frac{2}{L}}$$

- Second boundary condition:

$$\psi(a) = 0 \longrightarrow k_n = \frac{n\pi}{a}$$

- Solutions: $\psi_n(x) = \sqrt{\frac{2}{a}} \sin \frac{n\pi x}{a}, \quad n = 1, 2, \dots$



- But, don't forget the dynamics ... $k = \frac{P}{\hbar}$

- Classical action:

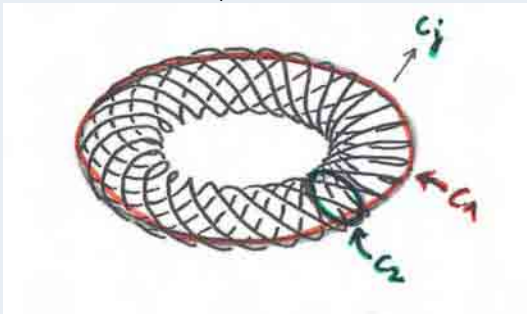
$$\oint P dx = 2 \int_0^a P dx = 2 \int_0^a k \hbar dx = 2k \hbar a = 2 \frac{n\pi}{a} \hbar a = nh$$

- Action is quantized!



Essential ingredients in QM

Action Quantization (Einstein–Brillouin–Kramers)

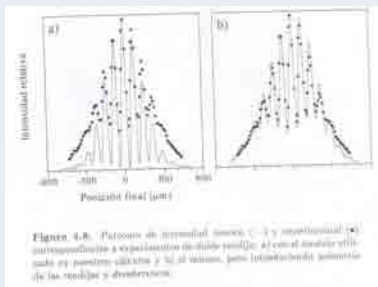


$$\oint_{C_j} \sum_i^N P_i dq_i = h \left(n_j + \frac{\alpha_j}{4} \right)$$

Classical information = Quantum condition

Essential ingredients in QM

• Interference



Tomonaga

• Coherence

What happens in the chaotic regime?

- Gutzwiller's theory (~ 1970 's)
- Based on the quantum mechanical Green function:

$$G(q, q'; E)$$

- Calculate trace

$$g(E) = \int G(q, q; E) dq = \sum \frac{1}{E - E_n}$$

- Semiclassical approximation:

$$g = \sum_P^{PO} \frac{T_P}{i} \sum_{r=1}^{\infty} \frac{\exp(irS_P/\hbar - i\pi r\mu_P/2)}{|\det[(M_P)^r - \mathbb{I}]|^{1/2}}$$



What to do?

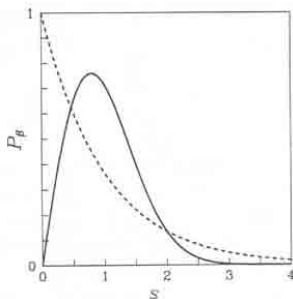
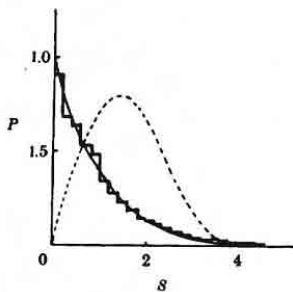
Level statistics



1. CADA UNA DE ESTAS DISTRIBUCIONES unidimensionales consta de 100 niveles. Los espectros, de derecha a izquierda, corresponden a: una formación periódica de líneas equidistantes; una sucesión aleatoria; una formación periódica perturbada por un ligero "bata" aleatoria de cada nivel; los estados energéticos del núcleo del arbi-166, todos con los mismos números cuánticos de espín y paridad; los 100 autovalores centrales de una matriz simétrica aleatoria de orden 300; las posiciones de los ceros de la función zeta de Riemann situados justo por en-

cima del cero 10^{27} -ésimo; un centenar de números primos consecutivos a partir de 103.613; la posición de los 100 variantes elevadas y soterradas más septentrionales de la autopista interestatal 85 estadounidense; posiciones de las travessas de una vía muerta de ferrocarril; posiciones de los anillos de crecimiento, desde 1884 hasta 1983, de un abeto del Monte Santa Helena, estado de Washington; fechas de los terremotos de California de magnitud 5.0 o mayor entre 1959 y 2001; longitudes de 100 paseos consecutivos en bicicleta.

Level statistics



$$\text{Poisson: } P(s) = \frac{1}{s_m} e^{-\frac{s}{s_m}}$$

$$\text{Wigner surmise: } P(s) = \frac{\pi s}{2s_m^2} e^{-\frac{s^2}{4s_m^2}}$$

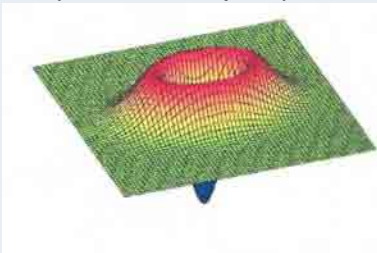


Phase space representations of QM

- Wigner transform (1932)
"On the quantum corrections to statistical thermodynamics"

$$W(q, P) = \int d\eta e^{i\eta P} \psi^*(q - \eta/2)\psi(q + \eta/2)$$

- Interpretation as a joint probability distribution



Harmonic oscillator

Interpretation of Wigner function

Trick: Use Dirac's notation

$$W(P, x) = \frac{1}{2\pi} \int \psi^*\left(x + \frac{s}{2}\right) \psi\left(x - \frac{s}{2}\right) e^{iPs} ds$$

- $\psi^*\left(x + \frac{s}{2}\right) = \langle \psi | x + \frac{s}{2} \rangle$
- $\psi\left(x - \frac{s}{2}\right) = \langle x - \frac{s}{2} | \psi \rangle$
- $e^{iPs} = \frac{1}{\sqrt{2\pi}} e^{iP(x+s/2)} \frac{1}{\sqrt{2\pi}} e^{-iP(x-s/2)} = \langle x + \frac{s}{2} | P \rangle \langle P | x - \frac{s}{2} \rangle$

$$W(P, x) = \int \langle \psi | x + \frac{s}{2} \rangle \langle x + \frac{s}{2} | P \rangle \langle P | x - \frac{s}{2} \rangle \langle x - \frac{s}{2} | \psi \rangle ds$$

- **1st:** Amplitude particle in state ψ is at position $x - s/2$
- **2nd:** Amplitude particle at $x - s/2$ has momentum P
- **3rd:** Amplitude particle with momentum P is at $x + s/2$
- **4th:** Amplitude particle in state ψ is at position $x + s/2$

But ...

- Problem: $W(q, P)$ can be negative
- **Why?**: Heisenberg's uncertainty principle
- Solution: **Husimi function** (Wigner average in cells of area \hbar^N)



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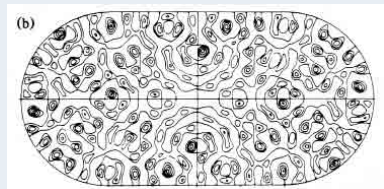
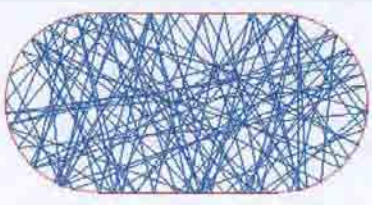
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Periodic orbits in quantum mechanics: Scars

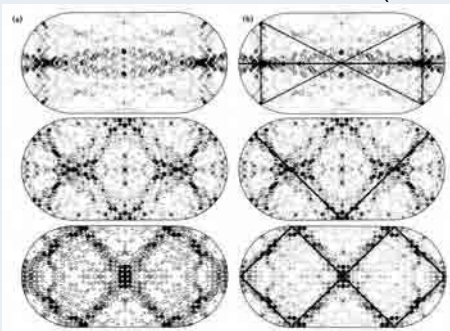
- What are scars?

Expected: Chaotic classical dynamics \longrightarrow uniform distributed quantum density



Scarred functions

- But in numerical calculations (McDonald&Kaufman) ...



Heller in 1984 coined the term **scar** to name an enhanced localization of quantum probability density of certain eigenstates on classical unstable **periodic orbits**

Heller's dynamical explanation

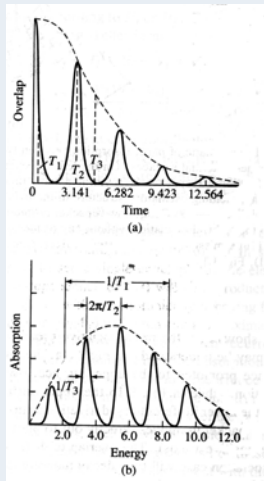
Recurrences

Fourier transform
between:

correlation function

$C(t) = \langle \phi(0) | \phi(t) \rangle$, and
corresponding spectrum

$$I(E) = \int dt e^{iEt/\hbar} C(t)$$



Some landmarks in scar theory

- Gutzwiller (1960's), Relevance of PO's
- Bogomolny (1988), expression for smoothed probability density over small intervals in energy and space
- Berry (1989) developed the corresponding theory in phase space (Wigner functions)
- P, Borondo and Benito (1994), Systematic construction of scar functions
- Vergini (2000)
- Keating and Prado (2001), superscars in mixed systems, influence of bifurcations on scarring

Scars in Optical Fibers

VOLUME 88, NUMBER 1

PHYSICAL REVIEW LETTERS

7 JANUARY 2002

Light Scarring in an Optical Fiber

Valérie Doya, Olivier Legrand, and Fabrice Mortessagne

Laboratoire de Physique de la Matière Condensée, CNRS UMR 6622, Université de Nice Sophia-Antipolis, 06108 Nice, France

Christian Miniatura

Laboratoire Ondes et Désordre, CNRS FRE 2302, 1361 route des Lucioles, Sophia-Antipolis, F-06560 Valbonne, France

(Received 31 July 2001; published 18 December 2001)

We report the first experimental study of wave scarring in an optical fiber with a noncircular cross section. This optical multimode fiber serves as a powerful tool to image waves in a system where light rays exhibit a chaotic dynamics. Far-field intensity measurements are used to provide a better identification of scars in the Fourier domain. This first experimental characterization of scarring effect in optics demonstrates the relevance of such an optical waveguide for novel experiments in wave chaos.



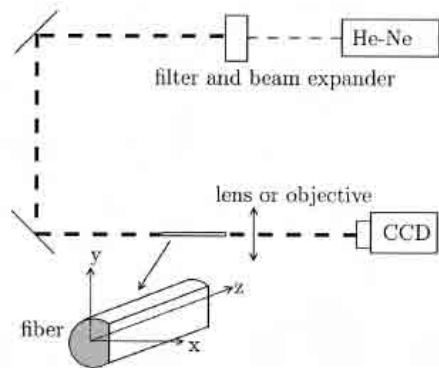
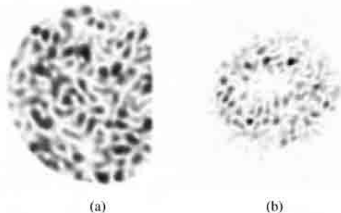
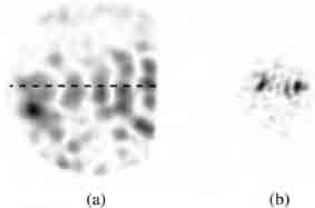


FIG. 14. Experimental setup.

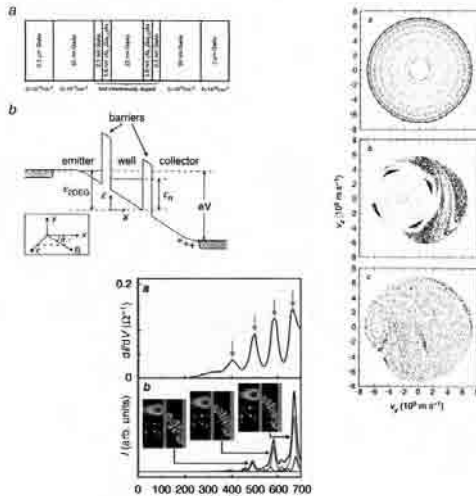
FIG. 1. Typical specklelike experimental intensity pattern at the output of a chaotic D-shaped fiber for a plane wave illumination at central wave vector $\kappa_c = 19.0R^{-1}$. (a) Near-field intensity; (b) far-field intensity.FIG. 3. Scar pattern for a plane wave illumination at central wave vector $\kappa_c = 11.4R^{-1}$ along the 2BO (see text): (a) Near-field intensity; (b) far-field intensity.

Billiards: Models in Nanotechnology

Wilkinson et al., 1996; Resonant Tunneling Diode



Billiards: Models in Nanotechnology



How to systematically construct scar function

Phys. Rev. Lett. 73, 1613 (1994)

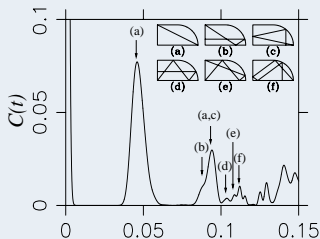
- Launch wavepacket initially localized on the PO

$$|\phi(0)\rangle = \left(\frac{2\alpha}{\pi}\right)^{1/4} e^{-\alpha(x-x_0)^2 - \alpha(y-y_0)^2} e^{i(P_x^0 x + P_y^0 y)}$$

- Propagate in time

$$|\phi(t)\rangle = e^{-i\hat{H}t}|\phi(0)\rangle = \sum_n |n\rangle \langle n|\phi(0)\rangle e^{-iE_n t}$$

- Compute $C(t) = \langle \phi(0)|\phi(t)\rangle$

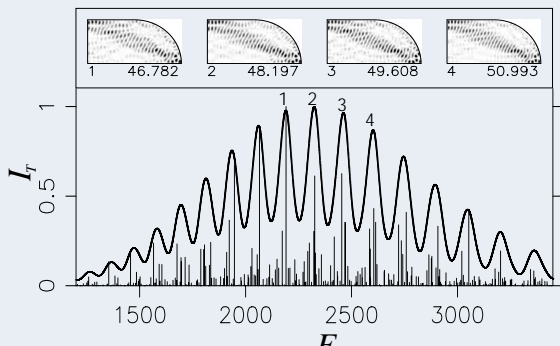


How to systematically construct scar function

- Compute spectrum by Fourier transforming **up** to the time of the first recurrence

$$I_T(E) = \frac{1}{2\pi} \int_{-\infty}^{\infty} dt C(t) W_T(t) e^{iEt}$$

$$I_T(E) = \frac{T}{(2\pi)^{1/2}} \sum_n |\langle n | \phi(0) \rangle|^2 e^{-T^2(E-E_n)^2/2}$$



How to systematically construct scar function

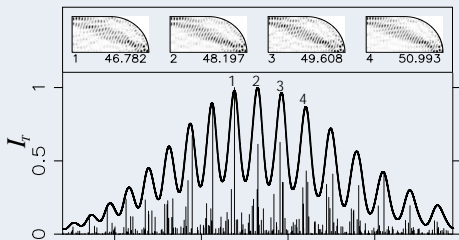
- Peaks at Bohr–Sommerfeld quantization condition

$$k = \frac{2\pi}{L} \left(n + \frac{\nu}{4} \right)$$

- Compute wave function **associated** to each peak

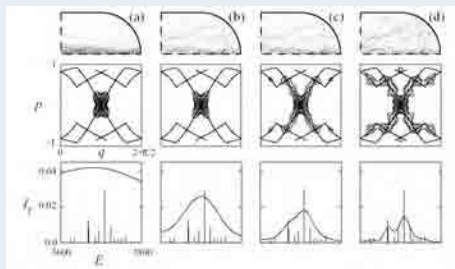
$$|\psi^{E_0}\rangle = \frac{1}{2\pi} \int_{-\infty}^{\infty} dt |\phi(t)\rangle W_T(t) e^{iE_0 t}$$

$$|\psi^{E_0}\rangle = \frac{T}{(2\pi)^{1/2}} \sum_n |n\rangle \langle n|\phi(0)\rangle e^{-T^2(E_0 - E_n)^2/2}$$



Properties of scar function

- Localized on **fixed points** and **manifolds** associated to the PO



- Cutoff T increases from (a) to (d), allowing longer dynamics (phase space exploration)

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Heteroclinic motion and cross-correlation function

Phys. Rev. E 70, 035202(R) (2004)

- To gauge interaction between POs A and B, we compute

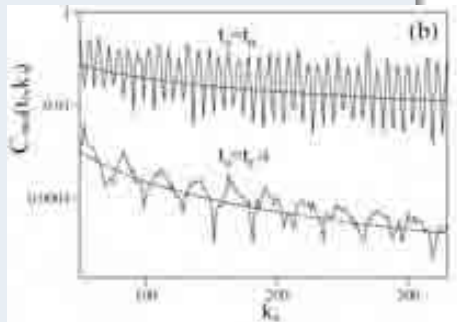
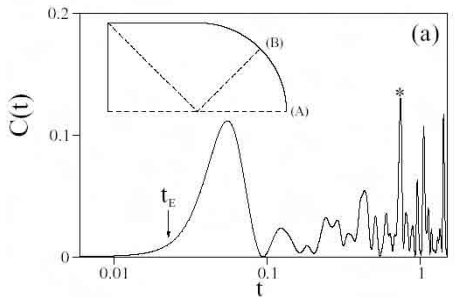
$$C(t) = |\langle \phi_B | e^{-i\hat{H}t} | \phi_A \rangle|^2$$

- $|\phi_{A,B}\rangle$ properly quantized (in the sense BS) scar functions

$$S(E) = 2\pi\hbar n + \frac{\pi}{2}\hbar\nu$$

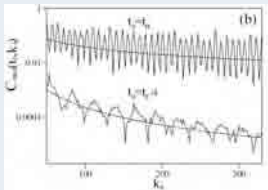


Results

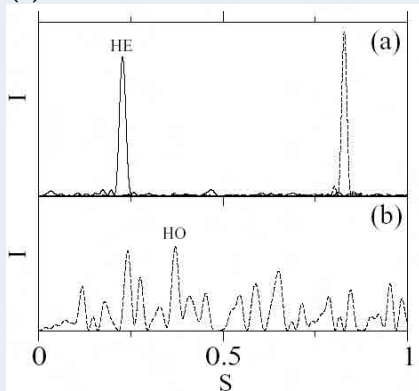


Different behavior below and above $\sim t_E$

Now, we Fourier transform $C(t)$

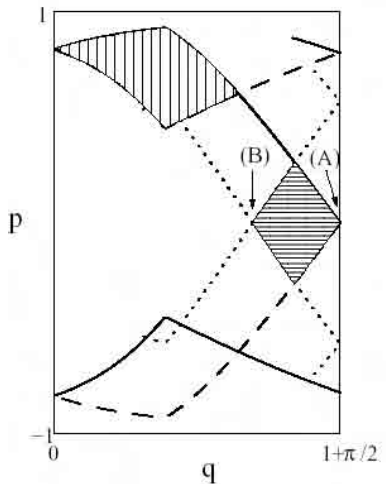


Full line: $t_0 = t_E/4$;
Dashed line: $t_0 = t_H$



- Peak HE (data for $T_E/4$) can be assigned to **heteroclinic area**
Also, $|\langle \phi_B | \hat{H} | \phi_A \rangle|^2 \propto \cos(S_{AB}k)$
- Peak (data for T_H) coincides with $k_A - k_B$
- Two different regimes below and above t_E (**Fermi golden rule**)
- Peak HO can be assigned to homoclinic area

Phase space portrait



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Homoclinic motion and eigenvalues

Phys. Rev. Lett. 94, 054101(2005)

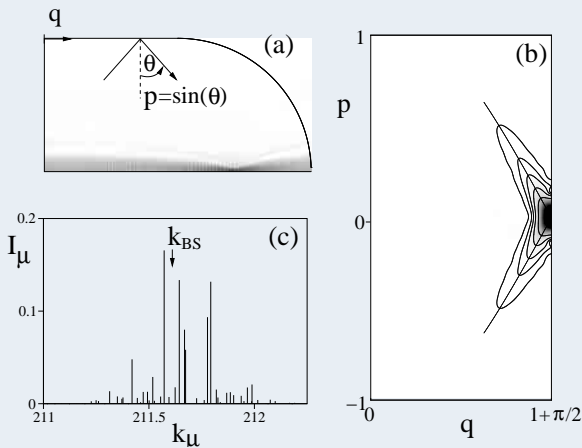
- We could also use the auto-correlation function

$$C(t) = |\langle \phi_A | e^{-i\hat{H}t/\hbar} | \phi_A \rangle|^2$$

- But, since: $e^{-i\hat{H}t} = 1 - i\hat{H}t/\hbar + \hat{H}^2/2\hbar^2 + \dots$,
- $C(t) \sim 1 - [\langle H^2 \rangle - \langle H \rangle^2] t^2/\hbar^2 = 1 - \sigma^2 t^2/\hbar^2$
and then it is simpler just to ...



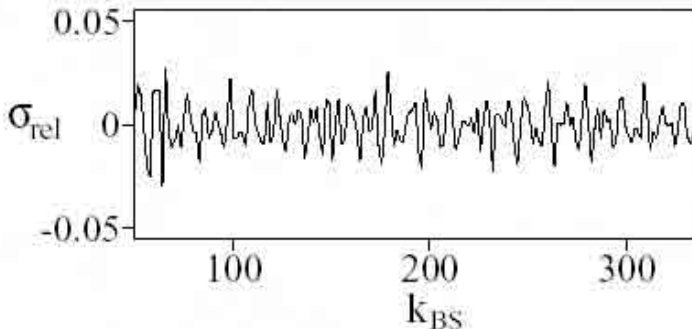
- Project **scar functions** on eigenstates spectrum



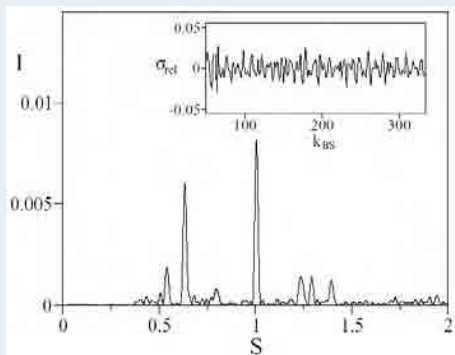
- Compute $\sigma = \sqrt{\sum_n |\langle n|\psi\rangle|^2 (k_n^2 - k_{BS}^2)}$

- Scale σ and make them adimensional

$$\sigma_{rel} = \frac{\sigma - \sigma_{sc}}{\sigma_{sc}}; \quad \sigma_{sc} = \frac{\pi \hbar \lambda}{|\ln \hbar|}; \quad \lambda \text{ Lyapunov exp}$$

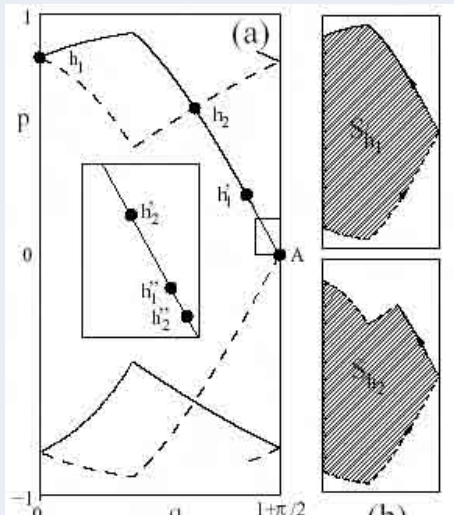


- Now Fourier analyze the signal
"The noise is the signal" (Landauer)

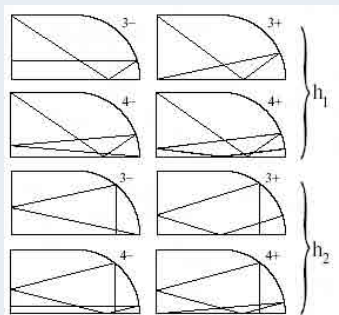


- Peaks at $S = 0.633$ and 1.007
 Also at $S = -3.367$ and -2.993 , since FT is $L_H = 4$ periodic

- Peaks coincide with the value of primary **homoclinic areas**



- The homoclinic motions (both h_1 and h_2) can be approximated by two families of satellite PO's (Ozorio de Almeida)



- Under which circumstances the satellite PO's **reinforce** the **quantization** of the central one?
 - Quantization horizontal PO: $kL_H - \frac{\pi}{2}\nu_H = 2\pi n_H$
 - Quantization homoclinic torus: $kL_m - \frac{\pi}{2}\nu_m = 2\pi n_m$
(approximated by m -th satellite PO):
 - $k(L_m - mL_H) - \frac{\pi}{2}(\nu_m - m\nu_H) = 2\pi(n_m - mn_H)$

m	$\overline{L_m - mL_H}$	
	Family h_1	Family h_2
3	-3.367 727 48	-2.990 915 39
4	-3.368 367 57	-2.991 131 87
5	-3.368 389 68	-2.991 141 81
6	-3.368 390 43	-2.991 142 21
7	-3.368 390 45	-2.991 142 22

Conclusion ...

- Additional quantization condition for the homoclinic torus

$$kS_{h_i} - \frac{\pi}{2}\nu_{h_i} = 2\pi n, \quad i = 1, 2$$



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Homoclinic motion and wave functions

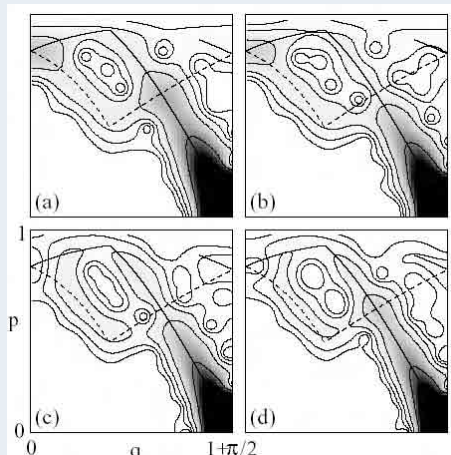
Phys. Rev. Lett. scheduled 30 Aug 2006

- Scar functions calculated in a slightly different way

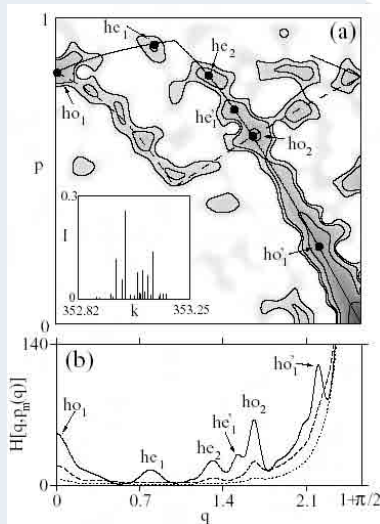
$$|\phi_{\text{scar}}\rangle = \int_{-T}^T dt \cos\left(\frac{\pi t}{2T}\right) e^{i(E_{\text{BS}} - \hat{H})t/\hbar} |\phi_{\text{tube}}\rangle$$

Husimidis for 4 scar function with quantization/antiquantization conditions on the homoclinic torus (all quantized on the PO)

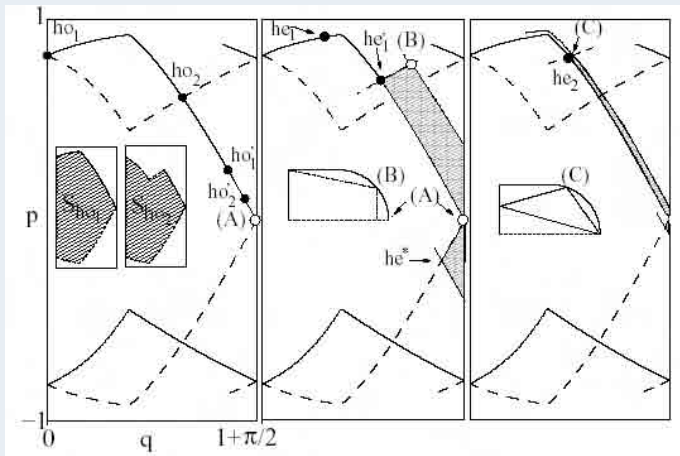
Label	n_H	k_{BS}	n_{ho_1}	n_{ho_2}
(a)	34	54.585	29.01	25.99
(b)	40	64.010	34.07	30.47
(c)	44	70.293	37.43	33.46
(d)	50	79.718	42.49	37.95



- Scar function $n = 224$
- Homoclinic quantization:
 $n_{h_1} = 189.01, n_{h_2} = 168.07$
- Extra quantization on heteroclinic orbits:
 $kS_{he} = 2\pi n_{he}$
 $n_{he_1} = 19.00, n_{he_2} = 5.98$
- Husimis for $T = 0.9t_E, 1.2t_E$
and $3.3t_E$



Classical phase space



How to play/dance this game?

- **Riemann zeta function:**

$$\zeta(z) = \sum_{n=1}^{\infty} n^{-z} = \prod_p (1 - p^{-z})^{-1}, \quad \text{Re}(z) > 1$$

- **Riemann's conjecture:** All (nontrivial) zeros have real part equal to $\frac{1}{2}$:

$$\zeta\left(\frac{1}{2} - iE_n\right) = 0$$

- Numerical evidence. RH has been checked with $1,500 \times 10^6$ primes above prime number 10^{22}
- Data can be found in Andrew Odlyzko web page
- **Conjecture:** $\{E_n\}$ behaves as the eigenvalues of a Hermitian (Hamiltonian) operator with a chaotic classical limit, in the sense that all PO's are isolated and unstable, with non time-reversal trajectories

Motivation

Periodic orbits in quantum mechanics

Unveiling heteroclinic motions in quantum mechanics

Unveiling homoclinic motions in quantum mechanics

Riemann zeta function



Thanks for your attention

