Classical and Quantum Chaos and the semiclassical approach

- Classical & Quantum Chaos
- Semiclassical Approach → Martin Sieber
- Random matrix theory → Thomas Guhr

References:
F. Haake, *Quantum Signatures of Chaos* (Spinger Verlag, Heidelberg, 2001)
P. Cvitanović, *Chaos, and what to do about it* ? www.ChaosBook.org
A.Bäcker, *Eigenfunctions in chaotic quantum systems*
https://tud.qucosa.de/api/qucosa%3A23663/attachment/ATT-0/?L=1

Lagrange-Equations

- Generalized coordinates and generalized velocities

$$\mathbf{q}(t) = (q_1(t), q_2(t), \cdots, q_N(t)), \dot{\mathbf{q}}(t) = (\dot{q}_1(t), \dot{q}_2(t), \cdots, \dot{q}_N(t))$$

- Lagrange-function $L(\mathbf{q}(t), \dot{\mathbf{q}}(t)) = T - V$

- Kinetic energy $T = \frac{1}{2} m \sum_{i=1}^{N} \dot{q}_i^2, \quad m = 1$, external potential $V = V(\mathbf{q})$

- Conservative system $\frac{\partial L}{\partial t} = 0 \Rightarrow E = T + V = const.$

- Lagrange equations

$$\frac{\partial L}{\partial q_i} - \frac{d}{dt}\left(\frac{\partial L}{\partial \dot{q}_i}\right) = 0$$

Hamiltonian Formalism

- Hamiltonian with N degrees of freedom

$$H(\mathbf{q},\mathbf{p}) = \sum_{i=1}^{N} p_i \dot{q}_i - L(\mathbf{q}(t), \dot{\mathbf{q}}(t))$$

- Coordinates and the conjugate momenta

$$\mathbf{q}(t) = (q_1(t), q_2(t), \cdots, q_N(t)),\ \mathbf{p}(t) = (p_1(t), p_2(t), \cdots, p_N(t)),\ p_i := \frac{\partial L}{\partial \dot{q}_i}$$

- Hamilton´s equations of motion

$$\frac{\partial H}{\partial p_i} = \dot{q}_i,\ \frac{\partial H}{\partial q_i} = -\dot{p}_i$$

- Conservative systems: Hamiltonian $H(\mathbf{q},\mathbf{p})=E$ is constant along the phase space trajectory $\xi(t) = (\mathbf{q}, \mathbf{p})$

$$\frac{\mathrm{d}}{\mathrm{d}t} H(\boldsymbol{q}(t), \boldsymbol{p}(t)) = \frac{\partial H}{\partial q_i}\dot{q}_i(t) + \frac{\partial H}{\partial p_i}\dot{p}_i(t) = \frac{\partial H}{\partial q_i}\frac{\partial H}{\partial p_i} - \frac{\partial H}{\partial p_i}\frac{\partial H}{\partial q_i} = 0$$

The Phase Space

- The phase space vector $\xi(t)$ specifies the trajectory of a particle in phase space

$$\xi(t) = (\mathbf{q}(t), \mathbf{p}(t))^T = (q_1(t), q_2(t), \cdots, q_N(t), p_1(t), p_2(t), \cdots, p_N(t))^T$$

- $2N$-dimensional gradient

$$\nabla := \frac{\partial}{\partial \xi} = \left(\frac{\partial}{\partial q_1}, \frac{\partial}{\partial q_2}, \cdots, \frac{\partial}{\partial q_N}, \frac{\partial}{\partial p_1}, \frac{\partial}{\partial p_2}, \cdots, \frac{\partial}{\partial p_N} \right)^T$$

- With this notation Hamilton‘s equations may be written as

$$\dot{\xi} = \begin{pmatrix} \frac{\partial}{\partial \mathbf{p}} H \\ -\frac{\partial}{\partial \mathbf{q}} H \end{pmatrix} = \mathbf{J} \nabla H(\xi), \quad \mathbf{J} := \begin{pmatrix} \mathbf{0} & \mathbf{1} \\ -\mathbf{1} & \mathbf{0} \end{pmatrix}$$

Properties of the Phase Space Trajectories

- For conservative systems (E=const.), the trajectory $\xi(t)$ is confined to the ($2N$-1)-dimensional energy shell
- Because of the uniqueness of Hamilton´s equations of motion for a given initial condition ξ_0, a phase space trajectory $\xi(t)$ can never cross itself
- A trajectory is called periodic if $\xi(t+T) = \xi(t)$ for some $0<T<\infty$

- Liouville´s Theorem

➢The divergence of the Hamiltonian flux $\nabla H(\xi,t)$ vanishes

$$\nabla \cdot \dot{\xi} = \sum_i \left(\frac{\partial \dot{q}_i}{\partial q_i} + \frac{\partial \dot{p}_i}{\partial p_i} \right) = 0$$

$\Leftrightarrow$ The phase space volume $\mathrm{d}\Gamma$ is invariant under canonical transformations

$$\mathrm{d}\Gamma = \left(\prod_{i=1}^{N} \mathrm{d}q_i \right) \left(\prod_{i=1}^{N} \mathrm{d}p_i \right) = \left(\prod_{i=1}^{N} \mathrm{d}Q_i \right) \left(\prod_{i=1}^{N} \mathrm{d}P_i \right)$$

Definition of Integrability

- A system of N degrees of freedom is integrable, if there are at least N constants of motion that are in involution

$$C_n(\mathbf{q},\mathbf{p}) = C_n = const., \quad n = 1,\cdots,N$$

$$\{C_n, C_m\} = \sum_{i=1}^{N}\left(\frac{\partial C_n}{\partial p_i}\frac{\partial C_m}{\partial q_i} - \frac{\partial C_n}{\partial q_i}\frac{\partial C_m}{\partial p_i}\right) = 0$$

- For conservative systems the Hamiltonian itself is a constant of motion

$$C_1 = E = H(\mathbf{q},\mathbf{p})$$

- Each separable system is integrable $E = \sum_{i=1}^{N} E_i = \sum_{i=1}^{N} H(q_i, p_i) \Rightarrow C_i = E_i$
- For some integrable systems a canonical transformation can be found such that $H(\mathbf{q},\mathbf{p}) \to \widetilde{H}(\mathbf{P})$
- Generating function: $F = F(\mathbf{q},\mathbf{P},t), \ \frac{\partial F}{\partial q_i} = p_i, \ \frac{\partial F}{\partial P_i} = Q_i, \ \widetilde{H} = H + \frac{\partial F}{\partial t}$

Integrable Hamiltonian Systems

- Consider systems for which a canonical transformation exists such that

$$H(\mathbf{q},\mathbf{p}) \rightarrow \widetilde{H}(\mathbf{P})$$

- Equations of motion:

$$\dot{P}_i = -\frac{\partial \widetilde{H}}{\partial Q_i} = 0 \quad \rightarrow \quad P_i(t) = const.$$

$$\dot{Q}_i = \frac{\partial \widetilde{H}}{\partial P_i} = const. \rightarrow \quad Q_i(t) = \omega_i t + \alpha_i$$

- The generating function is given up to a constant by

$$\frac{\partial S}{\partial \mathbf{q}} = \mathbf{p} \Rightarrow S(\mathbf{q}) = \int_{q_0}^{q} \mathbf{p} \cdot \mathrm{d}\mathbf{q} + const. = \sum_{i=1}^{N} \int_{q_i(0)}^{q_i(t)} p_i \mathrm{d}q_i + const.$$

- Generally for $N > 1$ a solution can only be found for integrable systems, the simplest ones being separable systems with

$$H(\mathbf{q},\mathbf{p}) = \sum_{i=1}^{N} h(q_i, p_i)$$

Torus Variables I

- Einstein (1917): The phase space trajectories $\xi(t)$ of an integrable system with N independent degrees of freedom lie on a manifold, which has the structure of an N-torus

- An N-torus is a connected N-dimensional manifold M_N with one hole. For N=1 it is a circle, for N=2 it is a torus

- The constants of motion C_n define vector fields $\mathbf{v}_n$ which are linearly independent and in the tangential plane of M_N

$$\mathbf{v}_n = \mathbf{J} \cdot \nabla C_n, \quad \mathbf{v}_1 = \mathbf{J} \cdot \nabla H = \dot{\boldsymbol{\xi}}$$

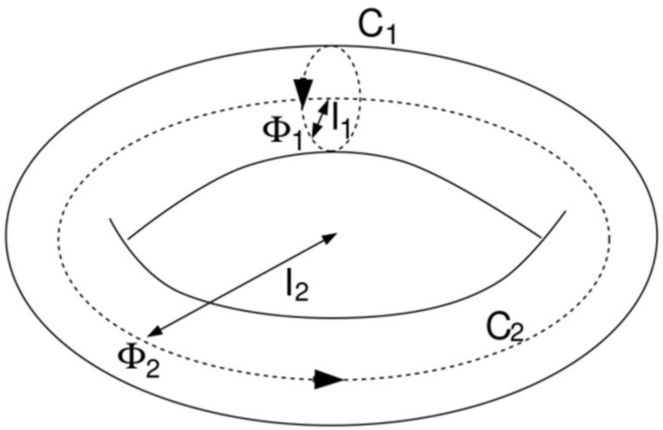
- On an N-torus always exist N independent loops C_n, that cannot be reduced to a point or mapped onto one another

- These elementary loops may be described by angle variables $\Phi_n \in [0,2\pi)$

Torus (Action-Angle) Variables II

- Each loop C_n can be mapped onto a circle with radius I_n corresponding to the momenta conjugate to the angle variables Φ_n
- Action variables $I_n > 0$:

$$I_n = \frac{1}{2\pi} \oint_{C_n} \mathbf{p}\, d\mathbf{q}, \quad n = 1, \cdots, N$$



- Canonical transformation:

$$(q_i, p_i) \rightarrow (\Phi_i, I_i)$$

$$H(\mathbf{q}, \mathbf{p}) \rightarrow \widetilde{H}(\mathbf{I})$$

- Equations of motion for these \`torus variables´

$$\dot{I}_n = -\frac{\partial \widetilde{H}}{\partial \Phi_n} = 0 \Rightarrow I_n = const.$$

$$\dot{\Phi}_n = \frac{\partial \widetilde{H}}{\partial I_n} = const. = \Omega_n \Rightarrow \Phi_n(t) = \Omega_n t + \alpha_n$$

Periodic Orbits on an *N*-Torus

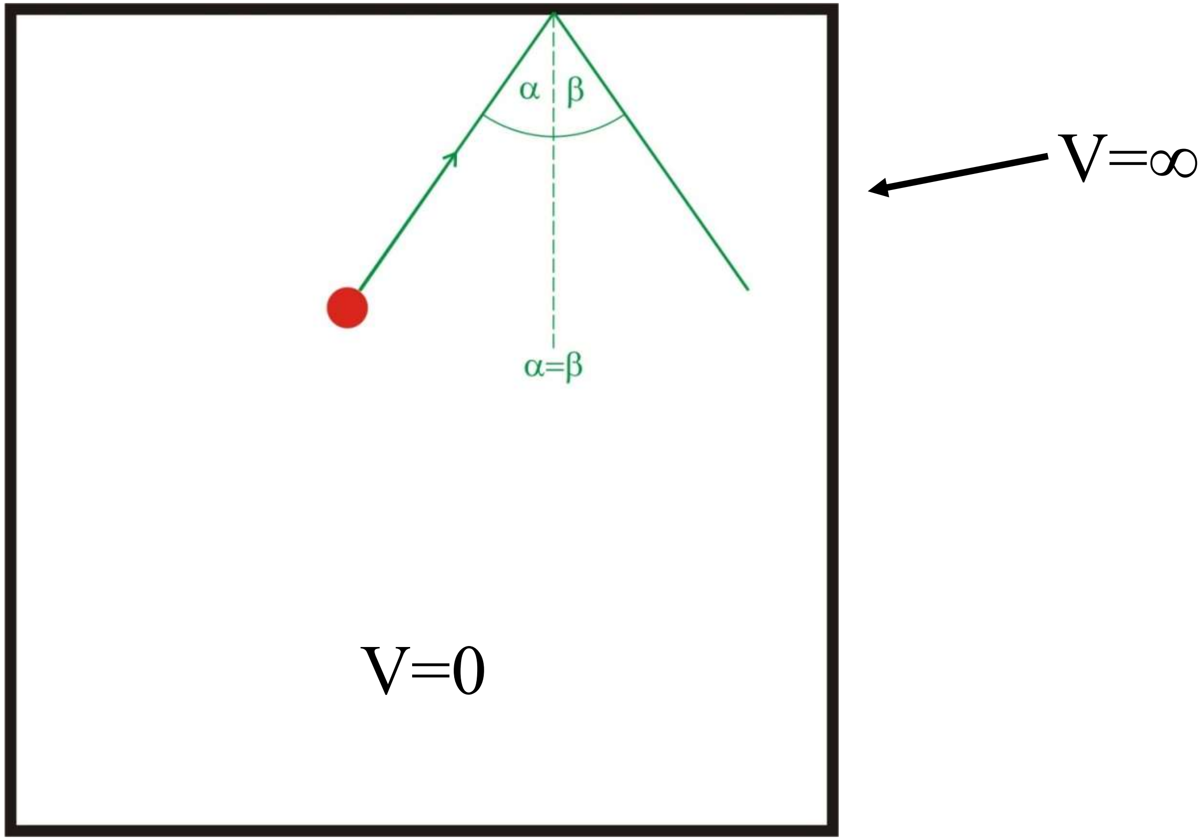
- $N=2$: Trajectories move on a 2-torus with frequencies Ω_1, Ω_2.
- Ω_1 / Ω_2 irrational: trajectories never close and cover the torus surface uniformly
- $\Omega_1 / \Omega_2 = n / m$ rational: periodic orbits $\Rightarrow$ trajectories are closed and never cover the whole torus surface
- Condition for the periodicity of a trajectory on an N-torus:

$$\frac{\Omega_i}{\Omega_j} = \frac{n_i}{n_j}; \quad n_i, n_j \in \mathrm{N}$$

$$\Omega_i = \frac{\partial \widetilde{H}}{\partial I_i} = \frac{2\pi}{T} n_i; \quad n_i \in \mathrm{N}; \quad i = 1, \cdots, N$$

- Note: Ω_i is constant but generally depends on $\mathbf{I}$

Classical Billiard

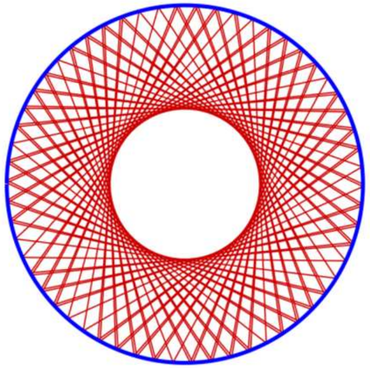


- Particle moves freely within the billiard along straight lines with constant velocity and is reflected specularly at boundary
- Shape of billiard determines chaoticity of classical dynamics

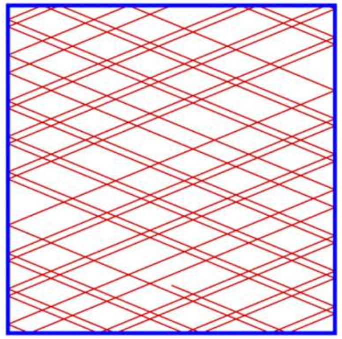
Integrable and Chaotic Billiards

- Integrable billiards:

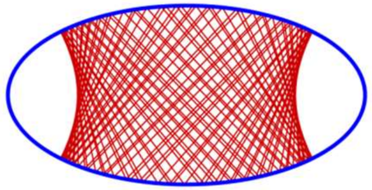
circle



square



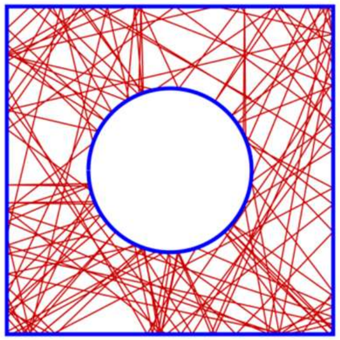
ellipse



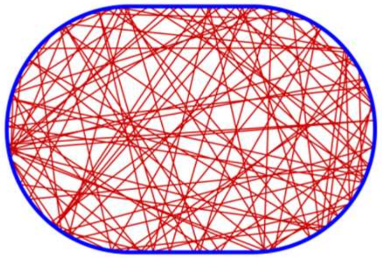
- Constants of motion: L p_x, p_y $L_1 L_2$

- Chaotic billiards:

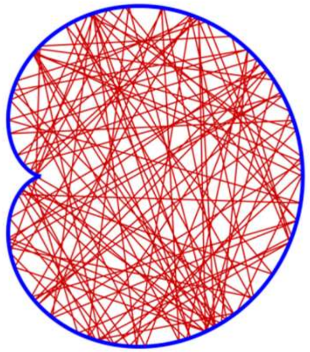
Sinai



Bunimovich stadium



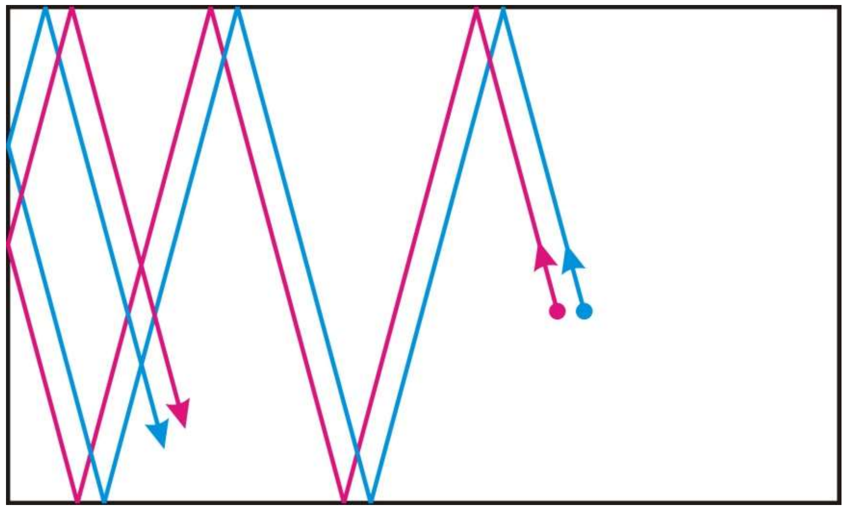
Limaçon



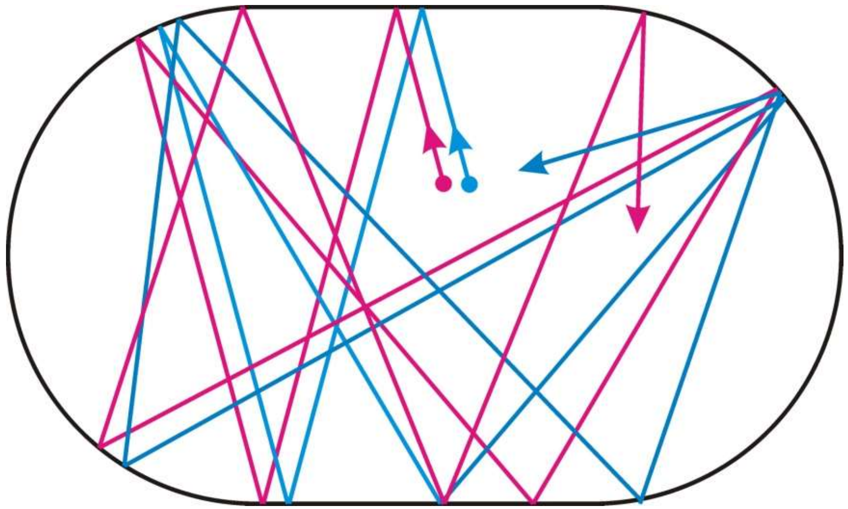
$r(\varphi) = 1 + \varepsilon \cos(\varphi),\ \varepsilon = 0.5$

Integrable and Chaotic Dynamics

Rectangular billiard (regular)



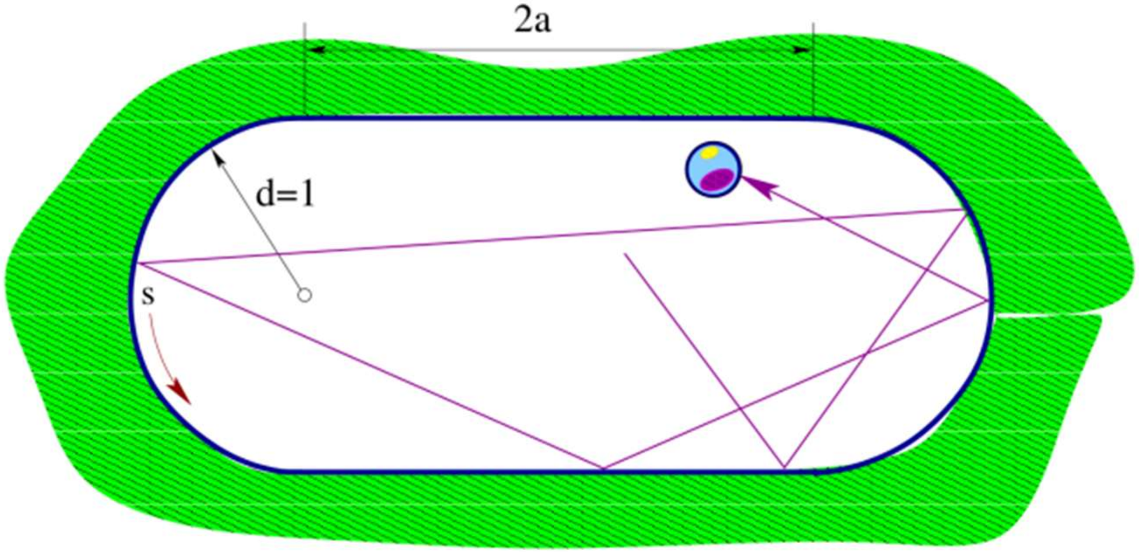
Bunimovich stadium (chaotic)

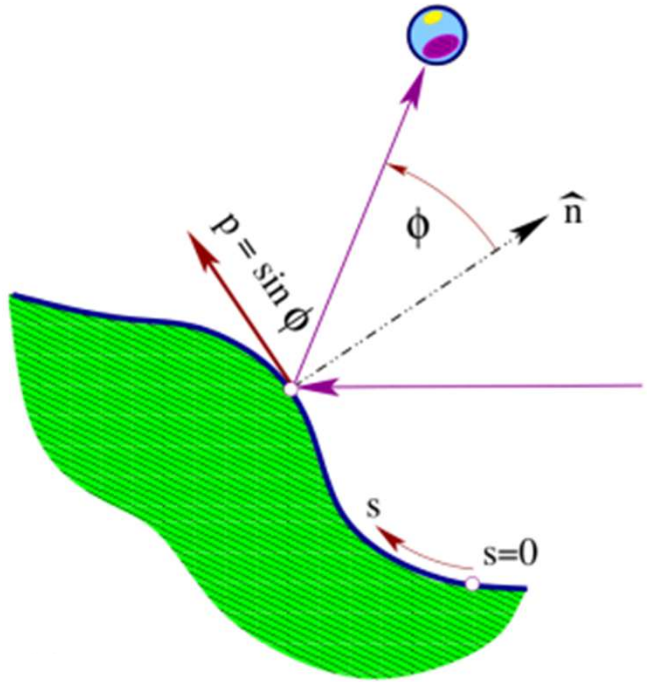


- Dynamical, exponential instability leading to unpredictability is a characteristic of chaos
- Deterministic chaos: sensitivity of the solutions of the equations of motion with respect to infinitesimal changes in the initial conditions

Poincaré Section Map (PSM)

Definition of Birkhoff coordinates



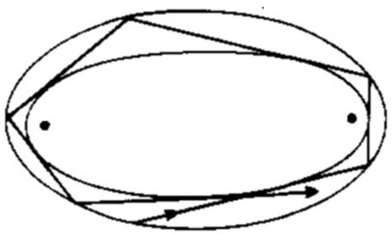


- The Poincaré map is defined in terms of the arclength s_n and the momentum $p_n = |\mathbf{p}| \sin \phi_n$ at n th bounce with the boundary
- Energy conservation: $|\mathbf{p}|=\text{const.}=1$

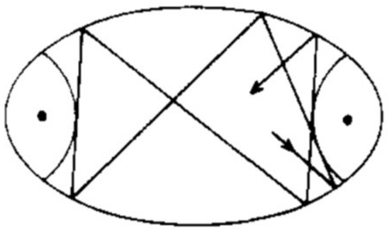
$$P:(s_n, p_n) \to (s_{n+1}, p_{n+1})$$

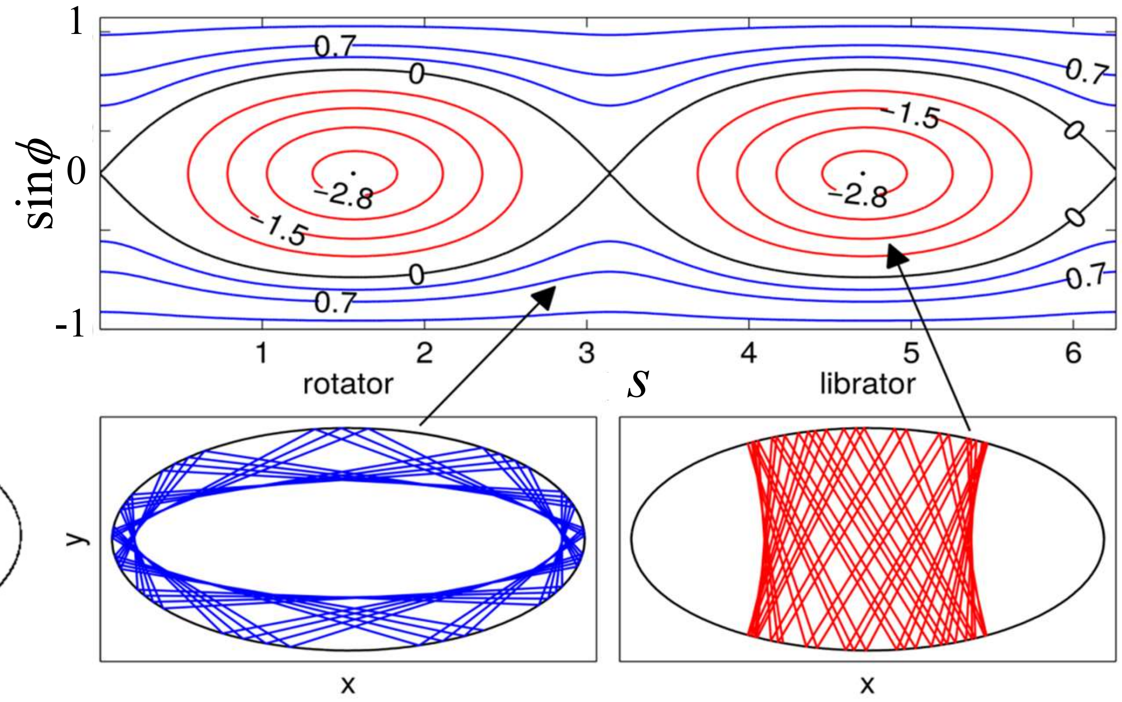
PSM of Ellipse

rotations



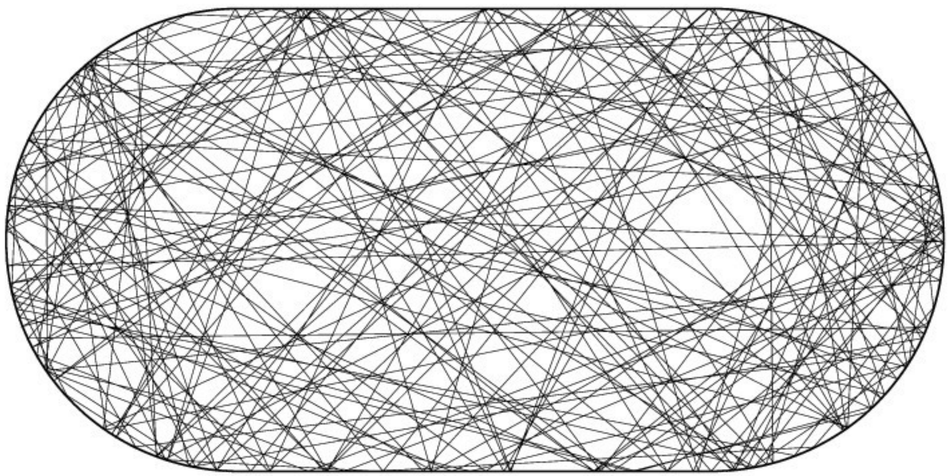
librations

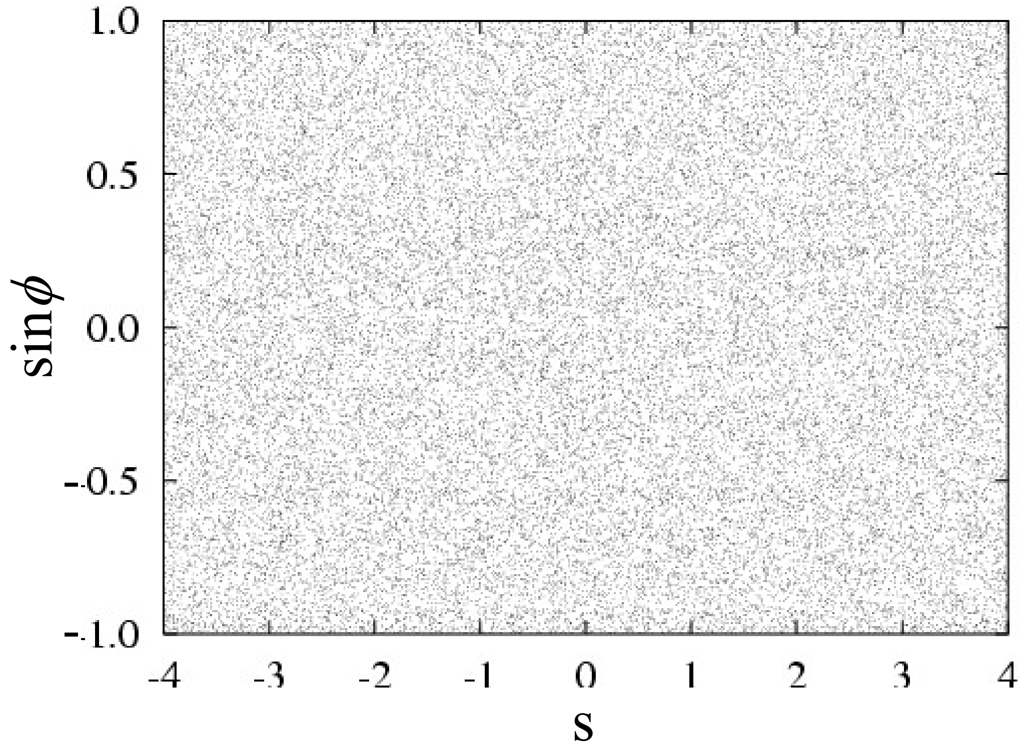




- Orbits encircling both foci touch an ellipse
- Orbits passing between the foci touch hyperbolas
- PSMs were generated by varying the initial angle ϕ

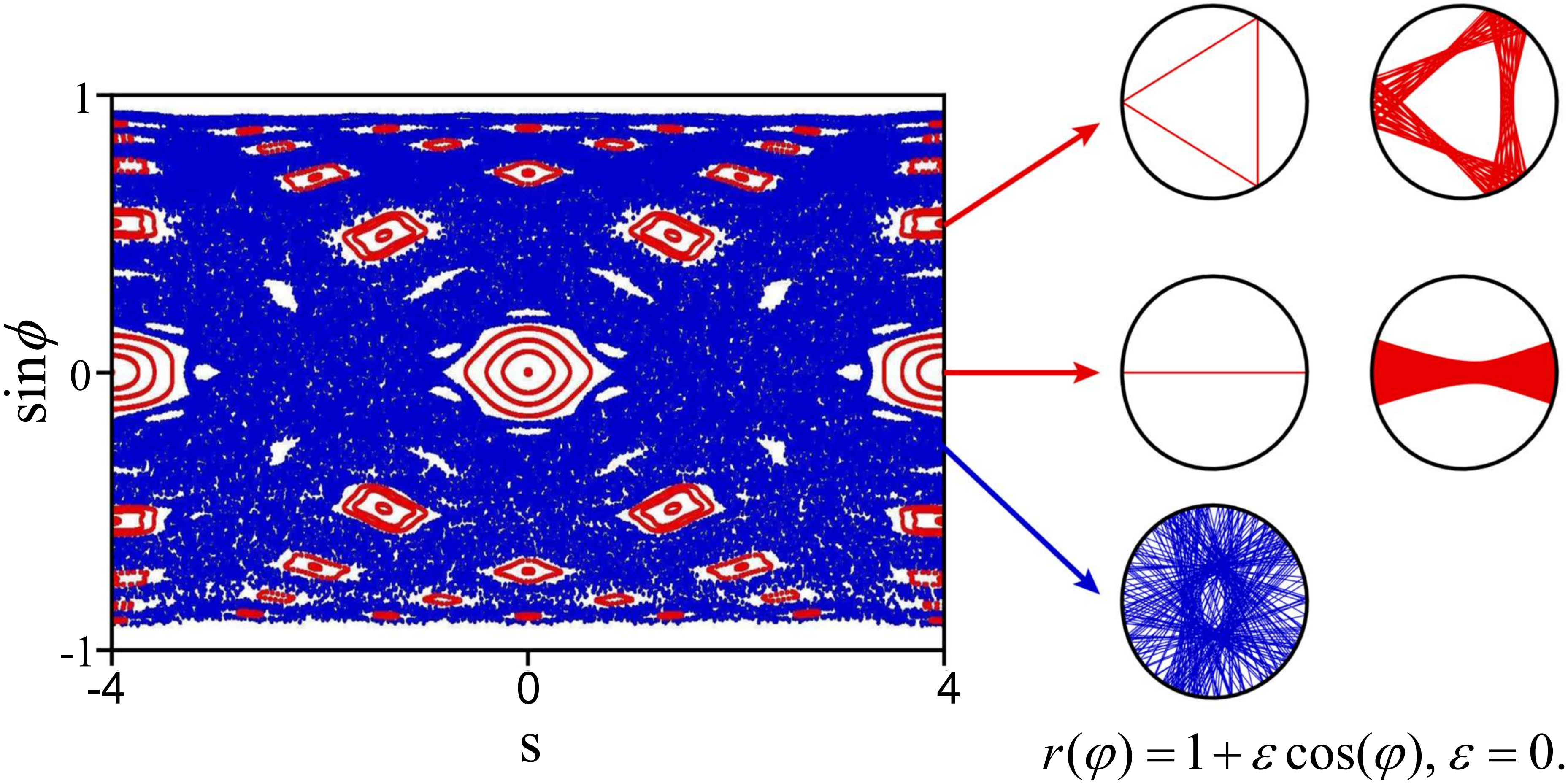
PSM of Stadium Billiard





- PSM was created by iterating one initial condition (s_0, p_0) over a large number of bounces with the boundary / long time

PSM of Limaçon Billiard



$r(\varphi) = 1 + \varepsilon\cos(\varphi),\ \varepsilon = 0.3$

- PSM was generated by varying the initial angle ϕ
- For $\varepsilon = 0.5$ the PSM is similar to that of the stadium billiard

Ergodicity of the Classical Dynamics

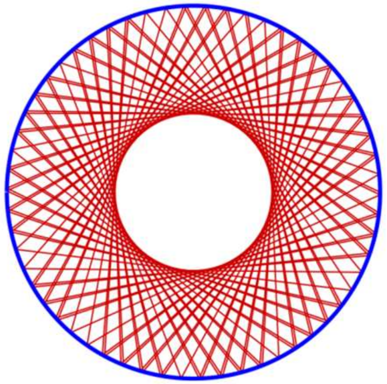
- Energy shell: $\Omega = \{(\boldsymbol{q},\boldsymbol{p}),\ H(\boldsymbol{q},\boldsymbol{p}) = E\}$

- Ergodicity: Almost all trajectories visit every part in the accessible phase space Ω

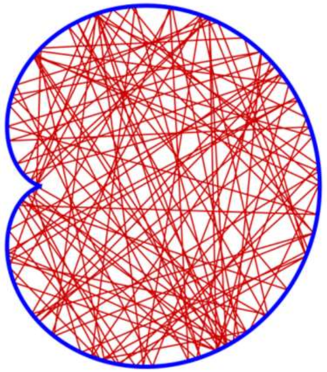
$\Leftrightarrow$ Spatial and temporal averages coincide:

$$\frac{\text{time spent in}\,\Omega_0\text{up to}\,T}{T} \rightarrow \frac{\text{vol}\,(\Omega_0)}{\text{vol}\,(\Omega)} \quad (T \rightarrow \infty)$$

Not ergodic:



Ergodic:



Central Question of Quantum Chaos

- How does the regular or chaotic behaviour of the classical dynamics manifest itself in those of the corresponding quantum system?
- Problem: a distinction between regularity and chaos in terms of the long-time evolution of trajectories is not possible in a quantum system
- Reason: Heisenberg's uncertainty relation $\Delta x \, \Delta p \geq \hbar / 2$
- But: due to the correspondence principle there must be a relation between a classical system and its quantum counter partner

  $\rightarrow$ quantum chaos

Quantum Billiard

- Schrödinger equation of a free particle

$$-\frac{\hbar^2}{2m}\nabla^2\psi(\boldsymbol{q},t) = i\hbar\frac{\partial}{\partial t}\psi(\boldsymbol{q},t)$$

- Confinement to billiard boundary $\partial B \rightarrow$ Dirichlet conditions at boundary

$$\psi(\boldsymbol{q},t) = 0 \text{ for } \boldsymbol{q} \in \partial B$$

- Time-independent Schrödinger equation

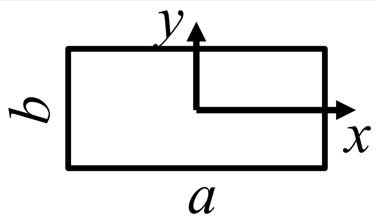
$$-\frac{\hbar^2}{2m}\nabla^2\psi_n(\boldsymbol{q}) = E_n\psi_n(\boldsymbol{q})$$

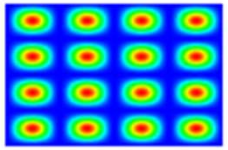
- Eigenfunctions $\psi_n(\boldsymbol{q})$

- Eigenvalues E_n

Wave Functions of the Rectangular Billiard

Eigenvalues: $E(m,n) = \frac{\pi^2}{8}\left[\frac{m^2}{a^2} + \frac{n^2}{b^2}\right]$



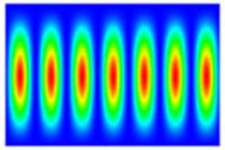


Dirichlet-Dirichlet

$\psi = 0$ at x & y axes

$$\Psi_{m,n}(x,y) = A \sin\left(\frac{m\pi x}{2a}\right) \sin\left(\frac{n\pi y}{2b}\right),$$

m even, n even,

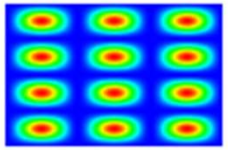


Neumann-Neumann

$\partial_n \psi = 0$ at x & y axes

$$\Psi_{m,n}(x,y) = A \cos\left(\frac{m\pi x}{2a}\right) \cos\left(\frac{n\pi y}{2b}\right),$$

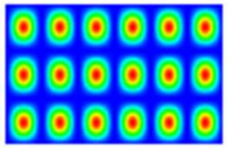
m odd, n odd,



Dirichlet-Neumann

$$\Psi_{m,n}(x,y) = A \sin\left(\frac{m\pi x}{2a}\right) \cos\left(\frac{n\pi y}{2b}\right),$$

m even, n odd,

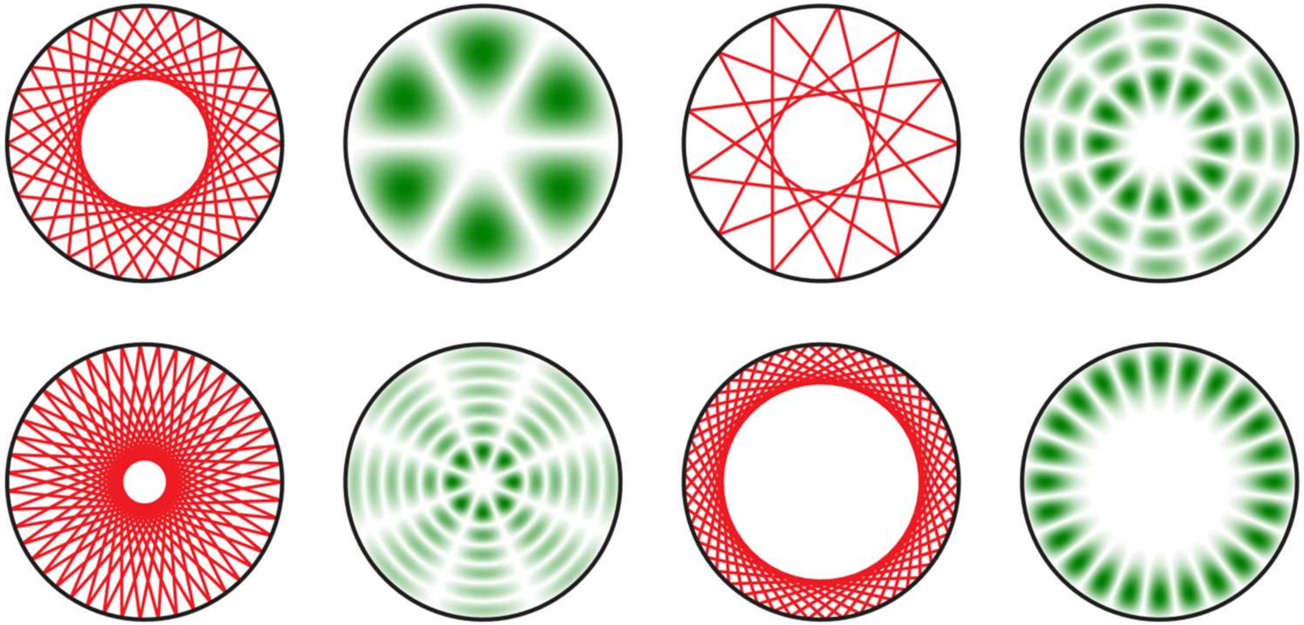


Neumann-Dirichlet

$$\Psi_{m,n}(x,y) = A \cos\left(\frac{m\pi x}{2a}\right) \sin\left(\frac{n\pi y}{2b}\right),$$

m odd, n even,

Wave Functions of the Circle Billiard

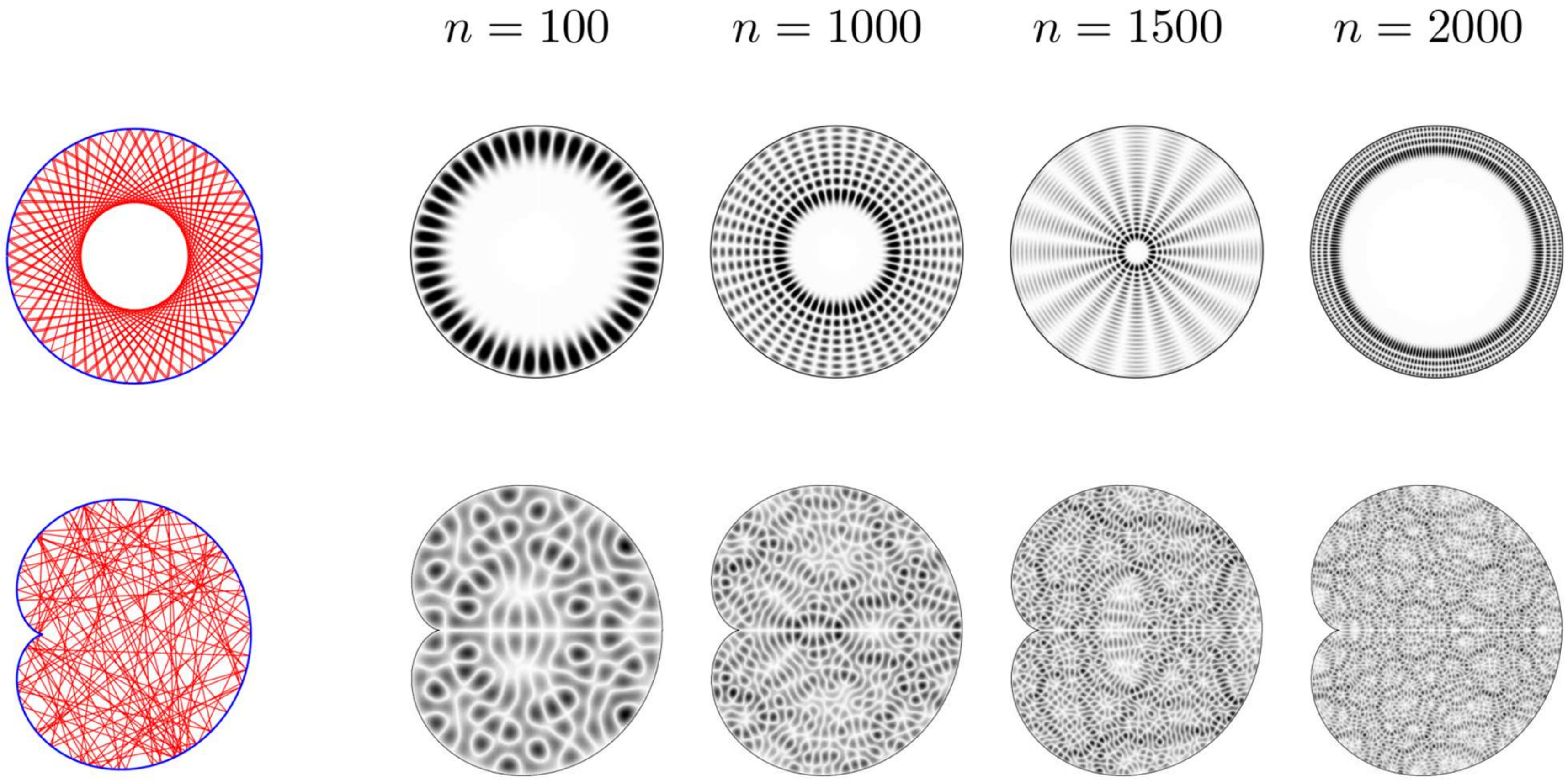


- Eigenfunctions and eigenvalues:

$$\psi_{nm}(r,\varphi) = J_m(k_{nm}r)e^{im\varphi},\ J_m(k_{nm}R) = 0$$

- Angular momentum of classical trajectory: $\sin\phi \approx \dfrac{m}{Rk_{1m}}$

Wave Functions of Circle and Limaçon Billiard for Increasing Energy



Ergodicity in Quantum Systems

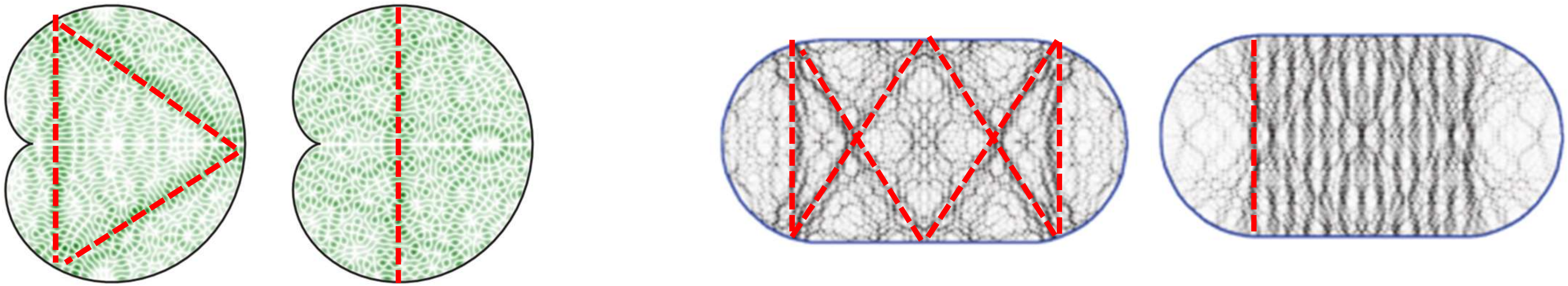
- Probability that a quantum particle in state n is found in a part B_0 of position space B:

$$\mu_n(B_0) = \int_{B_0} \mathrm{d}^2 q \, |\psi_n(\boldsymbol{q})|^2$$

- Quantum ergodicity:

$$\mu_n(B_0) \rightarrow \frac{\mathrm{Area}(B_0)}{\mathrm{Area}(B)}$$

- Exception: \`scar´ wave functions



Spectral Properties of Integrable Systems

Berry-Tabor Conjecture:

- The fluctuation properties in the eigenvalue spectra of a typical integrable system behave like independent random numbers from a Poisson process $\rightarrow$ Based on Einstein-Brillouin-Keller (EBK) quantization

Integrable Systems: Einstein-Brillouin-Keller (EBK) Quantization

- EBK quantization: $I_i = \frac{1}{2\pi} \oint_{C_i} p\mathrm{d}q = \left(n_i + \frac{\alpha_i}{4} \right) \hbar,\ n_i = 0, 1, 2, \cdots$
- Maslov index $\frac{\alpha_i}{4} = \left(\frac{\mu_i}{4} + \frac{b_i}{2} \right)$, μ = # turning points, b = # refl. at hard wall
- Applicable to N-dimensional integrable systems that can be described using torus variables
- EBK equation provides an implicit quantization condition for the energies

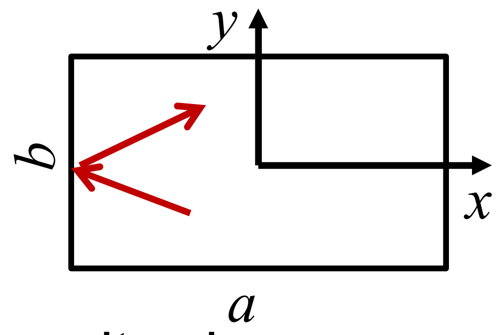
$$E = \widetilde{H}(\mathbf{I}) = \widetilde{H}(\hbar(\mathbf{n} + \boldsymbol{\alpha})) \Rightarrow E = E(n_1, \cdots, n_N)$$

- Generally, the EBK eigenvalues yield a good approximation for the quantum eigenvalues in the semiclassical limit

Action-Angle Variables of a Rectangular Billiard

- Constants of motion

$$E = \frac{p_x^2}{2} + \frac{p_y^2}{2}, \left|p_x\right| = const., \left|p_y\right| = \sqrt{2E - \left|p_x\right|^2} = const.$$



- At each reflection one of the momenta $p_i\,(i=x,y)$ changes its sign $p_i \to -p_i$

- Action variables

$$I_1 = \frac{1}{2\pi} \oint_{C_x} p_x dx = \frac{a}{\pi}\left|p_x\right|$$

$$I_2 = \frac{1}{2\pi} \oint_{C_y} p_y dy = \frac{b}{\pi}\left|p_y\right|$$

- Hamiltonian

$$H = \frac{\pi^2}{2}\left(\frac{I_1^2}{a^2} + \frac{I_2^2}{b^2}\right)$$

- Angle variables

$$\Phi_1(t) = \frac{\pi^2 I_1}{a^2} t + \alpha_1, \Phi_2(t) = \frac{\pi^2 I_2}{b^2} t + \alpha_2$$

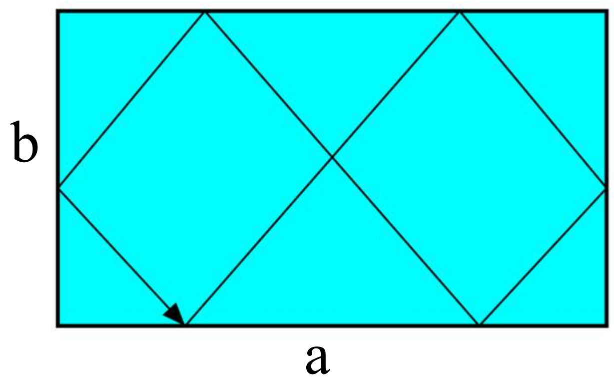
Rectangular Billiard

$\alpha_1 = \alpha_2 = 1$ (2 reflections at hard walls)

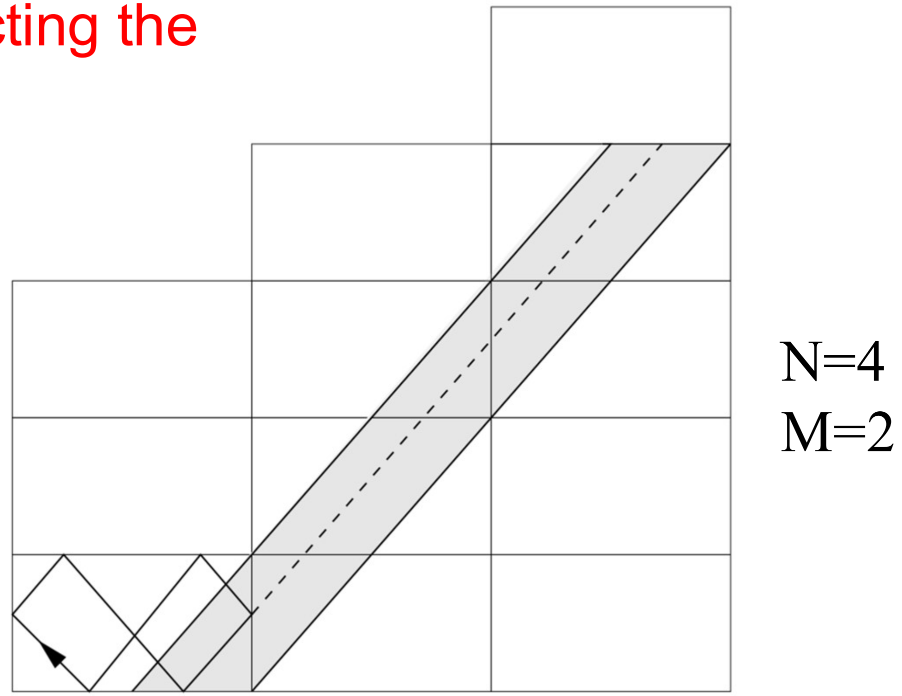
$$I_1 = \frac{a}{\pi}|p_x| = \hbar(n_1+1),\; I_2 = \frac{b}{\pi}|p_y| = \hbar(n_2+1),\; n_i = 0, 1, \cdots$$

$$E_{N,M} = \frac{\pi^2\hbar^2}{2}\left(\frac{N^2}{a^2}+\frac{M^2}{b^2}\right),\; N, M = 1, 2, \cdots \rightarrow$$ EBK eigenvalues exact!

- The trajectories are unfolded by reflecting the rectangular billiard at its boundaries
- Periodic folding $\Leftrightarrow$ 2-torus



$\rightarrow$



Trace Formula in Terms of Periodic Orbits

Sieber et al., JPA 28, 5041 (1995)

- Spectral density of a quantum system: $\rho(E)=\sum_{n,m=1}^{\infty}\delta(E-E_{nm})$
- Sum over periodic orbits with lengths $L_{pq}=2\sqrt{p^2L_x^2+q^2L_y^2}$

$$\rho(E)=\sum_{n,m=1}^{\infty}\delta(E-E_{nm})=\frac{L_xL_y}{4\pi}-\frac{L_x}{4\pi k}-\frac{L_y}{4\pi k}+\frac{1}{4}\delta(E)$$

$$+\frac{L_xL_y}{4\pi}\sum_{p,q\neq(0,0)}\sqrt{\frac{2}{\pi k L_{pq}}}\cos\left(kL_{pq}-\frac{\pi}{4}\right)$$

$$-\frac{L_x}{2\pi k}\sum_{p=1}^{\infty}\cos(2kpL_x)-\frac{L_y}{2\pi k}\sum_{q=1}^{\infty}\cos(2kqL_y)$$

- Weyl formula for the smooth part of the level density of 2D billiards

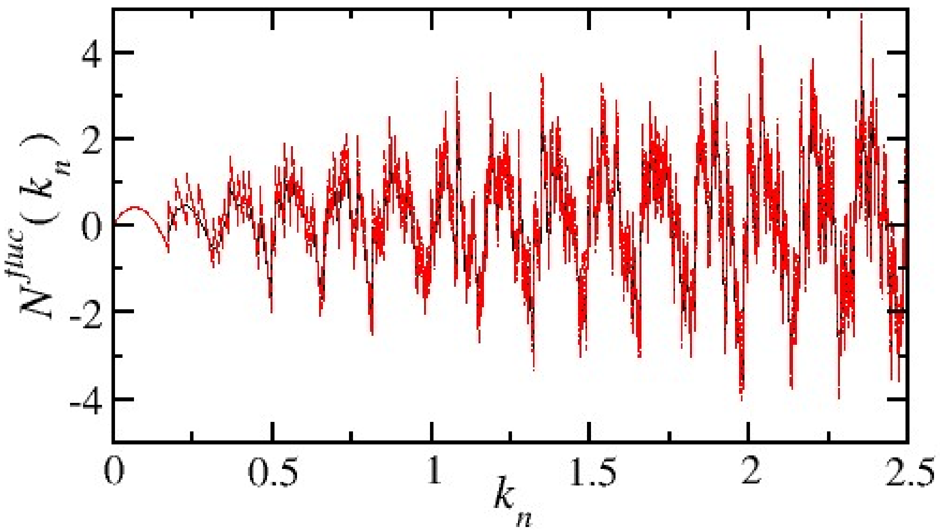
$$\bar{\rho}(E)=\frac{L_xL_y}{4\pi}-\frac{L_x}{4\pi k}-\frac{L_y}{4\pi k}$$

Numerical Test of the Trace Formula for Rectangular Billiards

— : numerical eigenvalues

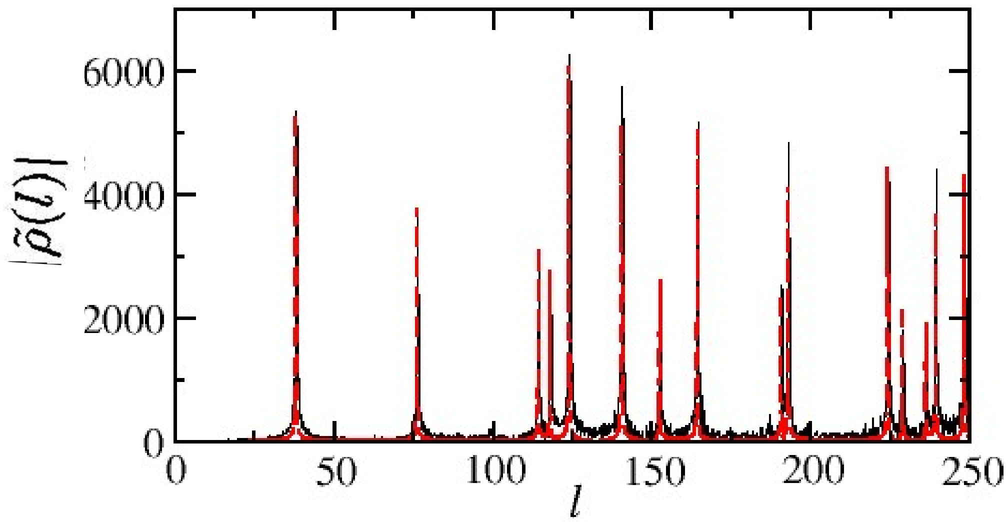
— : trace formula

$$N^{fluc}(k) = N(k) - N^{smooth}(k)$$

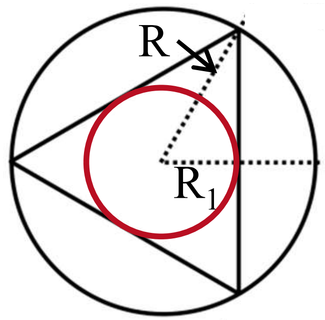


- Length spectrum

$$|\tilde{\rho}(l)| = |\int_0^{k_{max}} \mathrm{d}k e^{ikl} \rho_{fluc}(k)|$$



Action-Angle Variables of a Circle Billiard



- Polar coordinates

$$x = r\cos\phi, \quad \dot{x} = \dot{r}\cos\phi - r\dot{\phi}\sin\phi$$

$$y = r\sin\phi, \quad \dot{y} = \dot{r}\sin\phi + r\dot{\phi}\cos\phi$$

- Hamiltonian

$$H = E = \frac{1}{2}\left(\dot{x}^2 + \dot{y}^2\right) = \frac{1}{2}\left(\dot{r}^2 + r^2\dot{\phi}^2\right)$$

- Conjugate momenta

$$p_i = \frac{\partial L(r,\phi;\dot{r},\dot{\phi})}{\partial \dot{q}_i} \Rightarrow p_r = \dot{r},\ p_\phi = r^2\dot{\phi} = const. = \left|\vec{L}\right| \Rightarrow H = \frac{1}{2}\left(p_r^2 + \frac{p_\phi^2}{r^2}\right)$$

- Action variables

$$I_\phi = \frac{1}{2\pi}\oint p_\phi \mathrm{d}\phi = p_\phi = \left|\vec{L}\right|$$

$$I_r = \frac{1}{2\pi}\oint p_r \mathrm{d}r = \frac{1}{2\pi}\int_{R_1}^{R}\sqrt{2E - \frac{\left|\vec{L}\right|^2}{r^2}}\mathrm{d}r = \frac{1}{\pi}\left(\sqrt{2ER^2 - \left|\vec{L}\right|^2} - \left|\vec{L}\right|\arccos\frac{\left|\vec{L}\right|}{\sqrt{2E}R}\right)$$

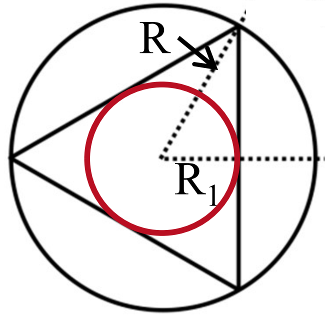
- Angle variables

$$\omega_\phi = \dot{\Phi}_\phi = \frac{\partial E}{\partial I_\phi} = \frac{2E}{\sqrt{2ER^2 - \left|\vec{L}\right|^2}}\arccos\frac{\left|\vec{L}\right|}{\sqrt{2E}R}$$

$$\omega_r = \dot{\Phi}_r = \frac{\partial E}{\partial I_r} = \frac{2\pi E}{\sqrt{2ER^2 - \left|\vec{L}\right|^2}}$$

Circle Billiard

$M_r = \#$ librations of the radial coordinate, $M_\phi = \#$ revolutions

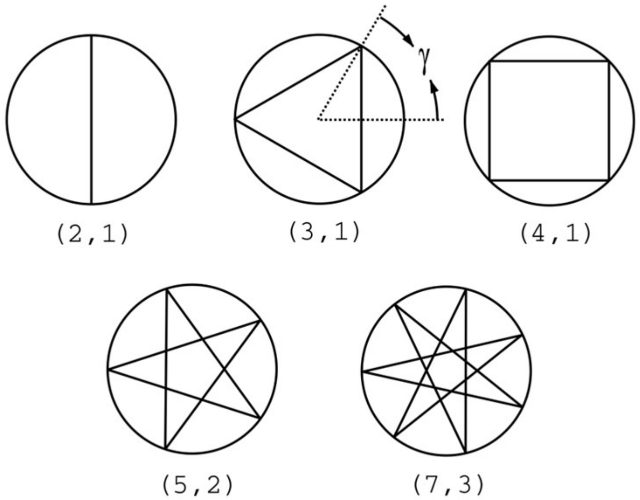


$$I_\phi = \left(M_\phi + \frac{\alpha_\phi}{4} \right) \hbar = M_\phi \hbar$$

$$I_r = \frac{\hbar}{\pi} \left(\sqrt{k^2 R^2 - M_\phi^{\ 2}} - |M_\phi| \arccos \frac{|M_\phi|}{kR} \right) = \hbar \left(M_r + \frac{1}{4} + \frac{1}{2} \right) = \hbar \left(M_r + \frac{3}{4} \right), k^2 = \frac{2E}{\hbar^2}$$

- Spectrum produced by the EBK quantization is not exact!

- Example: closed orbits in circle billiard, characterized by (M_r, M_ϕ)
  $M_r = \#$ vertices of polygon
  $M_\phi = \#$ revolutions around center



Trace Formula for Circle Billiard

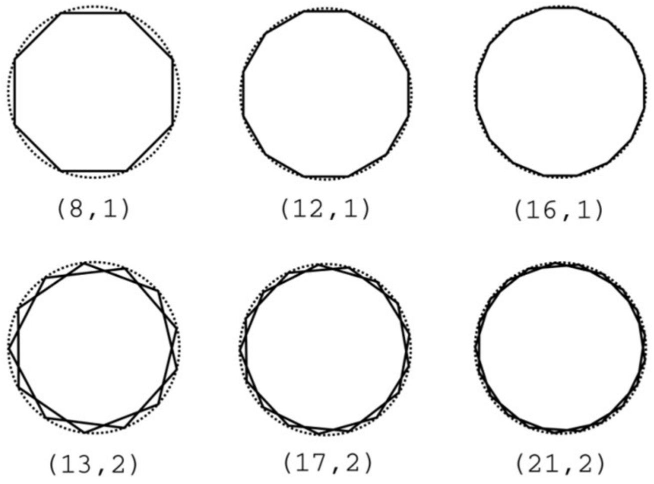
Berry & Tabor, JPA 10, 371 (1977)

- Periodic orbits: $$\frac{\omega_\phi}{\omega_r} = \frac{1}{\pi}\arccos\left(\frac{M_\phi}{kR}\right) = \frac{M_\phi}{M_r}$$
- Action of periodic orbits: $$S(\mathbf{M}) = 2\pi M_\phi I_\phi + 2\pi M_r I_r = 2kRM_r \sin\left(\frac{M_\varphi}{M_r}\pi\right) = kRs_{\mathbf{M}}$$
- Trace formula:

$$\rho^{fluc}(kR) = \sqrt{\frac{\pi}{2}}\sqrt{kR}\sum_{\mathbf{M}>0} m_{\mathbf{M}} \frac{s_{\mathbf{M}}^{3/2}}{M_r^2}\cos\left(kRs_{\mathbf{M}} - \frac{3}{2}M_r\pi - \frac{\pi}{4}\right), \quad m_M = \begin{cases} 1: M_r = 2M_\varphi \\ 2: M_r > 2M_\varphi \end{cases}$$

- Convergence problem: as $M_r \to \infty$ for fixed M_ϕ, the length $Rs_{\mathbf{M}} \to 2\pi M_\phi R$

$\Rightarrow$ Accumulation points of orbits at scaled actions of multiples of 2π

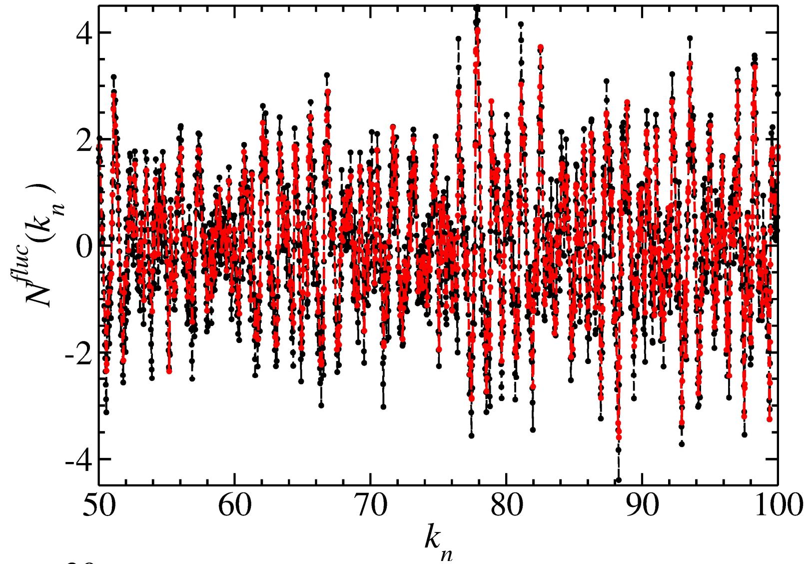


Numerical Test of the Trace Formula for Circle Billiards

— : numerical eigenvalues

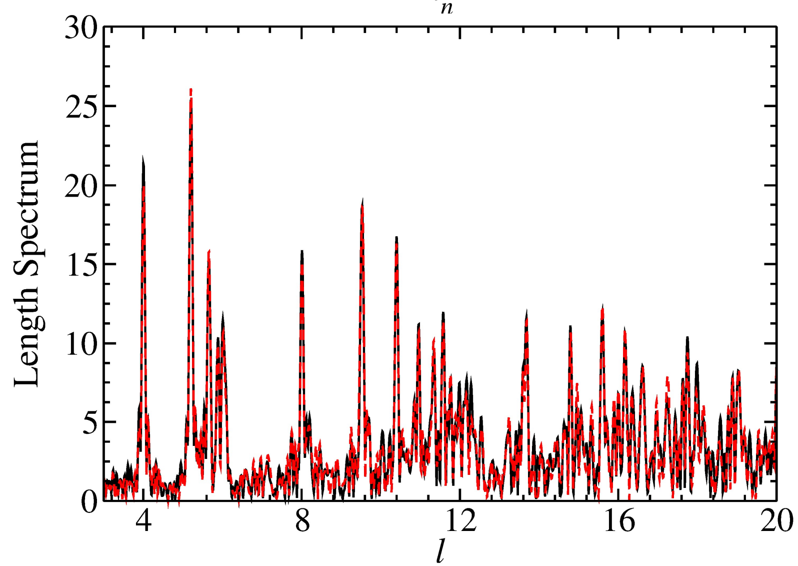
— : trace formula

$$N^{fluc}(k) = N(k) - N^{smooth}(k)$$



- Length spectrum

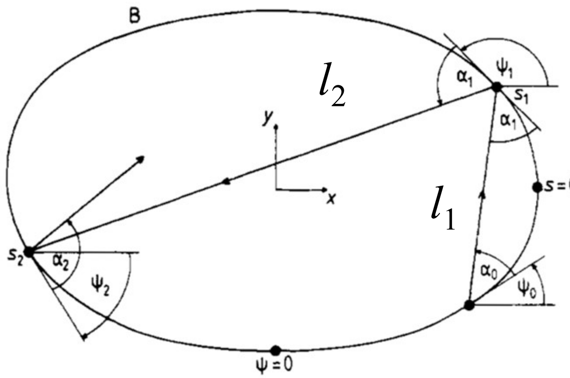
$$|\tilde{\rho}(l)| = |\int_0^{k_{max}} \mathrm{d}k e^{ikl} \rho_{fluc}(k)|$$



Gutzwiller‘s Trace Formula for Chaotic Billiards

$$\rho^{fluc}(k) = \sum_{po} \frac{l_{po}}{\pi \left| \det\left(M_{po} - 1\right) \right|^{1/2}} \cos\left(k l_{po} - \mu_{po} \frac{\pi}{2} \right)$$

l_{po}: length of periodic orbit po
μ_{po}: Maslov index of periodic orbit po
M_{po}: Monodromy matrix



$$M_{po} = \widetilde{M}_n \cdot \widetilde{M}_{n-1} \cdots \widetilde{M}_2 \cdot \widetilde{M}_1, \quad \widetilde{M}_i = \begin{pmatrix} -1 & 0 \\ \dfrac{2}{R_i \cos\alpha_i} & -1 \end{pmatrix} \begin{pmatrix} 1 & l_i \\ 0 & 1 \end{pmatrix}$$

R_i: Radius of curvature

- Trace formula was derived under the assumption that all involved periodic orbits should be isolated in phase space

$\rightarrow$ applicable to chaotic systems

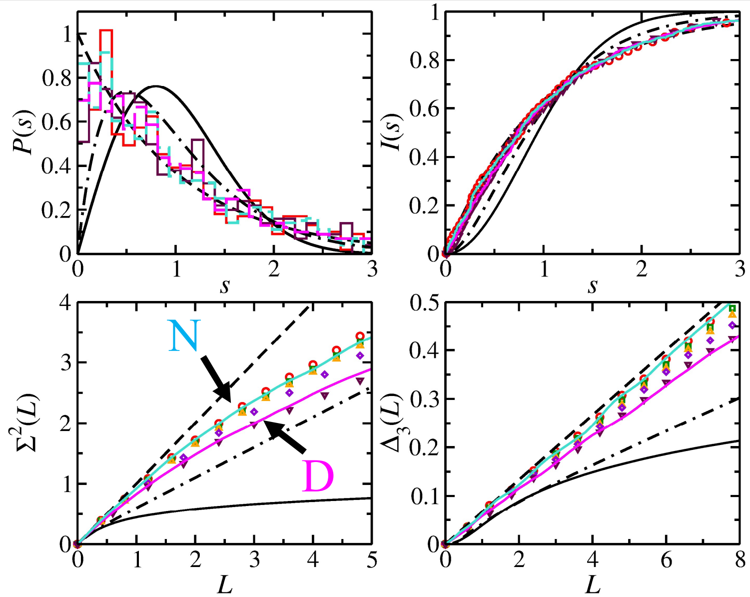
$\rightarrow$ Martin Sieber‘s lectures

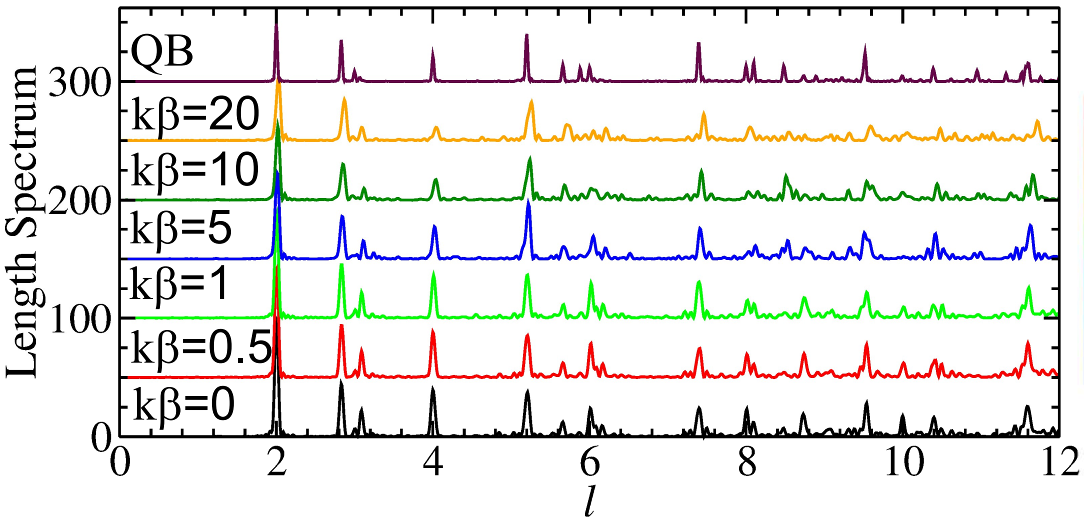
Spectral Properties of Robin Sector Billiard

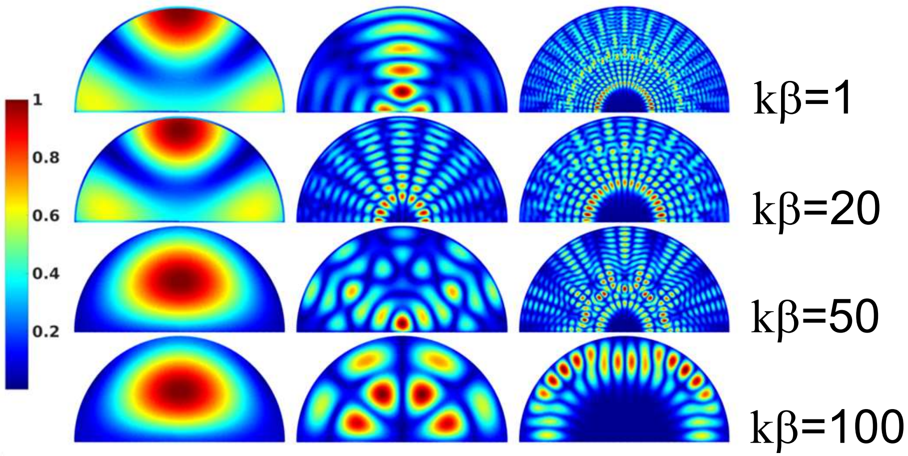
- Robin BC

$$\left[\tilde{\beta} + \frac{1}{2}\kappa(s)\right] \Phi_j(s) + \partial_n \Phi_j(n,s)\big|_{n \to 0^-} = 0$$

- Shown are the symmetric solutions







Spectral Properties of Chaotic Systems

Bohigas-Gianonni-Schmit Conjecture:

- The fluctuation properties in the eigenvalue spectra of a typical time-reversal invariant integer spin / time-reversal invariant 1/2 integer spin / time-reversal non-invariant chaotic system coincide with those of real-symmetric / quaternion real / complex Hermitian random matrices from the Gaussian ensembles (GOE / GSE / GUE)

Time-Reversal

- A classical Hamiltonian is called time-reversal invariant if H is invariant under the operation $t \to -t,\ \boldsymbol{x} \to \boldsymbol{x},\ \boldsymbol{p} \to -\boldsymbol{p},\ H(\boldsymbol{x},\boldsymbol{p}) \to H(\boldsymbol{x},-\boldsymbol{p})$
- The Schrödinger equation is time-reversal invariant if to each solution

$$i\hbar\frac{\partial}{\partial t}\psi(\boldsymbol{x},t) = H\psi(\boldsymbol{x},t)$$

another, uniquely related solution $\psi'(\boldsymbol{x}',t'=-t)$ exists

- Conventional time-reversal operator is the complex conjugation $\mathcal{K}$

$$t \to -t,\ \boldsymbol{x} \to \boldsymbol{x},\ \boldsymbol{p} \to -\boldsymbol{p},$$

$$\psi(\boldsymbol{x}) \to \psi^\star(\boldsymbol{x}) = \mathcal{K}\psi(\boldsymbol{x}),\ \mathcal{K}^2 = 1$$

- Property of antinunitary, which implies antilinearity:

$$\langle\mathcal{K}\psi|\mathcal{K}\phi\rangle = \langle\psi|\phi\rangle^\star = \langle\phi|\psi\rangle$$

- A complex conjugation operator can be defined with respect to any presentation $\mathcal{K} = U\mathcal{K}'$

Canonical Transformation for Hamiltonian without Time-Reversal Invariance

- Hamiltonian can be expressed by a Hermitian matrix with real eigenvalues

$$(H_{\mu\nu})^\star = \tilde{H}_{\mu\nu} = H_{\nu\mu}$$

- A Hermitian matrix is diagonalized by a unitary transformation

$$H_{\mu\nu} = \sum_{\lambda=1}^{N} U_{\mu\lambda} E_\lambda U^\dagger_{\lambda\nu} = \sum_{\lambda=1}^{N} U_{\mu\lambda} E_\lambda U^\star_{\nu\lambda}$$

- Canonical transformation changes H but not its eigenvalues and does not destroy Hermiticity

- Let $H' = AHA^{-1} = AEA^{-1}$, i.e., $H'_{\mu\nu} = \sum_{\lambda=1}^{N} A_{\mu\lambda} E_\lambda \left(A^{-1}\right)_{\lambda\nu}$

- Hermiticity: $\left(AHA^{-1}\right)^\dagger = AHA^{-1} \equiv \left[H, A^\dagger A\right] = 0$

- Unitary matrices constitute the class of canonical transformations

$$A^\dagger A = \mathbb{1}$$

Canonical Transformation for Time-Reversal Invariant Hamiltonians

- Invariance of H under antiunitary time-reversal operator T

$$[H,T] = 0,\; T^2 = 1$$

- T-invariant basis can be constructed from arbitrary $|\phi_\mu\rangle$ and complex a_μ

$$\psi_\mu = a_\mu \phi_\mu + T a_\mu \phi_\mu, \text{ with } \langle \psi_\mu | \phi_\nu \rangle = \delta_{\mu\nu}$$

- With respect to the T-invariant basis the Hamiltonian is real symmetric

$$\begin{aligned} H_{\mu\nu} &= \langle \psi_\mu | H \psi_\nu \rangle = \langle T\psi_\mu | T H \psi_\nu \rangle^\star \\ &= \langle \psi_\mu | T H T^2 \psi_\nu \rangle^\star = \langle \psi_\mu | T H T \psi_\nu \rangle^\star = H^\star_{\mu\nu} \end{aligned}$$

$\Rightarrow$ Hamiltonian can be made real without being diagonalized

- Orthogonal matrices constitute the class of canonical transformations

Random Matrix Theory: Gaussian Ensembles

- The Gaussian orthogonal / symplectic / unitary ensembles are defined in the space of real symmetric / quaternion real / Hermitian matrices by :

- GOE: The joint probability is invariant under orthogonal transformations O

$$P(H) = P(H'),\ H' = OH\tilde{O},\ \tilde{O} = O^{-1}$$

- GUE (GSE): The joint probability is invariant under unitary (+symplectic) transformations U

$$P(H) = P(H'),\ H' = UHU^{\dagger},\ U^{\dagger} = U^{-1}$$

- The matrix elements are statistically independent

$$P(H) = P_{11}(H_{11})P_{22}(H_{22})P_{12}(H_{12})\ ....$$

- The probability density $P(H)$ has the same form for GOE, GSE and GUE

$$\boxed{P(H) = \mathcal{N}e^{-ATrH^2}}$$

Threefold way

- Quantum systems with violated time-reversal invariance
- Hamiltonian (unitary universality class):

$$\hat{H} = \hat{H}^{\dagger}.$$

- Quantum Systems with integer spin and preserved time-reversal invariance
- Time-reversal operator

$$\hat{T} = \mathcal{C} \quad \hat{T}^2 = 1$$

- Hamiltonian (orthogonal universality class):

$$\hat{T}\hat{H}\hat{T}^{-1} = \hat{H} \quad \hat{H} = \hat{H}^T$$

- Quantum systems with 1/2-integer spin and preserved time-reversal invariance belong to the symplectic universality class

Hamiltonian with Symplectic Symmetry (GSE)

- Time-reversal operator of spin-1/2 systems $\hat{T} = \hat{Y}\mathcal{C},\, \hat{Y} = \begin{pmatrix} \hat{0}_N & -\mathbb{1}_N \\ \mathbb{1}_N & \hat{0}_N \end{pmatrix}$
- Time-reversal invariance $\hat{T}\hat{H}\hat{T}^{-1} = \hat{H}$
- Hermiticity implies that $\hat{H} = \hat{H}^\dagger$ is symplectic

$$\hat{H} = \hat{Y}\hat{H}^T\hat{Y}^T$$

- The eigenvalues are Kramer's degenerate $\hat{T}^2 = -1 \;\Rightarrow\; \langle\psi|\hat{T}\psi\rangle = 0$
- Define basis $\mathcal{B} = \{|1\rangle, |2\rangle \ldots, |N\rangle, |\hat{T}1\rangle, |\hat{T}2\rangle, \ldots, |\hat{T}N\rangle\}$
- Symplectic Hamiltonian $\hat{H} = \begin{pmatrix} \hat{H}_0 & \hat{V} \\ -\hat{V}^* & \hat{H}_0^* \end{pmatrix},\, \hat{H}_0 = \hat{H}_0^\dagger,\, \hat{V} = -\hat{V}^T$

Eigenvalue Distributions of $N\times N$ Random Matrices from the GEs

- Joint probability distribution of the eigenvalues of $N\times N$ dimensional real symmetric random matrices from the GOE (β=1) / Hermitian random matrices from the GUE (β=2) / quaternion-real random matrices from the GSE (β=4)

$$\boxed{P_N(E_1,\cdots,E_N) = \mathcal{N}_\beta \prod_{\mu<\nu}^{N} |E_\mu - E_\nu|^\beta \exp\left(-A\sum_{\mu=1}^{N} E_\mu^2\right)}$$

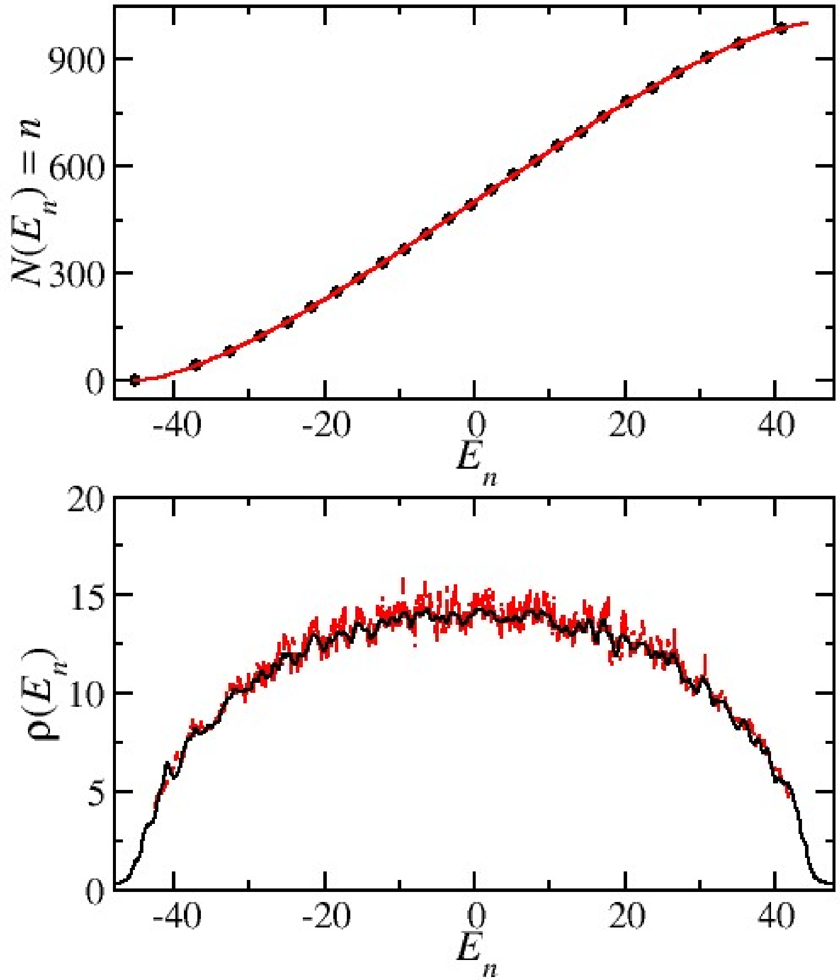
- Ensemble-averaged level density

$$\begin{aligned}\langle\rho(E)\rangle &= \left\langle \sum_{i=1}^{N} \delta(E - x_1)\right\rangle \\ &= N\int_{-\infty}^{\infty}\cdots\int_{-\infty}^{\infty} P_N(E, x_2,\cdots,x_N))\mathrm{d}x_2\cdots\mathrm{d}x_N\end{aligned}$$

- Wigner´s semicircle law

$$\langle\rho(E)\rangle = \begin{cases} \frac{1}{\pi}\sqrt{2N - E^2} & |E| \leq \sqrt{2N} \\ 0 & |E| > \sqrt{2N}\end{cases}$$

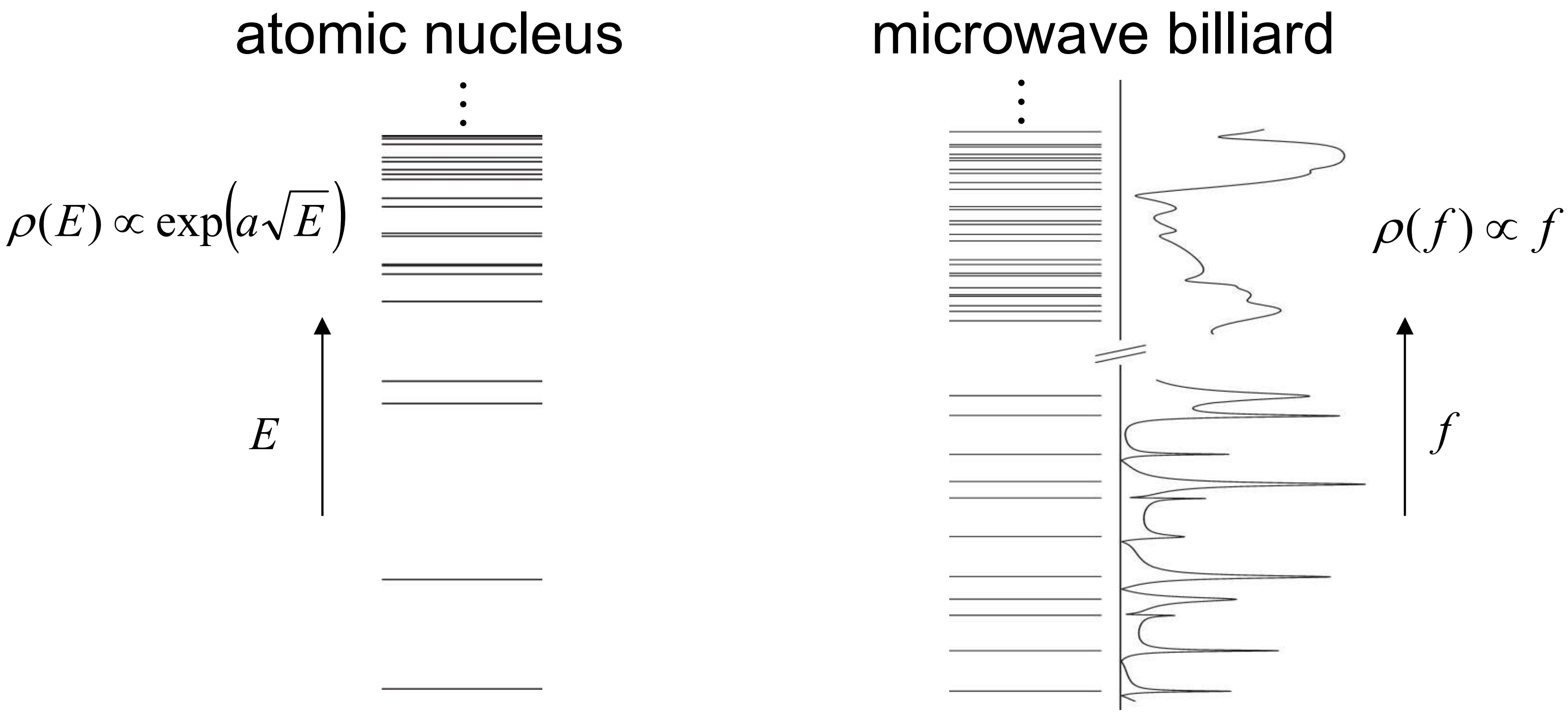
Level Density and Integrated Level Density



- The level density fluctuates around a non-uniform average density $\langle \rho(E) \rangle$

$\rightarrow$ System specific property, i.e., non-universal feature

Equivalence of Ensemble Averages and Spectral Averages



- Ergodicity: Ensemble average = spectral average
- Spectral averages are performed over different parts of the level sequence
- Uniform average level density $\overline{\rho}(E) = \overline{\rho}$ needed $\rightarrow$ unfolding of spectra

Unfolding

- Replace E_i by $e_i = f(E_i)$
- The unfolded e_i should have unit average spacing / density in interval of ΔN levels

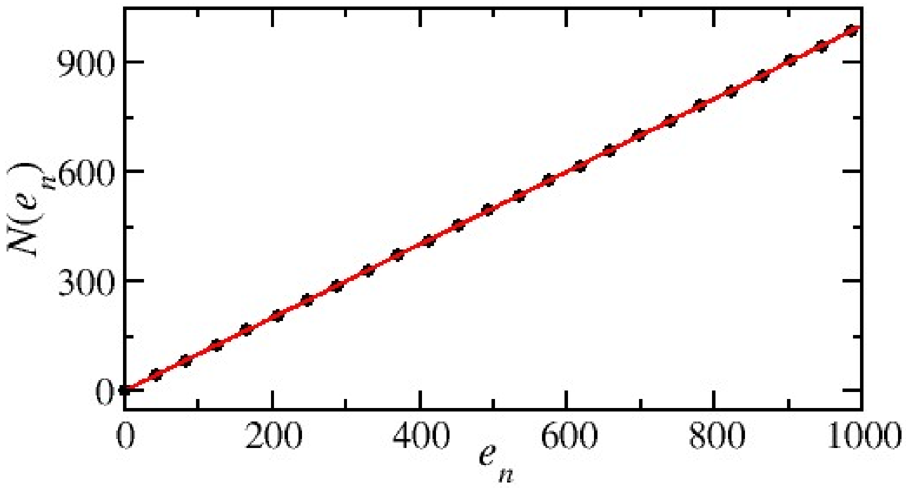
$$\begin{aligned} 1 &= \frac{\Delta e}{\Delta N} = \frac{1}{\Delta N}\left[f(E+\Delta E/2) - f(E-\Delta E/2)\right] \\ &= \frac{\Delta E}{\Delta N} f'(E) = f'(E)/(\bar{\rho}(E)) \end{aligned}$$

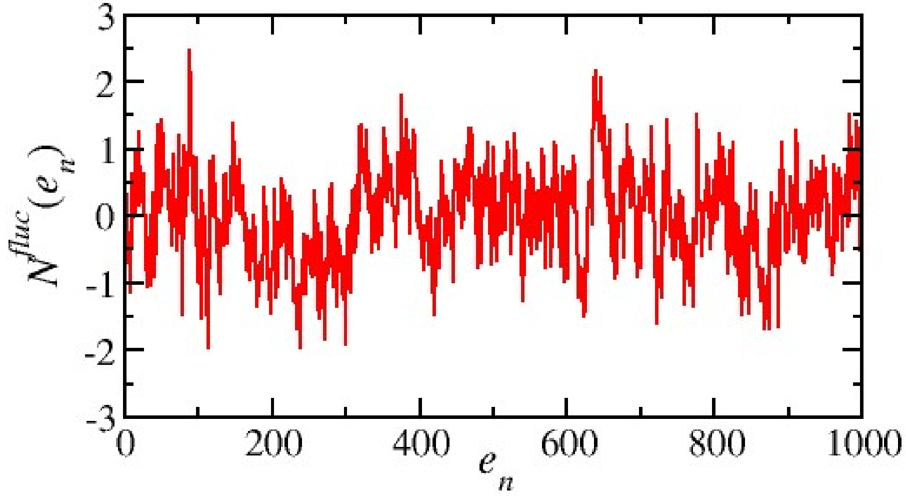
$\Rightarrow$ unfolding implies replacement of E_i by the integrated level density evaluated up to E_i

$$f(E) = \overline{N}(E) = \int_{-\infty}^{E} \mathrm{d}E' \, \overline{\rho}(E')$$

- Unfolding: $e_i = \overline{N}(E_i)$

Integrated Level Density of the Unfolded Eigenvalues





$$N^{fluc}(e_n) = N(e_n) - \overline{N}(e_n),\ \overline{N}(e_n) = e_n$$

Nearest-Neighbor Spacing Distribution `Wigner Surmise´

- The distribution of the spacings between adjacent eigenvalues may be derived using 2×2 random matrices ($\beta=1$: GOE, $\beta=2$: GUE, $\beta=4$: GSE)

$$P(S) \propto \int_{-\infty}^{\infty} \mathrm{d}E_+ \int_{-\infty}^{\infty} \mathrm{d}E_- \delta\left(S - |E_+ - E_-|\right) |E_+ - E_-|^{\beta} e^{-A\left(E_+^2 + E_-^2\right)}$$

- Normalize to average spacing one and $P(S)$ to one

$$\langle S \rangle = \int_0^{\infty} \mathrm{d}S\, S P(S) = 1, \int_0^{\infty} \mathrm{d}S\, P(S) = 1$$

- The result are the Wigner distributions:

$$P(S) = \begin{cases} (S\pi/2)\mathrm{e}^{-S^2\pi/4} & \text{orthogonal} \\ (S^2 32/\pi^2)\mathrm{e}^{-S^2 4/\pi} & \text{unitary} \\ (S^4 2^{18}/3^6\pi^3)\mathrm{e}^{-S^2 64/9\pi} & \text{symplectic.} \end{cases}$$

- Generally used for comparison of numerical and experimental data with random matrix predictions
- Very good approximation of exact distribution (see below)

n-Point Correlation- and Cluster Functions

- n-point correlation function: probability density to find a level around each of the points E_1, E_2, …, E_n, while the positions of the remaining levels are unobserved

$$R_n(E_1,...,E_n) = \left\langle \sum_{i_1\neq i_2\neq\cdots\neq i_n=1}^{N} \delta(E_1-x_{i_1})\delta(E_2-x_{i_2})\cdots\delta(E_n-x_{i_n}) \right\rangle$$

$$= \frac{N!}{(N-n)!}\int_{-\infty}^{\infty}\cdots\int_{-\infty}^{\infty} P_N(E_1,E_2,\cdots,E_n,x_{n+1},\cdots,x_N))\mathrm{d}x_{n+1}\cdots\mathrm{d}x_N$$

$$\langle\rho(E)\rangle = R_1(E)$$

- Each R_n is grouped into clusters depending on $E_{i_1}, E_{i_2}, \cdots, E_{i_m}, m \le n$
- Irreducible cluster functions vanish for large $|E_i - E_j|$

$$T_n(x_1,\cdots,x_n) = \sum_G (-1)^{n-m}(m-1)!\prod_{j=1}^{m} R_{G_j}(x_k,\, k\in G_j)$$

- Unfolding necessary to obtain definite limits as $N\to\infty$

$$Y_n(e_1,e_2,\cdots,e_n) = \lim_{N\to\infty}\frac{T_n(E_1,E_2,\cdots,E_n)}{R_1(E_1)R_1(E_2)\cdots R_1(E_n)}$$

Long-Range Correlations

- Number variance $\Sigma^2(L) = \langle n^2 \rangle - \langle n \rangle^2$
- Related to the 2-point cluster function by

$$\Sigma^2(L) = L - 2\int_0^L (L-r) Y_2(r) \mathrm{d}r$$

- Dyson-Mehta statistic (rigidity): least-mean square deviation of $N(e)$ from the straight line best fitting it in an interval of length L

$$\Delta_3(L) = \frac{2}{L^4}\int_0^L (L^3 - 2L^2 r + r^3)\Sigma^2(r)\mathrm{d}r$$

- The 2-point cluster function is known explicitly:

$$\boxed{Y_2(e = |e_1 - e_2|) = \begin{cases} s(e)^2 - J(e)D(e) & \beta = 1\,\mathrm{GOE} \\ s(e)^2 & \beta = 1\,\mathrm{GUE} \end{cases}}$$

$$s(e) = \frac{\sin \pi e}{\pi e}, \quad I(e) = \int_0^e \mathrm{d}e' s(e')$$

$$D(e) = \frac{\partial s}{\partial e}, \quad J(e) = I(e) - \frac{1}{2}\mathrm{sgn}(e)$$

Spectral Properties of Uncorrelated Random Numbers from a Poisson Process

- Poissonian fluctuations: no correlations between neighboring levels!

$$P(E_1, E_2, \cdots, E_N) = \left(\frac{1}{2\Lambda}\right)^N, \; -\Lambda \le E_i \le \Lambda$$

- Constant level density:

$$\rho(E) = \frac{1}{2\Lambda}$$

- Gap probability and nearest-neighbor spacing distribution are Poisson distributions:

$$\begin{aligned} E(s) &= \left(\frac{1}{2\Lambda}\right)^N \left[\prod_{i=1}^{N} \int_{-\Lambda+\frac{\Lambda s}{N}}^{\Lambda-\frac{\Lambda s}{N}} \mathrm{d}E_1\right] \\ &= \left(1 - \frac{s}{N}\right)^N \xrightarrow{N\to\infty} e^{-s}, P(s) = \frac{\partial^2 E(s)}{\partial^2 s} = e^{-s} \end{aligned}$$

- All cluster functions Y_n with $n > 1$ vanish

$$\begin{aligned} Y_n(r) &= 0, \; n = 2, 3, \cdots N \\ \Sigma^2(L) &= L \\ \Delta_3(L) &= \frac{L}{15} \end{aligned}$$

Ratio Distributions

Y.Y. Atas, E. Bogomolny, O. Giraud *et al.*, PRL 110, 084101 (2013)

- Consider ratio of two consecutive spacings of nearest-neighbors

$$r_i = \frac{f_{i+1} - f_i}{f_i - f_{i-1}}$$

- Advantage: ratios are dimensionless $\rightarrow$ no unfolding required

- Ratio distribution of Gaussian ensembles (β=1,2,4):

$$P_W(r) = \frac{1}{Z_\beta} \frac{(r + r^2)^\beta}{(1 + r + r^2)^{1+(3/2)\beta}}$$

- Ratio distribution of Poissonian random numbers:

$$\mathcal{P}_0(r) = 1/(1 + r)^2$$

Thank you

for

your attention

Canonical Transformations

- Consider a transformation $$q_i \to Q_i(\mathbf{q},\mathbf{p},t)$$ $$p_i \to P_i(\mathbf{q},\mathbf{p},t)$$ $$H(\mathbf{q},\mathbf{p},t) \to \widetilde{H}(\mathbf{Q},\mathbf{P},t)$$

- Canonical transformation $$\frac{\partial \widetilde{H}}{\partial P_i} = \dot{Q}_i, \ \frac{\partial \widetilde{H}}{\partial Q_i} = -\dot{P}_i$$

$$\delta \int_{q_i(t_1)}^{q_i(t_2)} \left(\sum_i \mathrm{p_i d}q_i - Hdt \right) = \delta \int_{Q_i(t_1)}^{Q_i(t_2)} \left(\sum_i \mathrm{P_i d}Q_i - \widetilde{H}dt \right) = 0$$

- Generating function $$dF = \left(\sum_i \mathrm{p_i d}q_i - Hdt \right) - \left(\sum_i \mathrm{P_i d}Q_i - \widetilde{H}dt \right)$$

- Example $$F = F(\mathbf{q},\mathbf{P},t), \ \frac{\partial F}{\partial q_i} = p_i, \ \frac{\partial F}{\partial P_i} = Q_i, \ \widetilde{H} = H + \frac{\partial F}{\partial t}$$

Semiclassical Approximation for Level Density of the Rectangular Billiard

- Starting point of the derivation of the semiclassical level density is the EBK quantization $E_{nm} = \frac{n^2\pi^2}{L_x^2} + \frac{m^2\pi^2}{L_y^2}$

$$\sum_{n,m=1}^{\infty} \delta(E-E_{nm}) = \frac{1}{4}\left[\sum_{n,m=-\infty}^{\infty} \delta(E-E_{nm}) - \sum_{n=-\infty}^{\infty} \delta(E-E_{n0}) - \sum_{m=-\infty}^{\infty} \delta(E-E_{0m}) + \delta(E-E_{00}) \right]$$

- Employ Poisson´s summation formula

$$\sum_{n=-\infty}^{\infty} f(n) = \sum_{M=-\infty}^{\infty} \int_{-\infty}^{+\infty} \mathrm{d}n\, f(n) e^{2\pi i M n}$$

$$\sum_{n,m=-\infty}^{\infty} \delta(E-E_{nm}) = \sum_{p,q=-\infty}^{\infty} \int_{-\infty}^{+\infty} \mathrm{d}n \int_{-\infty}^{+\infty} \mathrm{d}m\, \delta\left(E - \frac{n^2\pi^2}{L_x^{\ 2}} - \frac{m^2\pi^2}{L_y^{\ 2}} \right) e^{2\pi i (pn+qm)}$$

$$\frac{n\pi}{L_x} = \rho\cos\varphi, \quad \frac{m\pi}{L_y} = \rho\sin\varphi$$

$$\sum_{n,m=-\infty}^{\infty} \delta(E-E_{nm}) = \frac{1}{2}\frac{L_x L_y}{\pi^2} \sum_{p,q=-\infty}^{\infty} \int_0^{2\pi} d\varphi\, e^{i\pi\left(2pL_x\sqrt{E}\cos\varphi + 2qL_y\sqrt{E}\sin\varphi\right)} \equiv \frac{1}{2}\frac{L_x L_y}{\pi} \sum_{p,q=-\infty}^{\infty} J_0\left(k2\sqrt{p^2L_x^2 + q^2L_y^2}\right)$$

Nearest-Neighbor Spacing Distributions

- Probability that an interval of length S in units of the mean spacing $2\pi/N$ is empty

$$E_\beta(S)=\left[\prod_{i=1}^{N}\int_{-\pi+\pi S/N}^{\pi-\pi S/N} \mathrm{d}\varphi_i\right] P_\beta(\{\varphi_i\}),\; P_\beta(S)=\frac{\partial^2 E_\beta(S)}{\partial^2 S}$$

- CUE:

$$E_2(S)=\det\left(\delta_{kl}-\frac{\sin(\pi(k-l)\,S/N)}{\pi(k-l)}\right).$$

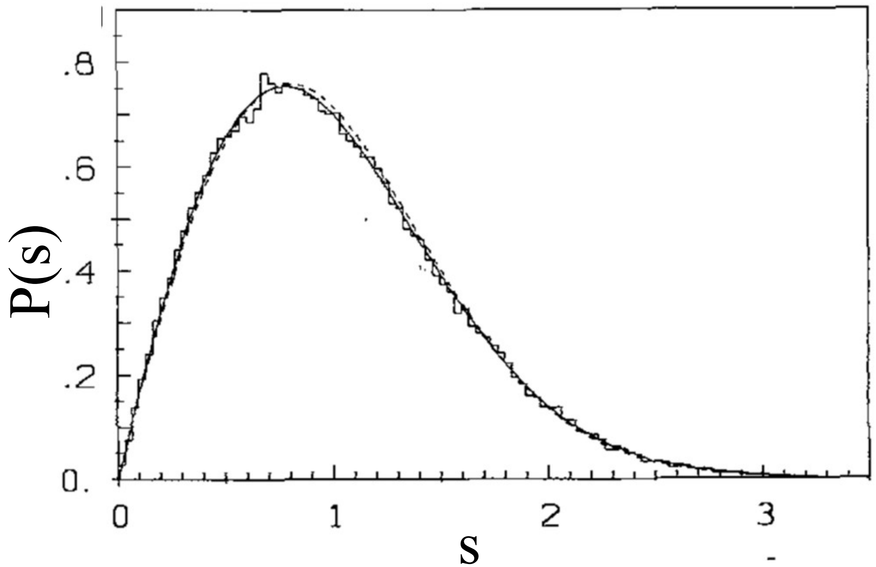
- Expand in a Taylor series:

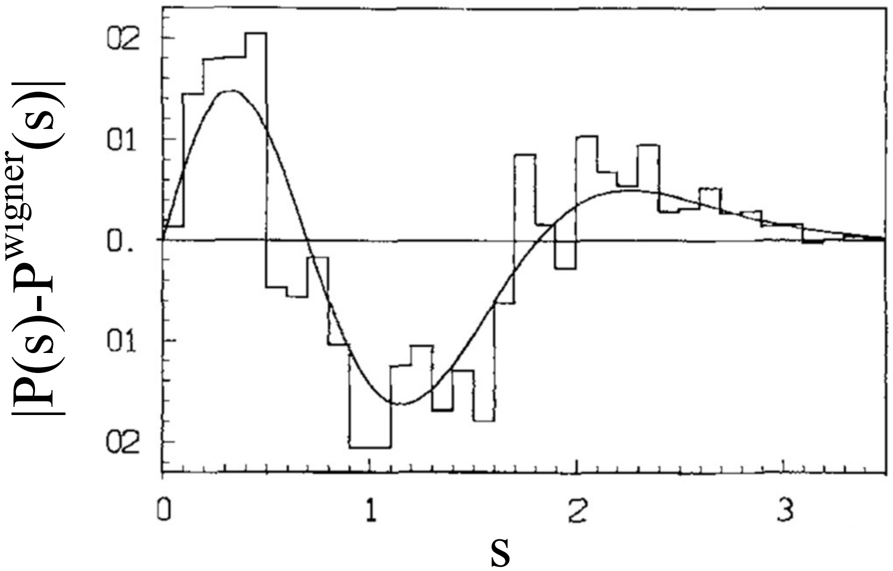
$$E_2(S)=\sum_{l=0}^{\infty} E_l\,S^l$$

- Taylor coefficients:

$$E_l^{(\mathrm{UE})}=\sum_{n=1,2,\dots}^{n^2\leq l}\pi^{l-n}\frac{(-1)^{(l+n)/2}}{n!}\sum_{l_1\dots l_n}^{1,2,\dots}\delta\left(\sum_{i=1}^{n} l_i,\frac{l-n}{2}\right)$$
$$\cdot\sum_{t_1}^{0\dots 2l_1}\dots\sum_{t_n}^{0\dots 2l_n}\det\left(\frac{1}{2l_i-t_i+t_j+1}\right)\prod_{k}^{1\dots n}$$
$$\cdot\left(\frac{1}{(2l_k+1)!}\binom{2l_k}{t_k}(-1)^{t_k}\right)$$

Comparison of the Exact NND with the Wigner Surmise





- Kicked top: $H(t) = \frac{\pi}{2} J_y + k \frac{J_z^2}{2j} \sum_{n=-\infty}^{\infty} \delta(t-n)$, $\langle \mathbf{J}^2 \rangle = j(j+1)$, j=500, 8.5≤k≤ 9.5
- Stroboscopic temporal behavior described by unitary Floquet operator

$$F = \exp\left(-i\frac{\pi}{2}J_y\right)\exp\left(-ik\frac{J_z^2}{2j}\right)$$

- 10^5 eigenphases were computed