Quantum chaos on graphs

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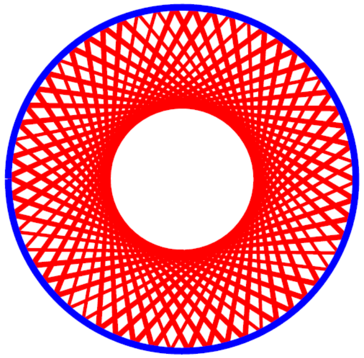
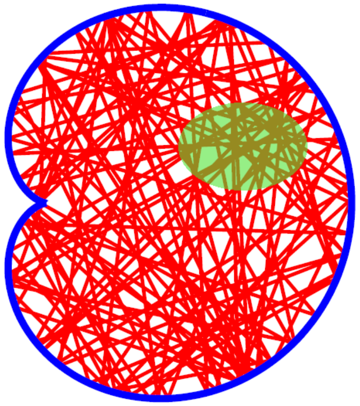
Overview:

- What is quantum chaos?
- Quantum graphs
- The trace formula
- The form factor
- Other graph models

Classical Chaos



integrable billiard
regular trajectories



chaotic billiard
irregular trajectories

Ergodicity implies for almost all trajectories $\Phi(t)$

$$\lim_{T\to\infty}\frac{1}{T}\int_0^T \chi_D(\Phi(t))\mathrm{d}t = \frac{\text{Area } D}{\text{Area } \Omega} \tag{1}$$

Quantum Mechanics on a billiard

Schrödinger eqn

$$\mathrm{i}\hbar\frac{\partial\Psi}{\partial t} = -\frac{\hbar^2}{2m}\Delta\Psi \tag{2}$$

Time-independent eqn: $(\hbar = 2m = 1)$ $\Psi(\mathbf{x}, t) = \psi(\mathbf{x})\mathrm{e}^{-\mathrm{i}Et}$

$$\boxed{-\Delta\psi_j = E_j\psi_j}$$

Billiard domain $\Omega \subset \mathbb{R}^2$, Hilbert space $L^2(\Omega)$.

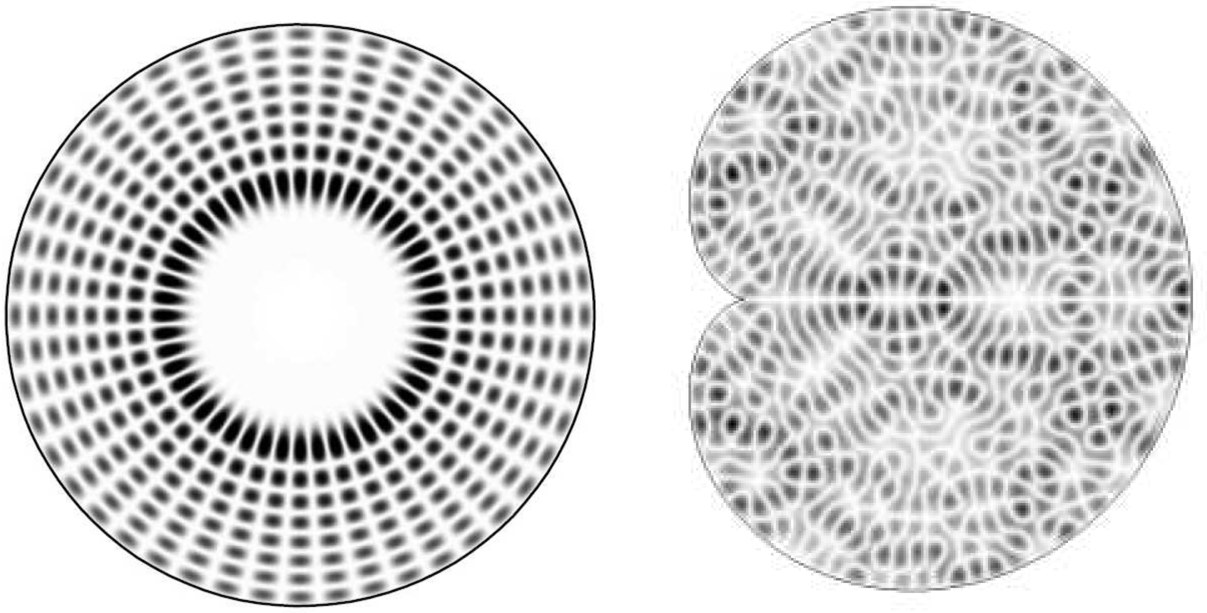
Dirichlet boundary conditions $\psi(\mathbf{x}) = 0$ on $\partial\Omega$.

Discrete spectrum of energy levels

$$E_0 \leq E_1 \leq E_2 \leq \ldots$$

Wavefunction ψ_j normalized so $\displaystyle\int_\Omega |\psi_j(\mathbf{x})|^2 \mathrm{d}\mathbf{x} = 1$.

$\displaystyle\int_B |\psi(\mathbf{x})|^2 \mathrm{d}\mathbf{x}$ probability of finding particle in $B \subset \Omega$.



Pictures from Arnd Bäcker: `http://www.physik.tu-dresden.de/~baecker/`

Quantum Chaology

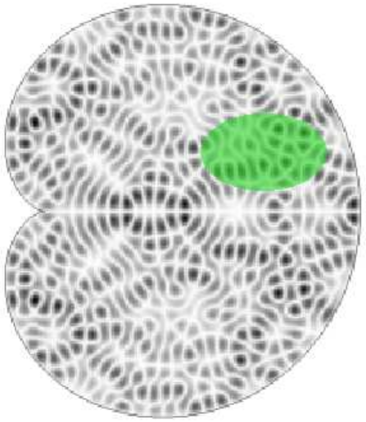
Quantum chaology is roughly the study of quantum mechanical systems whose classical analogue is chaotic.

Quantum Ergodicity Theorem

– Shnirelman 74, Colin de Verdiére 85, Zelditch 87, Zelditch & Zworski 96

For an ergodic billiard there exists a subsequence $\{\psi_{n_j}\}$ *of density one such that*

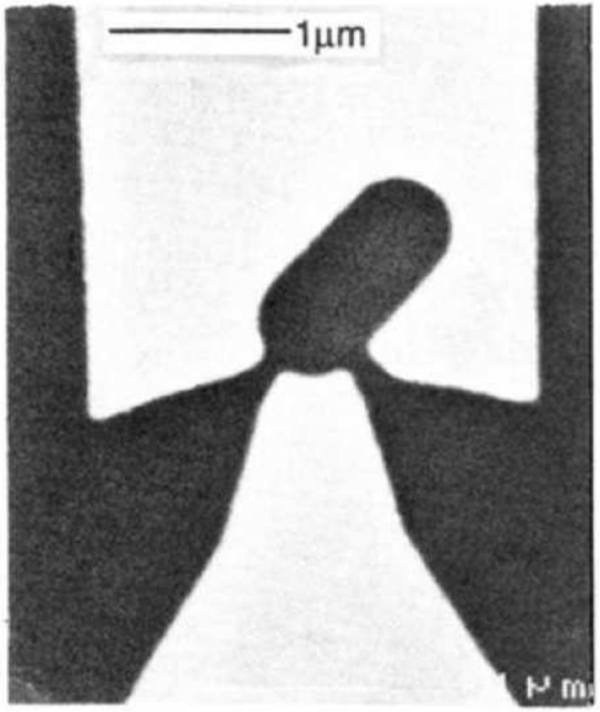
$$\lim_{j\to\infty}\int_D |\psi_{n_j}(\mathbf{x})|^2 \mathrm{d}\mathbf{x} = \frac{\text{Area } D}{\text{Area } \Omega} \tag{3}$$



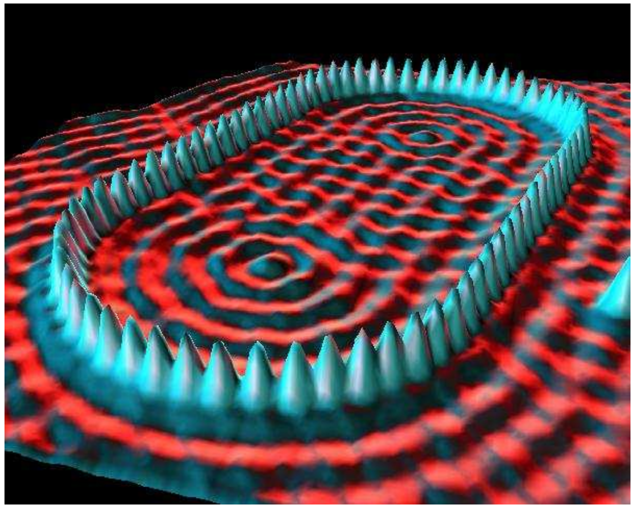
Applications:

Mesoscopic systems

Quantum dot



Quantum Corral

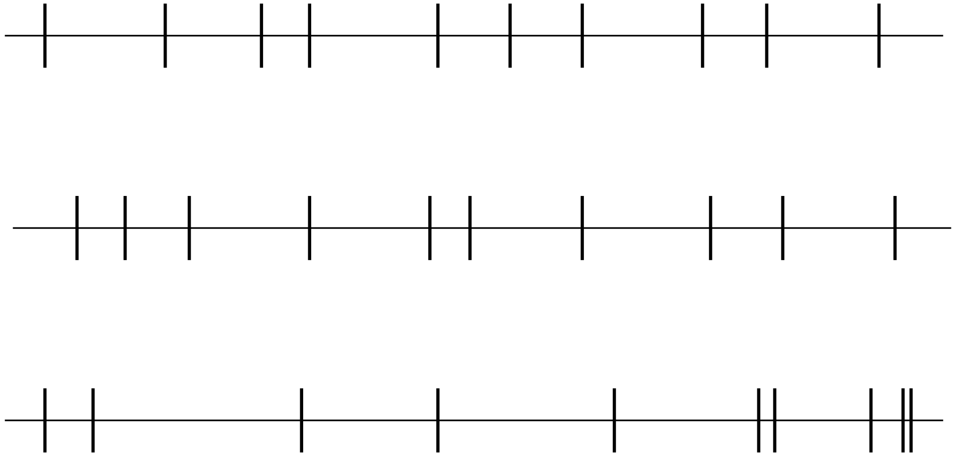


Quantum computers

Microprocessors

C. M. Marcus *et al.*, Phys. Rev. B, **48**, 2460 (1993)

STM Image Gallery: `www.almaden.ibm.com/vis/stm/corral.html`



spectrum of chaotic quantum system

eigenvalues of random matrix

uniformly distributed random numbers

The Gaussian Unitary Ensemble (GUE)

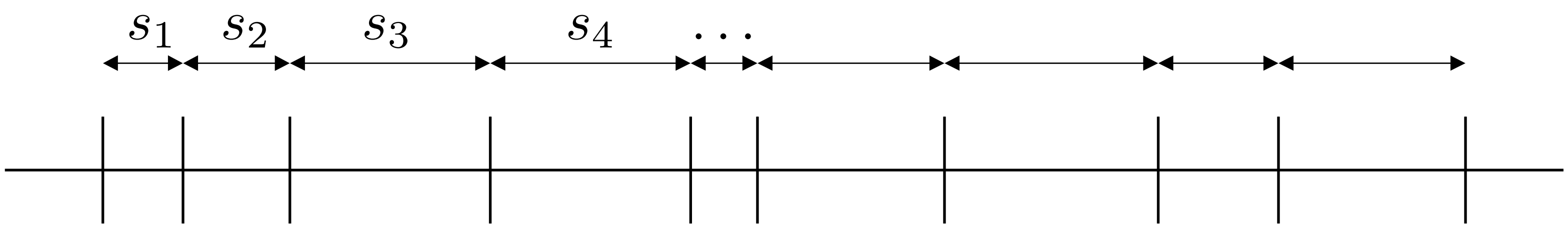
Ensemble of $N \times N$ Hermitian matrices, $H^* = H$.

- Independent matrix elements uncorrelated.
- Probability density $P(H)$ invariant under unitary transformations.

Uniquely determines $P(H) = C\mathrm{e}^{-A\,\mathrm{tr}(H^2)}$.

Eigenvalues $\lambda_1 \leqslant \lambda_2 \leqslant \cdots \leqslant \lambda_N$ real.
Scale so mean separation is one: $x_1 \leqslant x_2 \leqslant \cdots \leqslant x_N$.

Nearest neighbor spacing statistics



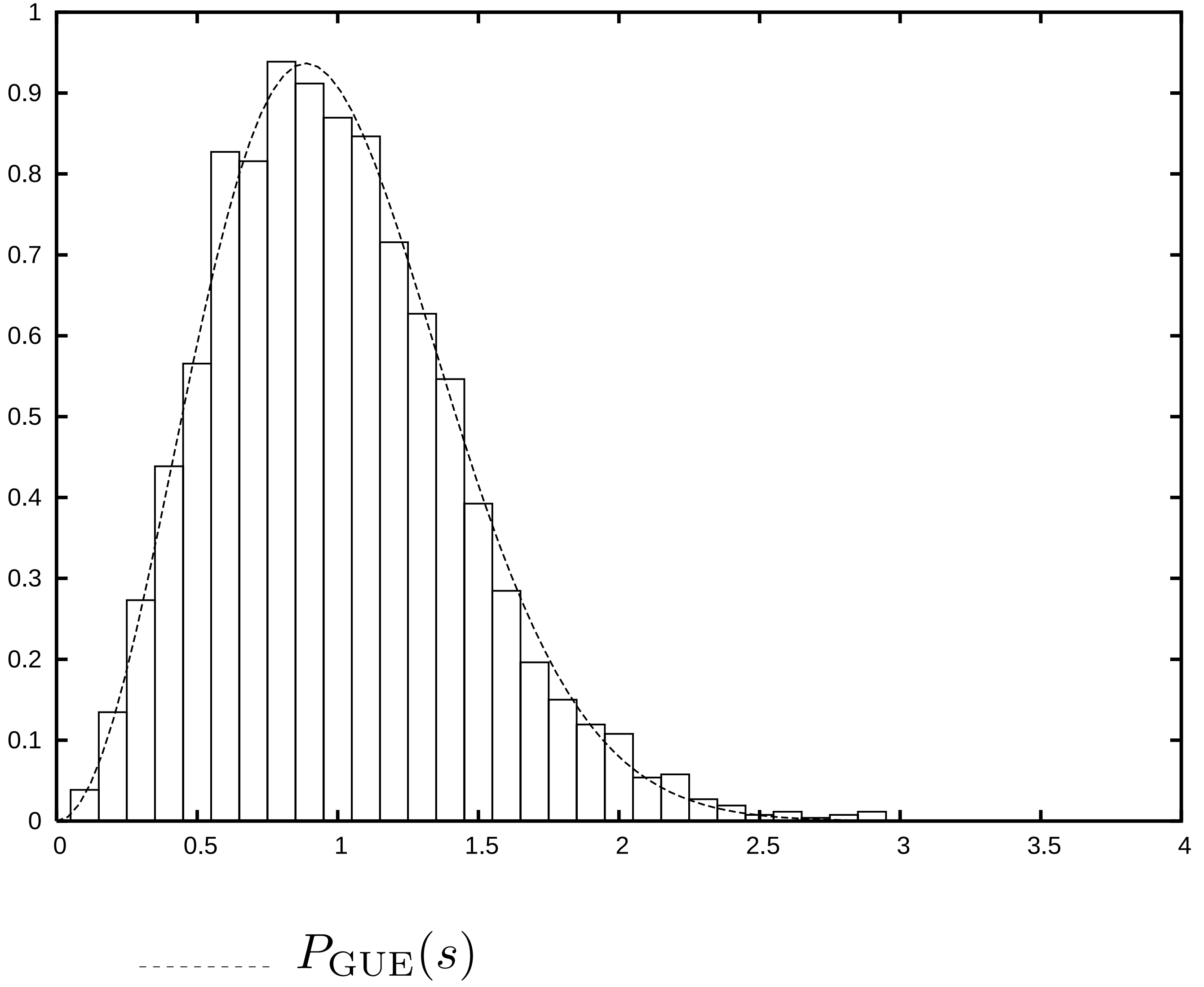
$p(s)$ probability density of spacings between consecutive eigenvalues on scale of mean spacing.

Level spacing distribution, $N \to \infty$.

$$P_{\mathrm{GUE}}(s) \approx \frac{32 s^2}{\pi^2} \mathrm{e}^{\frac{-4s^2}{\pi}} \tag{4}$$

Poisson distribution for random numbers $P_{\mathrm{Poisson}}(s) = \mathrm{e}^{-s}$.

Spacings of the eigenvalues of a large random matrix.



Conjecture: - Bohigas, Giannoni, Schmit

In the semiclassical limit energy level statistics of a quantum system whose classical analogue is chaotic correspond to eigenvalue statistics of random matrix ensembles. The ensemble of random matrices depends on the symmetries of the quantum system.

Gaussian Unitary Ensemble (GUE)	no time-reversal symmetry
Gaussian Orthogonal Ensemble (GOE)	time-reversal symm., $T^2 = \mathrm{I}$
Gaussian Symplectic Ensemble (GSE)	time-reversal symm., $T^2 = -\mathrm{I}$

Models of quantum chaos

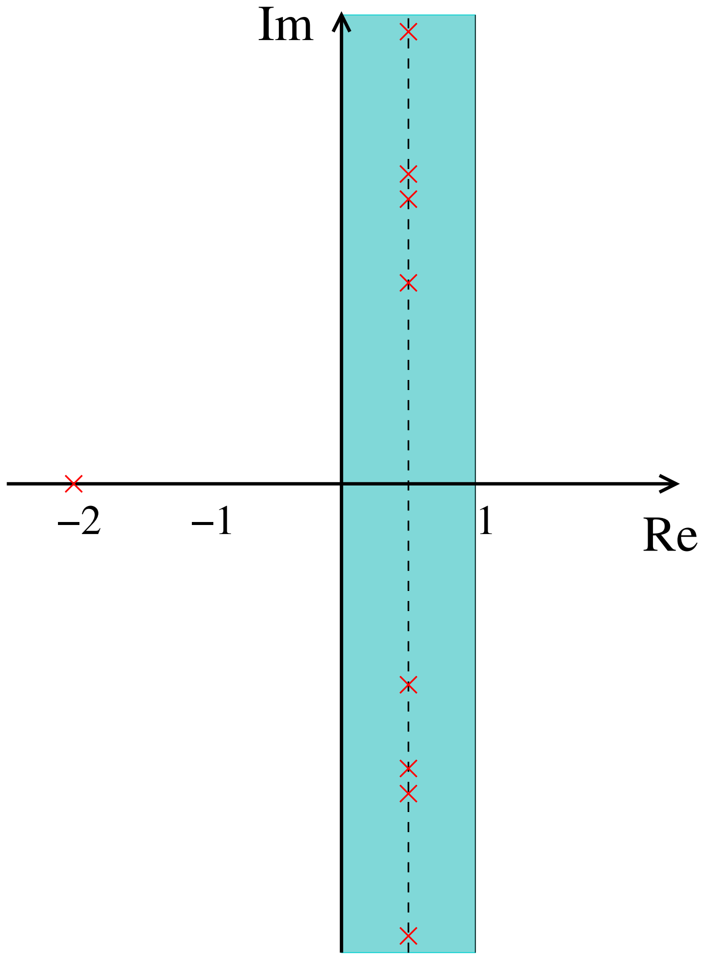
- Billiards
- Laplace-Beltrami operator on spaces of constant negative curvature
- Quantum maps: quantized automorphisms of 2-torus
- **Quantum graphs**
- Riemann zeta function

The zeta function

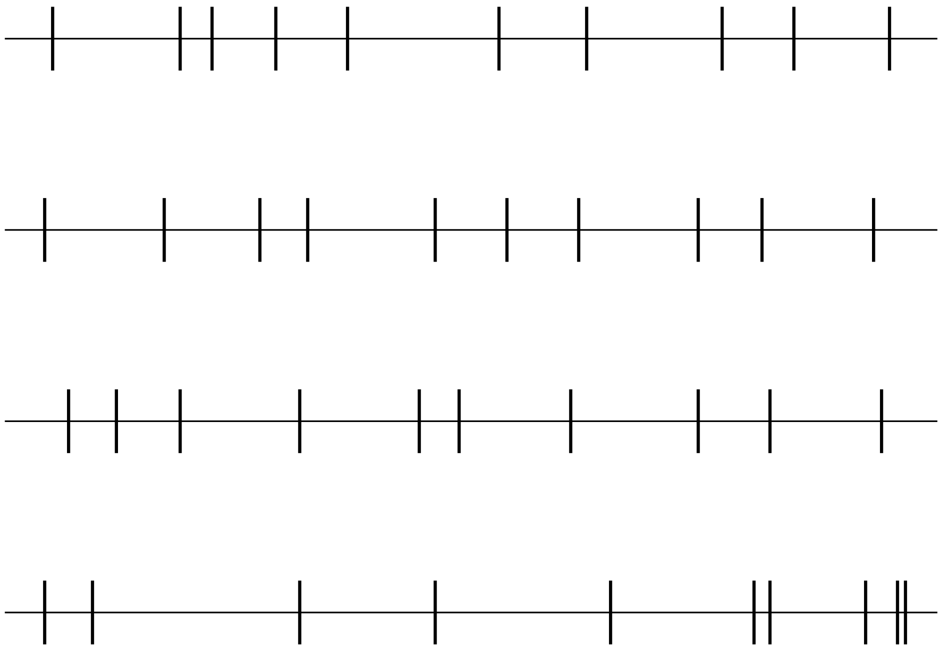
$$\zeta(s) = \prod_{p \text{ prime}} \left(1 - \frac{1}{p^s}\right)^{-1}$$

Defined for $\mathrm{Re}(s) > 1$,
analytically continued to $\mathbb{C}$.

Trivial zeros $s = -2, -4, \ldots$.
Other zeros in critical strip
$0 < \mathrm{Re}(s) < 1$.



Riemann Hypothesis: *All complex zeros lie on the line* $\mathrm{Re}(s) = \dfrac{1}{2}$.



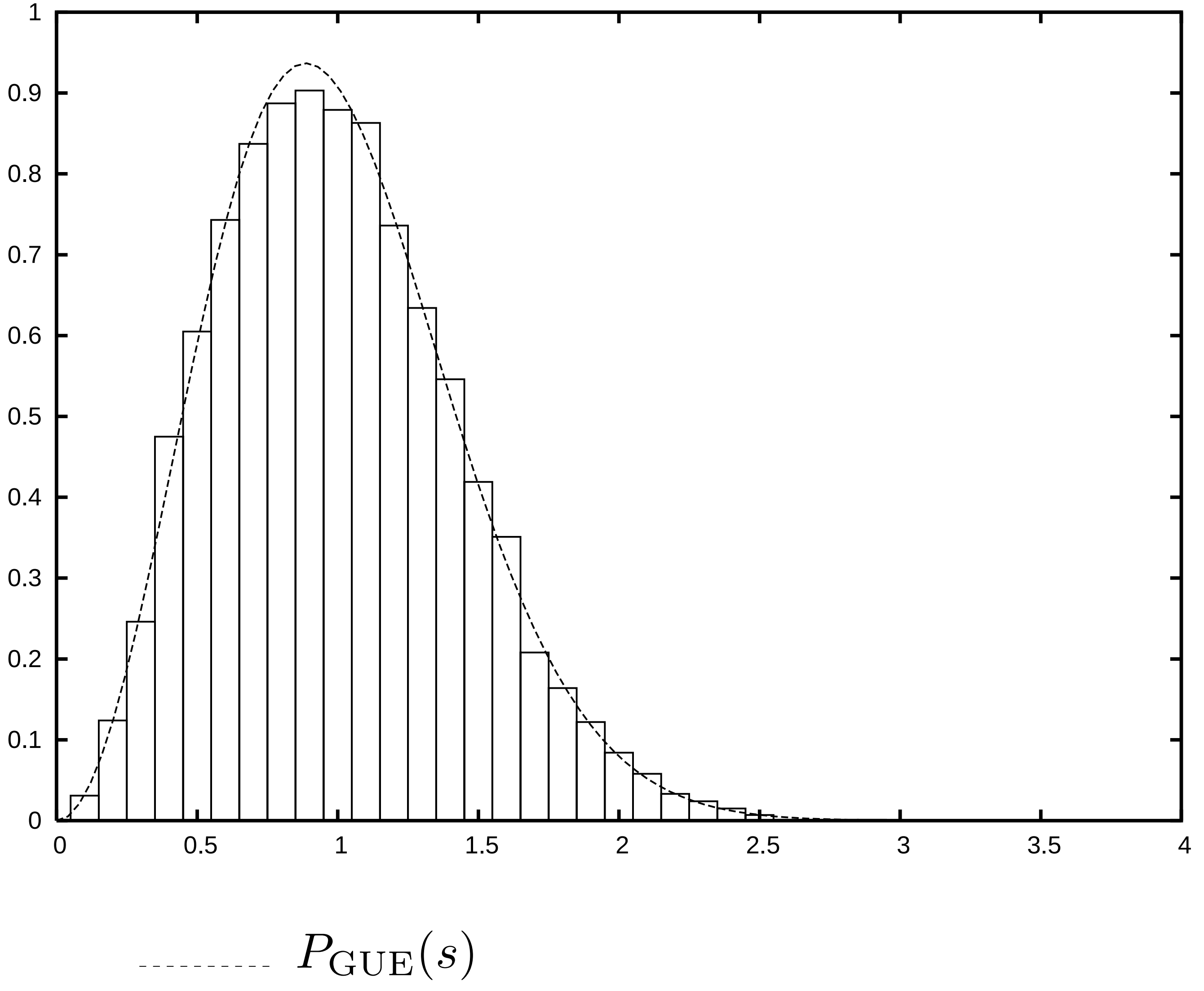
zeros of zeta

spectrum of chaotic quantum system

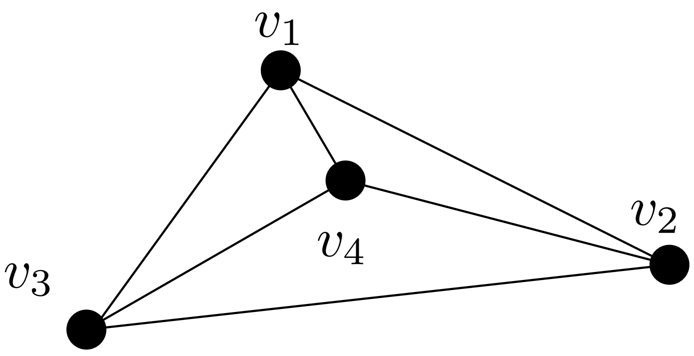
eigenvalues of random matrix

uniformly distriputed random numbers

Spacings of the zeros of zeta.



2. Metric graphs



set of vertices $V = \{v_j\}$

set of edges $E = \{e_j\}$

Metric graph Γ.

Each edge $e = (v_i, v_j)$ is an interval $[0, L_e]$.

Distance between two points $x, y \in \Gamma$ is $\rho(x, y)$.

Hilbert space

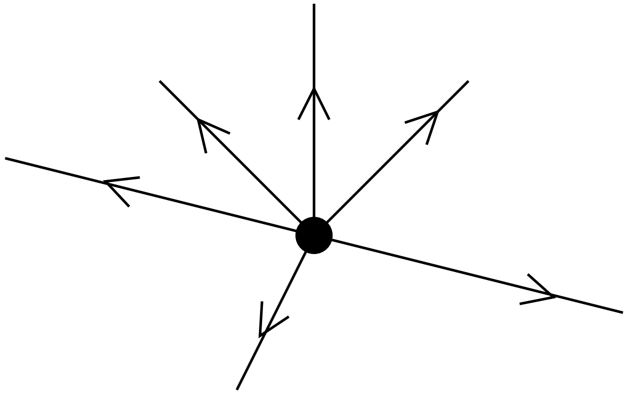
$$\mathcal{H} := \bigoplus_{e \in E} L^2\big([0, L_e]\big)$$

Laplace operator on a graph

Operator on edge $-\dfrac{\mathrm{d}^2}{\mathrm{d}x_e^2}$.

Define a domain on which the operator is self-adjoint.

Vertex boundary conditions:

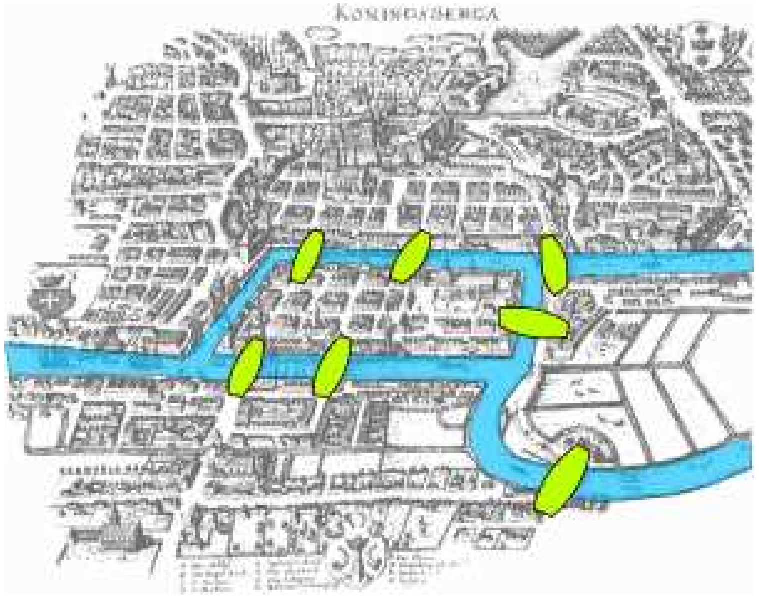


$$\mathbb{A}\boldsymbol{f}(0) + \mathbb{B}\boldsymbol{f}'(0) = \mathbf{0}$$

Theorem – Kostrykin & Schrader

The boundary conditions define a self-adjoint operator iff $\mathrm{rank}(\mathbb{A}, \mathbb{B})$ *maximal and* $\mathbb{A}\mathbb{B}^* = \mathbb{B}\mathbb{A}^*$.

Potted history of graph models



1736 Seven bridges of Königsburg - Euler

1950s Organic molecules

1980s Thin networks

1980s Photonic crystals

1997 Quantum Chaos
– Kottos & Smillansky

Dirac operator on a graph

Dirac eqn. in 1d, $\alpha\beta + \beta\alpha = 0$ and $\alpha^2 = \beta^2 = \mathrm{I}$.

$$\mathrm{i}\hbar \frac{\partial}{\partial t}\mathbf{\Psi}(x,t) = \left(-\mathrm{i}\hbar c\,\alpha\,\frac{\partial}{\partial x} + mc^2\,\beta\right)\mathbf{\Psi}(x,t) \tag{5}$$

e.g. $\alpha = \begin{pmatrix} 0 & -\mathrm{i} \\ \mathrm{i} & 0 \end{pmatrix}$ $\beta = \begin{pmatrix} 1 & 0 \\ 0 & -1 \end{pmatrix}$

Boundary conditions: $\mathbb{A}\boldsymbol{\psi}_1 + \mathbb{B}\boldsymbol{\psi}_2 = \mathbf{0}$

$$\boldsymbol{\psi}_1 := \left(\psi_1^1(0), \ldots, \psi_1^{|E|}(0), \psi_1^1(L_1), \ldots, \psi_1^{|E|}(L_{|E|})\right)^T$$

$$\boldsymbol{\psi}_2 := \left(\psi_2^1(0), \ldots, \psi_2^{|E|}(0), -\psi_2^1(L_1), \ldots, -\psi_2^{|E|}(L_{|E|})\right)^T$$

Theorem – J. Bolte & J. H.

The boundary conditions define a self-adjoint realization of the Dirac operator iff $\mathrm{rank}(\mathbb{A}, \mathbb{B})$ *maximal and* $\mathbb{A}\mathbb{B}^* = \mathbb{B}\mathbb{A}^*$.

3. The Quantum graph trace formula

Eigenvalue problem on an edge

$$-\frac{\mathrm{d}^2}{\mathrm{d}x_e^2}\psi_j(x_e) = k_j^2\,\psi_j(x_e)$$

Theorem – Roth, Kottos & Smilansky

$$\sum_{j\in\mathbb{Z}} h(k_j) = \frac{L}{\pi}\int_{-\infty}^{\infty} h(k)\mathrm{d}k + \frac{1}{\pi}\sum_p \frac{L_p}{r_p} A_p \hat{h}(L_p) + Ch(0) \qquad (6)$$

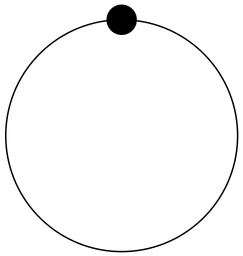
$p=(e_1,\ldots,e_n)$ periodic orbit on Γ, L_p length of p, $L=\sum_{e\in E} L_e$.

A_p product of transition amplitudes σ at vertices of p.

$$A_p = \sigma_{e_1e_2}\sigma_{e_2e_3}\ldots\sigma_{e_ne_1} \qquad (7)$$

Poisson summation formula $\sum_{j\in\mathbb{Z}} h(j) = \sum_{p\in\mathbb{Z}} \hat{h}(2\pi p)$.

This is the trace formula for a graph with a single edge $L = 2\pi$.



Trace formula for Dirac operator – J. Bolte & J. H.

$$\sum_{j\in\mathbb{Z}} h(k_j) = \frac{2L}{\pi}\int_{-\infty}^{\infty} h(k)\mathrm{d}k + \frac{1}{\pi}\sum_{p}\frac{L_p}{r_p}A_p \mathrm{tr}(d_p)\hat{h}(L_p) + Ch(0) \tag{8}$$

$$d_p = u_{e_1e_2}u_{e_2e_3}\dots u_{e_ne_1} \qquad d_p, u \in \mathrm{SU}(2) \tag{9}$$

u_{ef} spin rotation from e to f.

Classical dynamics on graphs

The Quantum graph defines transition amplitudes σ_{ef}.

$$M_{ef} = |\sigma_{ef}|^2 \tag{10}$$

The matrix Σ is unitary (equivalent to current conservation).
Consequently M is doubly stochastic

– rows and columns sum to one.

M defines a Markov chain on the graph.

$$\rho_{n+1} = M\rho_n \tag{11}$$

Chaotic properties:

For a connected graph the Markov chain is **ergodic**, $(M^q)_{ef} > 0$ for some q.

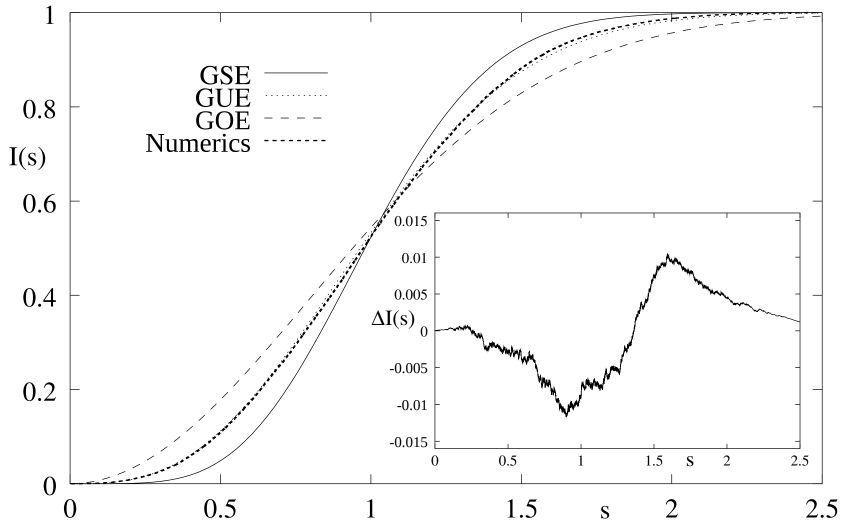
M has an eigenvalue 1. If there are no other eigenvalues on the unit circle the graph is **mixing**:

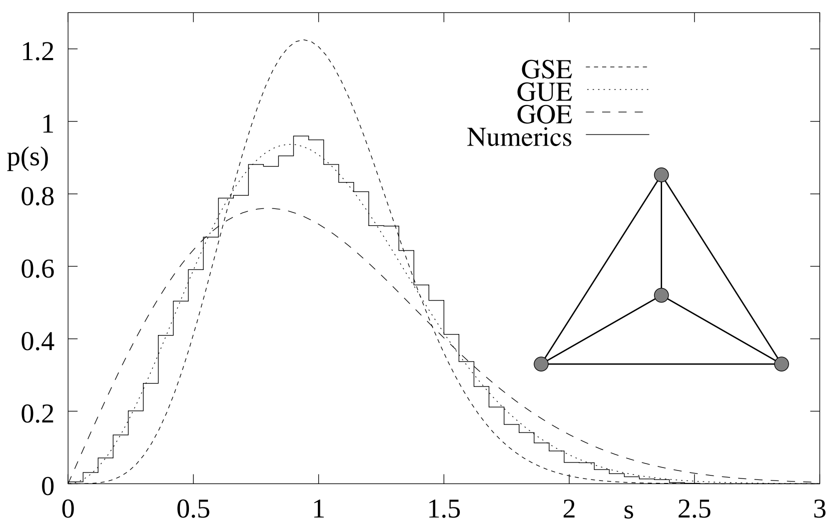
$$\lim_{n\to\infty} M^n \rho = \frac{1}{2|E|}(1,\ldots,1)^T \quad \text{or} \quad \lim_{n\to\infty} (M^n)_{ef} = \frac{1}{2|E|} \tag{12}$$

Note: for P_n the set of periodic orbits of length n,

$$n \sum_{p\in P_n} |A_p|^2 = \operatorname{tr} M^n = 1 \ . \tag{13}$$

Nearest neighbor spacing distributions for a quantum graph
no time-reversal symmetry, 25275 levels.





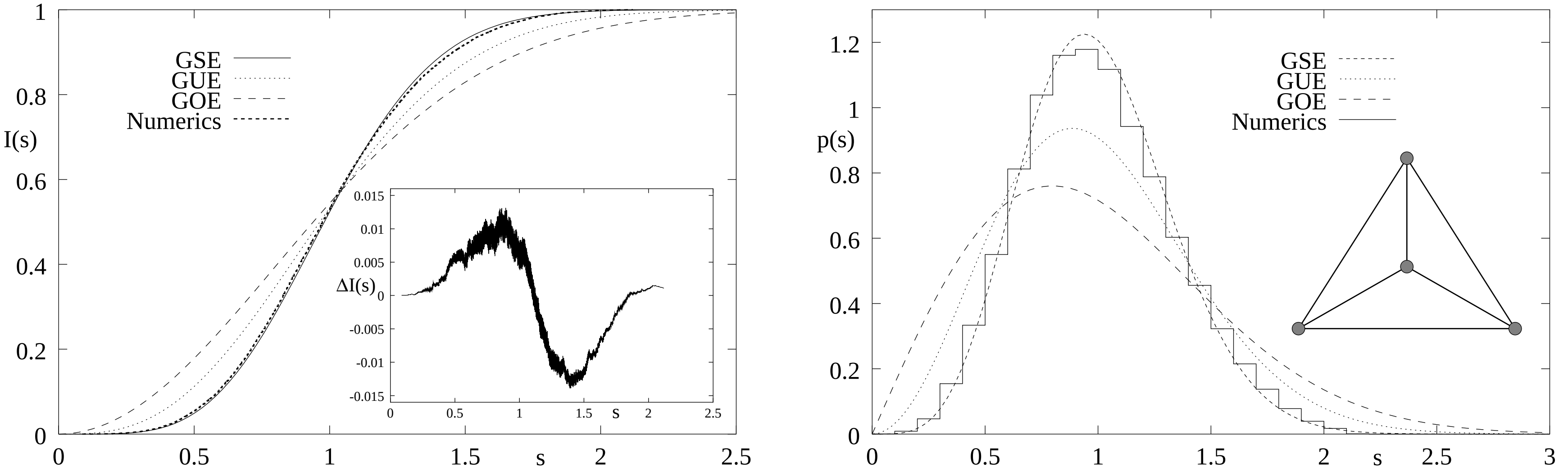
Time-reversal symmetry

For the Schrödinger eqn. the time-reversal operator is complex conjugation. Time-reversal symmetry implies $\sigma_{ef} = \sigma_{\overline{f}\overline{e}}$. Conjectured GOE spectral statistics.

For the Dirac equation the time-reversal operator squares to $-\mathrm{I}$. Time-reversal symmetry implies $\sigma_{ef} = \sigma_{\overline{f}\overline{e}}$ and $u_{ef} = u_{\overline{f}\overline{e}}^{-1}$. Conjectured GSE spectral statistics.

Nearest neighbor spacing distributions for the Dirac op.

Time-reversal symmetric, 24233 levels.



4. The form factor

Unfolded spectrum $\cdots \leqslant x_0 \leqslant x_1 \leqslant x_2 \leqslant \ldots$

Two point correlation function

$$R_2(x) = \lim_{\Lambda\to\infty} \frac{1}{\Lambda} \int_0^\Lambda \left(\sum_{i=-\infty}^{\infty} \delta(y - x_i) \right) \left(\sum_{j=-\infty}^{\infty} \delta(y - x - x_j) \right) \mathrm{d}y \tag{14}$$

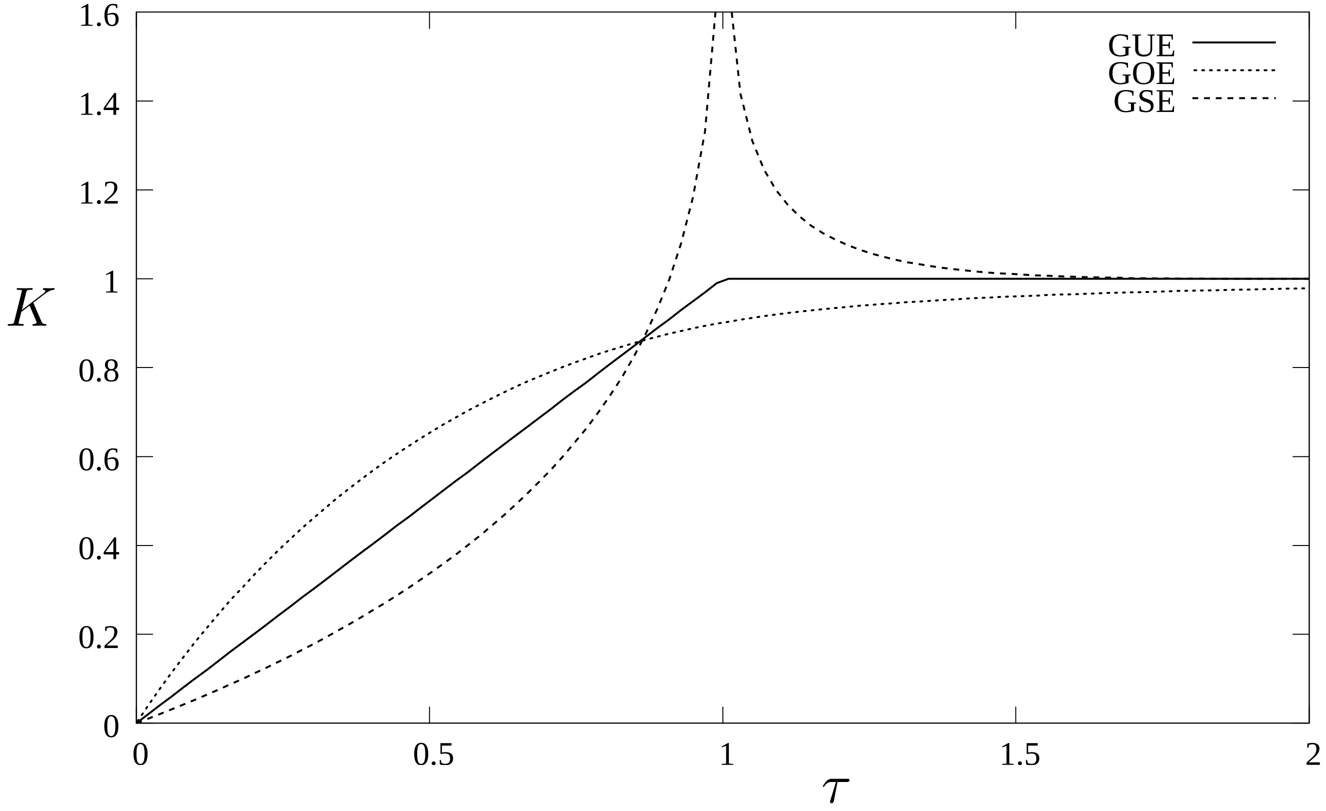
Form factor

$$K_2(\tau) = \int_{-\infty}^{\infty} R_2(x) \mathrm{e}^{2\pi \mathrm{i} x \tau} \mathrm{d}x \tag{15}$$

$$\approx \frac{1}{\Lambda} \left| \sum_{n=1}^{\Lambda} \mathrm{e}^{2\pi \mathrm{i} x_n \tau} \right|^2 \tag{16}$$

$(0, \Lambda)$ is an interval containing approx Λ eigenvalues.

$$K_{\mathrm{Poisson}}(\tau) \approx \begin{cases} \Lambda & \tau = 0 \\ 1 & \text{otherwise} \end{cases} \qquad K_{\mathrm{GUE}}(\tau) = \begin{cases} \tau & 0 < \tau \leq 1 \\ 1 & 1 \geq \tau \end{cases}$$



Quantum graph Form Factor

$$K(\tau) = \frac{1}{4(2L)^2} \sum_{p,q} \frac{L_p L_q}{r_p r_q} A_p A_q^* \mathrm{tr}(d_p)\, \mathrm{tr}(d_q) \delta\left(\tau - \frac{L_p}{2L}\right) \delta_{L_p, L_q} \quad (17)$$

Diagonal approximation - *Berry, Hannay & Ozorio de Almeida*
Evaluate sum for orbit pairs with $p = q$.
(Also assume $r_p = 1, L_p \approx n\overline{L}$.)

$$\begin{aligned} K(\tau) &= \sum_n \left(\frac{n}{2|E|}\right)^2 \delta\left(\tau - \frac{n}{2|E|}\right) \sum_{p \in P_n} A_p^2 \\ &\sim \sum_n \frac{1}{2|E|} \frac{n}{2|E|} \delta\left(\tau - \frac{n}{2|E|}\right) \\ &\sim \tau \end{aligned} \quad (18)$$

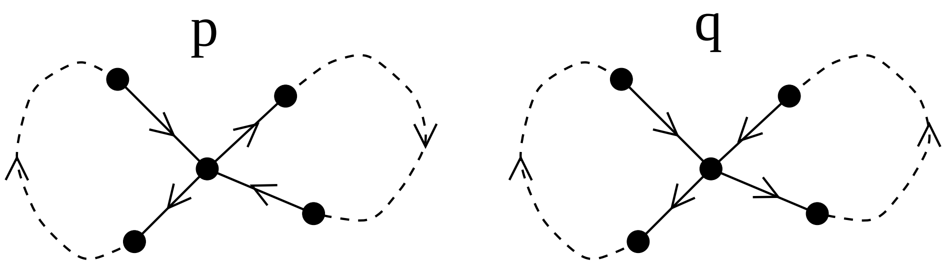
In limit $L \to \infty$, $\tau \to 0$ with $L\tau \to \infty$.
Used classical dynamics mixing, $\lim_{n \to \infty} \sum_{p \in P_n} A_p^2 = \frac{1}{n}$.

Let $G \subset \mathrm{SU}(2)$ with $R(G)$ an irreducible representation.

Theorem – J. Bolte & J. H.

$$\frac{1}{|G|^n} \sum_{u_{b_1} \in G} \cdots \sum_{u_{b_n} \in G} \mathrm{tr}(R(d_p))\, \mathrm{tr}(R(d_q)) = \left(\frac{c_R}{2}\right)^t$$

where t is the number of self-intersections at which the orbit p has been rearranged to produce q. $C_R = 1$ if R is a real representation and $C_R = -1$ if R is quaternionic.



A pair of orbits where q is obtained from p by rearranging the order of edges at a single self-intersection.

RMT correspondence

For u chosen randomly from a quaternionic representation the contribution to the form factor is $\left(-\frac{1}{2}\right)^{t+2}$ multiplied by the contribution to the form factor of the Laplacian for the same set of orbit pairs.

This is consistent with the relationship between form factors of the GSE and GOE of random matrices with the hypothesis that orbit pairs reordered at t self intersections contribute to the power series expansion at order $t+1$ – (*Sieber/Sieber & Richter*).

$$K_{\mathrm{GSE}}(\tau) = \frac{\tau}{2} + \frac{\tau^2}{4} + \frac{\tau^3}{8} + \frac{\tau^4}{12} + \dots \ ,$$
$$\frac{1}{2}K_{\mathrm{GOE}}\left(\frac{\tau}{2}\right) = \frac{\tau}{2} - \frac{\tau^2}{4} + \frac{\tau^3}{8} - \frac{\tau^4}{12} + \dots \ .$$

Other graph models

k_j^2 eigenvalue of quantum graph.

- Vacuum energy E_c, constant term in asymptotic expansion of

$$\frac{1}{2}\sum_{j=0}^{\infty} k_j \mathrm{e}^{tk_j} \ .$$

Using the trace formula,

$$E_c = -\frac{1}{2\pi}\sum_p \frac{A_p}{L_p r_p} \ . \tag{19}$$

- Chiral condensate

Conclusions:

- Quantum graphs are a simple model for complex spectral problems.
- In the semi-classical limit spectral statistics and eigenfunction behaviour prefigure classical chaos.
- Random matrix behaviour for systems with spin are expected when the spin transformations form an irreducible quaternionic representation of $G \subset \mathrm{SU}(2)$.

Future work:

- Precise conditions for RM behaviour of quantum graph spectra.
- Examples of intermediate statistics for systems with spin.
- Quantum ergodicity of eigenfunctions on a graph.
- Develop other graph models.