The variance of coefficients of the characteristic polynomial of regular quantum graphs

Jon Harrison¹ and Tori Hudgins²

¹Baylor University, ²University of Kansas

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Dynamical approach to spectral statistics

- '71 Gutzwiller's trace formula for the density of states in the semiclassical limit.
- '85 Berry Diagonal approximation to the form factor using Hannay-Ozorio de Almeida sum rule.
- '99 Kottos and Smilansky trace formula for the density of states of quantum graphs.
- '01 Sieber and Richter 2nd order contribution to the small parameter asymptotics of the form factor from figure 8 orbits with one self-intersection.
- '03 Berkolaiko, Schanz and Whitney 2nd and 3rd order contributions on quantum graphs.
- '04 Müller, Heusler, Braun, Haake and Altland all higher order contributions.



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- Assign unitary vertex scattering matrix $\sigma^{(v)}$ to each vertex v.

A democratic choice is the discrete Fourier transform matrix,

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Quantum evolution op. $U(k) = \Sigma e^{ikL}$, with $L = \text{diag}\{L_1, \ldots, L_B\}$, defines a unitary stochastic matrix ensemble - Tanner '01.

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Characteristic polynomial of $\mathbf{U}(k)$

$$\det \left(\mathsf{U}\left(k\right) - \zeta \mathsf{I} \right) = \sum_{n=0}^{B} a_n(k) \zeta^{B-n}$$

- Secular equation det $(\mathbf{U}(k) \mathbf{I}) = 0$.
- Riemann-Siegel lookalike formula, $a_n = a_{B-n}^*$ Kottos and Smilansky '99
- Variance of coeffs of characteristic polynomial of binary graphs in semiclassical limit using a diagonal approximation
 - Tanner '02, Band-Harrison-Sepanski '19

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- A *periodic orbit* γ = (b₁,..., b_m) is the equivalence class of closed paths under cyclic shifts, t(b_j) = o(b_{j+1}).
- A *primitive periodic orbit* is a periodic orbit that is not a repetition of a shorter orbit.
- Topological length of γ is m.
- Metric length of γ is $L_{\gamma} = \sum_{b_i \in \gamma} L_{b_i}$.
- Stability amplitude is $A_{\gamma} = \sum_{b_2 b_1} \sum_{b_3 b_2} \dots \sum_{b_m b_{m-1}} \sum_{b_1 b_m}$.



• A *pseudo orbit* $\bar{\gamma} = \{\gamma_1, \dots, \gamma_M\}$ is a set of periodic orbits.

- $m_{\bar{\gamma}} = M$ no. of periodic orbits in $\bar{\gamma}$.
- Metric length $L_{\bar{\gamma}} = \sum_{j=1}^{M} L_{\gamma_j}$.
- Stability amplitude $A_{\bar{\gamma}} = \prod_{j=1}^{M} A_{\gamma_j}$.
- A *primitive pseudo orbit (PPO)* is a set of distinct primitive periodic orbits.
- \mathcal{P}^n set of PPO with *n* bonds.

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Theorem 1 (Band-Harrison-Joyner '12)

Coefficients of the characteristic polynomial are given by,

$$\mathsf{a}_n = \sum_{ar{\gamma}\in\mathcal{P}^n} \left(-1
ight)^{m_{ar{\gamma}}} \mathsf{A}_{ar{\gamma}} e^{i\mathsf{k} \mathsf{L}_{ar{\gamma}}} \; .$$

Idea

- Expand det $(\mathbf{U}(k) \zeta \mathbf{I})$ as a sum over permutations.
- A permutation ρ ∈ S_B can contribute iff ρ(b) is adjacent to b for all b in ρ.
- Representing ρ as a product of disjoint cycles each cycle is a primitive periodic orbit.

Variance of coefficients of the characteristic polynomial

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$$\langle a_n \rangle = \begin{cases} 1 & n = 0\\ 0 & \text{otherwise} \end{cases}$$

$$\langle |a_n|^2 \rangle_k = \sum_{\bar{\gamma}, \bar{\gamma}' \in \mathcal{P}^n} (-1)^{m_{\bar{\gamma}} + m_{\bar{\gamma}'}} A_{\bar{\gamma}} \bar{A}_{\bar{\gamma}'} \lim_{K \to \infty} \frac{1}{K} \int_0^K e^{ik(L_{\bar{\gamma}} - L_{\bar{\gamma}'})} dk$$

$$= \sum_{\bar{\gamma}, \bar{\gamma}' \in \mathcal{P}^n} (-1)^{m_{\bar{\gamma}} + m_{\bar{\gamma}'}} A_{\bar{\gamma}} \bar{A}_{\bar{\gamma}'} \delta_{L_{\bar{\gamma}}, L_{\bar{\gamma}'}}$$
(3)

Diagonal contribution

 $\bar{\gamma}, \bar{\gamma}' \in \mathcal{P}^n$

$$\langle |\boldsymbol{a}_n|^2
angle_{\mathrm{diag}} = \sum_{\bar{\gamma} \in \mathcal{P}^n} |\boldsymbol{A}_{\bar{\gamma}}|^2 = 2^{-n} |\mathcal{P}^n| \; .$$

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Theorem 2 (Harrison-Hudgins '22)

For a 4-regular quantum graph with $\{L_b\}$ incommensurate,

$$\langle |a_n|^2 \rangle = \frac{1}{2^n} \left(|\mathcal{P}_0^n| + \sum_{N=1}^n 2^N |\widehat{\mathcal{P}}_N^n| \right)$$

where $\mathcal{P}_0^n \subset \mathcal{P}^n$ with no self-intersections and $\widehat{\mathcal{P}}_N^n \subset \mathcal{P}^n$ with N self-intersections, all of which are 2-encounters of length zero.

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Self-intersections



- 2-encounter: $\bar{\gamma} = (\gamma_1, \dots, \gamma_m)$ with no self-intersections in $\gamma_2, \dots, \gamma_m$ and $\gamma_1 = (1, 2)$, link 1 followed by link 2.
- 3-encounter: Define $\bar{\gamma}$ similarly but with $\gamma_1 = (1, 2, 3)$.
- Encounter *length zero* if it contains no bonds, $v_0 = v_r$.

Example: Binary de Bruijn graph with $B = 2^4$



п	$ \mathcal{P}_0^n $	$ \widehat{\mathcal{P}}_1^n $	$ \widehat{\mathcal{P}}_2^n $	$\langle a_n ^2 \rangle$	Numerics	Error
0	1	0	0	1	1.000000	0.000000
1	2	0	0	1	0.999991	0.000009
2	2	0	0	1/2	0.499999	0.000001
3	4	0	0	1/2	0.499999	0.000001
4	8	0	0	1/2	0.499999	0.000001
5	8	8	0	3/4	0.749998	0.000002
6	8	20	0	3/4	0.749986	0.000014
7	16	16	8	5/8	0.624989	0.000011
8	16	16	24	9/16	0.562501	-0.000001

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Figure 1: Variance of coefficients of the characteristic polynomial for the family of 4-regular binary de Bruijn graphs with 2^r vertices.

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Example: Binary graph with $B = 3 \cdot 2^2$



n	$ \mathcal{P}_0^n $	$ \widehat{\mathcal{P}}_1^n $	$\langle a_n ^2 \rangle$	Numerics	Error
0	1	0	1	1.000000	0.000000
1	2	0	1	1.000000	0.000000
2	3	0	3/4	0.750001	-0.000001
3	6	0	3/4	0.750003	-0.000003
4	10	4	7/8	0.874999	0.000001
5	8	4	1/2	0.499998	0.000002
6	8	8	3/8	0.374999	0.000001

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Figure 2: Variance of coefficients of the characteristic polynomial for the family of 4-regular binary graphs with $3 \cdot 2^r$ vertices.

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The sum over PPO can be replaced by a sum over *irreducible* pseudo orbits where no bonds are repeated $\widehat{\mathcal{P}}^n$.

where $\mathcal{P}_{\bar{\gamma}}$ is the set of irreducible PPO length $L_{\bar{\gamma}}$.

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• A PPO with a single 2-encounter length zero if $\bar{\gamma}' \neq \bar{\gamma}$ then $m_{\bar{\gamma}'} = m_{\bar{\gamma}} \pm 1$ and $\bar{A}_{\bar{\gamma}'} = -A_{\bar{\gamma}}$, hence $C_{\bar{\gamma}} = 2 \cdot 2^{-n}$.

- For quantum graphs the semiclassical limit is the limit of a sequence of graphs with B → ∞.
- For the variance fix *n*/*B* and consider long orbits on large graphs.

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- For quantum graphs the semiclassical limit is the limit of a sequence of graphs with $B \rightarrow \infty$.
- For the variance fix n/B and consider long orbits on large graphs.
- In the semiclassical limit half of PPO with a single 2-encounter have encounter length zero, as the probability to follow the orbit at the initial encounter vertex is 1/2.

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$$\langle |\boldsymbol{a}_n|^2 \rangle = 2^{-n} \left(|\mathcal{P}_0^n| + \sum_{N=1}^n 2^N |\widehat{\mathcal{P}}_N^n| \right) \approx 2^{-n} \sum_{N=0}^n |\mathcal{P}_N^n| = 2^{-n} |\mathcal{P}^n|$$



• For 4-regular graphs the variance only depends on primitive pseudo orbits where all self-intersections are 2-encounters of length zero.

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- To extend results to 2k-regular graphs requires averaging over assignments of the vertex scattering matrices.

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- J.M. Harrison and T. Hudgins, "Complete dynamical evaluation of the characteristic polynomial of binary quantum graphs," *J. Phys. A* **55** (2022) 425202 arXiv:2011.05213
- J.M. Harrison and T. Hudgins, "Periodic-orbit evaluation of a spectral statistic of quantum graphs without the semiclassical limit," *EPL* **138** (2022) 30002 arXiv:2101.00006
- R. Band, J. M. Harrison and C. H. Joyner, "Finite pseudo orbit expansions for spectral quantities of quantum graphs," J. Phys. A 45 (2012) 325204 arXiv:1205.4214

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