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Lyndon word decompositions and pseudo orbits on q-nary graphs

R. Band [a,*], J.M. Harrison [b], M. Sepanski [b]

[a] Department of Mathematics, Technion – Israel Institute of Technology, Haifa 32000, Israel
[b] Department of Mathematics, Baylor University, Waco, TX 76798, USA

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ABSTRACT

A foundational result in the theory of Lyndon words (words that are strictly earlier in lexicographic order than their cyclic permutations) is the Chen–Fox–Lyndon theorem which states that every word has a unique non-increasing decomposition into Lyndon words. This article extends this factorization theorem, obtaining the proportion of these decompositions that are strictly decreasing. This result is then used to count primitive pseudo orbits (sets of primitive periodic orbits) on q-nary graphs. As an application we obtain a diagonal approximation to the variance of the characteristic polynomial coefficients of q-nary quantum graphs.

1. Introduction

A fundamental tool used to understand the combinatorics of words is the Lyndon factorization [5] (see also Ref. [11]); every word has a unique standard decomposition into a non-increasing sequence of Lyndon words. Lyndon words being those words that occur strictly earlier in lexicographic order than any of their rotations.

So, for example, the Lyndon words on the binary alphabet with length ≤ 3 arranged in lexicographic order are

$$0 <_{\text{lex}} 001 <_{\text{lex}} 01 <_{\text{lex}} 011 <_{\text{lex}} 1\ . \tag{1}$$

And the unique standard decompositions of the binary words of length 3 into non increasing sequences of Lyndon words are,

$$(0)(0)(0),\quad (\mathbf{001}),\quad (\mathbf{01})(\mathbf{0}),\quad (\mathbf{011}),\quad (1)(0)(0),\quad (\mathbf{1})(\mathbf{01}),\quad (1)(1)(0),\quad (1)(1)(1). \tag{2}$$

* Corresponding author.
E-mail addresses: ramband@technion.ac.il (R. Band), jon_harrison@baylor.edu (J.M. Harrison), mark_sepanski@baylor.edu (M. Sepanski).

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The Lyndon factorization finds applications in diverse problems from the theory of free Lie algebras [11], to quasi-symmetric functions [8] and data compression techniques [12]. In this article we extend this foundational result to obtain the proportion of the standard decompositions that are strictly decreasing, so the standard decomposition has no repetitions. For words of a fixed length on an alphabet of q letters the proportion that have strictly decreasing Lyndon factorizations is shown to be $(q-1)/q$, independent of the word length. Returning to the example above, the strictly decreasing standard decompositions of binary words length of 3 in (2) are indicated in bold, we see half, $(2-1)/2$, of the standard decompositions are strictly decreasing.

The remainder of the article applies this new combinatorial result to a problem in the field of quantum chaos. We focus on quantum graphs, which are a widely studied model of quantum chaos introduced by Kottos and Smilansky [9,10]. Quantum graphs are also used in other diverse areas of mathematical physics including Anderson localization, microelectronics, nanotechnology, photonic crystals and superconductivity, see Ref. [2,6] for an introduction. In Ref. [1] the authors showed that spectral properties of quantum graphs are precisely encoded in finite sums over collections of primitive periodic orbits called primitive pseudo orbits. Here, we introduce graph families which we call q-nary graphs, where there is a bijection between primitive pseudo orbits on those graphs and strictly decreasing standard decompositions.

The spectrum of the graph is encoded in the characteristic polynomial of the quantum evolution operator, defined in terms of the scattering matrices at the vertices, see section 5. It was shown in Ref. [1] that the coefficients of the characteristic polynomial a_n can be expressed as a sum over primitive pseudo orbits of the graph. It is the variance of these coefficients, averaged over the spectral parameter, which we treat for families of q-nary graphs. A q-nary graph has vertices labeled by words of length m on an alphabet of q letters. By counting the number of strictly decreasing standard decompositions we obtain a diagonal approximation for the variance,

$$\langle |a_n|^2 \rangle_{\mathrm{diag}} = \frac{q-1}{q} \ . \tag{3}$$

This can be compared to the corresponding random matrix result [7],

$$\langle |a_n|^2 \rangle_{\mathrm{CUE}} = 1 \ . \tag{4}$$

The grounds for such a comparison is the Bohigas–Giannoni–Schmidt conjecture [4] which asserts that typically the spectrum of a classically chaotic quantum system corresponds, in the semiclassical limit, to that of an ensemble of random matrices determined by the symmetries of the quantum system. In quantum mechanics the semiclassical limit is the limit of large energies or equivalently the limit $\hbar \to 0$. The appropriate semiclassical limit for graphs is a limit of a sequence of graphs with increasing number of edges, which corresponds to increasing the length of the words labeling the vertices m. The deviation we see from random matrix theory is consistent with previous investigations of the variance [10,15,16]. From our result it is clear that the deviation does not vanish for a given family of q-nary graphs in the semiclassical limit. However, the discrepancy would disappear for a sequence of graphs where the degree of the vertices increases, which is equivalent to increasing q. This suggests that random matrix results for the variance may be recovered under stronger conditions than those typically required for other spectral properties.

The article is laid out as follows. In Section 2 we introduce the terminology associated with Lyndon factorizations. In Section 3 we count the number of strictly decreasing standard decompositions (Theorem 2) which is a main result of this article. In Section 4 we introduce q-nary graphs which are families of directed graphs and use Theorem 2 to count the primitive pseudo orbits on these graphs. Section 5 describes how coefficients of the graph's characteristic polynomial can be expressed as finite sums over primitive pseudo orbits. In Section 6 we apply the primitive pseudo orbit count to obtain a diagonal approximation for the variance of coefficients of the characteristic polynomial of q-nary quantum graphs and compare it to predictions from random matrix theory.

2. Introduction to Lyndon words

In this article we consider factorizations of words over a totally ordered alphabet $\mathcal{A}$ of q letters. The lexicographic order of words is defined in the following natural way. Let,

$$w = a_1 a_2 \dots a_l \tag{5}$$

$$w' = b_1 b_2 \dots b_k \tag{6}$$

with $a_i, b_j \in \mathcal{A}$. Then $w >_{\text{lex}} w'$ iff there exists $i \leq \min\{l, k\}$ such that $a_1 = b_1, \dots, a_{i-1} = b_{i-1}$ and $a_i > b_i$ or $l > k$ and $a_1 = b_1, \dots, a_k = b_k$.

Two words, w and w' are said to be conjugate if $w = uv$ and $w' = vu$ for some words u and v. Hence, two words are conjugate if and only if one may be obtained as a rotation (or cyclic shift) of the other and conjugacy is clearly an equivalence relation. A word is a *Lyndon* word if it is strictly less than all other words in its conjugacy class. So, going back to the binary example, the Lyndon words on the binary alphabet with length ≤ 4 are

$$0 <_{\text{lex}} 0001 <_{\text{lex}} 001 <_{\text{lex}} 0011 <_{\text{lex}} 01 <_{\text{lex}} 011 <_{\text{lex}} 0111 <_{\text{lex}} 1 \ . \tag{7}$$

For a fixed alphabet we denote the set of Lyndon words of length l by $\text{Lyn}_q(l)$ and $L_q(l) = |\text{Lyn}_q(l)|$. A useful classical result involving the number of Lyndon words is the following lemma (see e.g., Ref. [11]).

Lemma 1.

$$\sum_{l|m} l L_q(l) = q^m \tag{8}$$

The lemma [11] follows from the fact that every word of length m is a repetition of some word w of length $l|m$, where w is in the conjugacy class of some Lyndon word. There are $L_q(l)$ conjugacy classes and each conjugacy class has l distinct words.

The Chen–Fox–Lyndon factorization theorem [5] (see also Ref. [11]) is the following fundamental result in the theory of Lyndon words.

Theorem 1. *Any non-empty word w can be uniquely written as a concatenation of Lyndon words in non-increasing lexicographic order,*

$$w = v_1 v_2 \dots v_k \ , \tag{9}$$

where each v_j is a Lyndon word and $v_j \geq_{\text{lex}} v_{j+1}$.

We call the unique factorization (9) the *standard decomposition* (or *Lyndon factorization*) of w. So for example the Lyndon factorization of the word `LYNDON` is `(LYN)(DON)`.

Furthermore, we say that a standard decomposition is *strictly decreasing* if $v_j >_{\text{lex}} v_{j+1}$ for $j = 1, \dots, k-1$. We will denote by $\text{Str}_q(n)$ the number of strictly decreasing standard decompositions of words of length n from an alphabet of q letters. So, for example, the standard decompositions of binary words of length 4 are shown below where the strictly decreasing standard decompositions are indicated in bold,

$$\begin{array}{cccc}
(0)(0)(0)(0), & (\mathbf{0001}), & (\mathbf{001})(\mathbf{0}), & (\mathbf{0011}), \\
(01)(0)(0), & (01)(01), & (\mathbf{011})(\mathbf{0}), & (\mathbf{0111}), \\
(1)(0)(0)(0), & (\mathbf{1})(\mathbf{001}), & (\mathbf{1})(\mathbf{01})(\mathbf{0}), & (\mathbf{1})(\mathbf{011}), \\
(1)(1)(0)(0), & (1)(1)(01), & (1)(1)(1)(0), & (1)(1)(1)(1).
\end{array}$$

We see that precisely half of the binary words of length 4 have strictly decreasing standard decompositions. In general, for an alphabet of q letters, the proportion of words that have strictly decreasing standard decompositions is $(q-1)/q$, which we prove in the next section.

3. Counting strictly decreasing standard decompositions

The following theorem is the main combinatorial result of the paper.

Theorem 2. *For words of length $n \geq 2$,*

$$\mathrm{Str}_q(n) = (q-1)q^{n-1} \ . \tag{10}$$

We formally define a generating function for the number of strictly decreasing standard decompositions as

$$p\,(x) = \sum_{n=0}^{\infty} \mathrm{Str}_q(n) \cdot x^n \ , \tag{11}$$

where we set $\mathrm{Str}_q(0) = 1$ and $\mathrm{Str}_q(1) = q$. If we also define a function,

$$f\,(x) = \frac{qx^2 - 1}{qx - 1} = 1 + qx + \sum_{n=2}^{\infty} (q-1)\, q^{n-1} x^n \ , \tag{12}$$

then proving the theorem is equivalent to showing that $p = f$ on some interval. To do this we use the following lemma.

Lemma 2.

$$p\,(x) = \prod_{l=1}^{\infty} \left(1 + x^l\right)^{L_q(l)} \tag{13}$$

Proof. Observe that the set of words with strictly decreasing standard decomposition is in bijection with the set of subsets of all Lyndon words. The bijection is implemented by taking any collection of distinct Lyndon words, arranging them in (strictly) decreasing order, and concatenating. That this is invertible follows from the Chen–Fox–Lyndon theorem, as every word has a unique non-increasing standard decomposition. □

Proof of Theorem 2. As $p(0) = f(0) = 1$ we note that $p = f$ on $(-1, 1)$ if

$$\frac{\mathrm{d}}{\mathrm{d}x} \log p = \frac{\mathrm{d}}{\mathrm{d}x} \log f \tag{14}$$

on $(-1, 1)$. From Lemma 2,

$$\log p = \sum_{l=1}^{\infty} L_q(l) \log\left(1 + x^l\right) \tag{15}$$

$$= \sum_{l=1}^{\infty} L_q(l) \sum_{j=1}^{\infty} \frac{(-1)^{j+1}}{j} x^{lj} \ , \tag{16}$$

where the second equality is valid for $|x| < 1$. Hence,

$$\frac{\mathrm{d}}{\mathrm{d}x} \log p = -\frac{1}{x} \sum_{l=1}^{\infty} \sum_{j=1}^{\infty} (-1)^j l L_q(l) x^{lj} \tag{17}$$

$$= -\frac{1}{x} \sum_{m=1}^{\infty} \sum_{l|m} (-1)^{\frac{m}{l}} l L_q(l) x^m \ . \tag{18}$$

Splitting the sum over m into sums over odd and even terms respectively,

$$\frac{\mathrm{d}}{\mathrm{d}x} \log p = \frac{1}{x} \sum_{m=1}^{\infty} \sum_{l|2m-1} l L_q(l) x^{2m-1} - \frac{1}{x} \sum_{m=1}^{\infty} \sum_{l|2m} (-1)^{\frac{2m}{l}} l L_q(l) x^{2m} \tag{19}$$

$$= \frac{1}{x} \sum_{m=1}^{\infty} \sum_{l|m} l L_q(l) x^m - \frac{1}{x} \sum_{m=1}^{\infty} \sum_{l|2m} \left(1 + (-1)^{\frac{2m}{l}}\right) l L_q(l) x^{2m} \tag{20}$$

$$= \frac{1}{x} \sum_{m=1}^{\infty} \sum_{l|m} l L_q(l) x^m - \frac{2}{x} \sum_{m=1}^{\infty} \sum_{l|m} l L_q(l) x^{2m}, \tag{21}$$

where, in the last step we used the fact that coefficients in the second sum vanish unless l divides m. Applying Lemma 1,

$$\frac{\mathrm{d}}{\mathrm{d}x} \log p = \frac{1}{x} \sum_{m=1}^{\infty} (qx)^m - \frac{2}{x} \sum_{m=1}^{\infty} (qx^2)^m \tag{22}$$

$$= \frac{1}{x} \frac{qx}{1 - qx} - \frac{2}{x} \frac{qx^2}{1 - qx^2} \ . \tag{23}$$

Finally comparing this to,

$$\frac{\mathrm{d}}{\mathrm{d}x} \log f = \frac{q}{1 - qx} - \frac{2qx}{1 - qx^2} \ , \tag{24}$$

completes the proof. □

4. Quantum q-nary graphs and their pseudo-orbits

A graph $\mathcal{G}$ is a set of vertices $\mathcal{V}$ connected by a set of edges $\mathcal{E}$. We consider graphs with directed edges where each edge $e = (u, v) \in \mathcal{E}$, connects an origin vertex $o(e) = u$ to a terminal vertex $t(e) = v$. We write $e \sim v$ if v is a vertex in e. The number of edges $e \sim v$ is d_v the *degree* of v. The total number of edges is $E = |\mathcal{E}|$.

Let q and m be positive integers. We define a q-nary graph of order m in the following way. We use an alphabet, $\mathcal{A}$, of q letters and let the set of graph vertices be labeled by the q^m words of length m. The edges of the graph are labeled by words of length q^{m+1} where the first m letters of the edge label designate the origin vertex and the last m letters denote the terminal vertex. Consequently every vertex of the q-nary

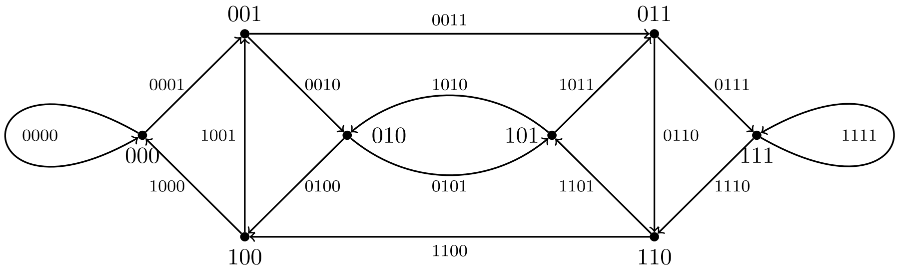

Fig. 1. A binary graph with 2^3 vertices.

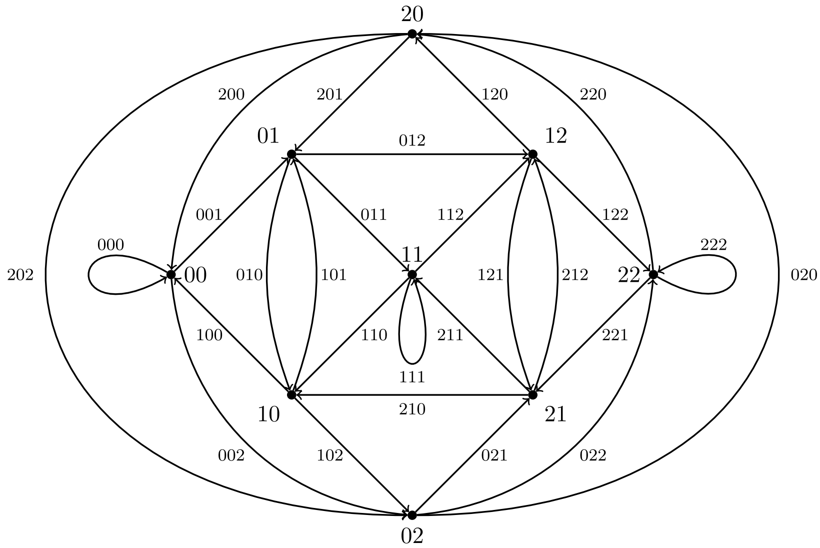

Fig. 2. A ternary graph with 3^2 vertices.

graph has q incoming edges and q outgoing edges. See Fig. 1 for an example of a binary graph with 2^3 vertices and Fig. 2 for a ternary graph with 3^2 vertices.

A *path* $p = (v_1, v_2, \dots, v_{l+1})$ of topological length $E_p = l$ can be labeled by a sequence of $l+1$ connected vertices or alternatively by the corresponding connected l edges $p = (e_1, \dots, e_l)$ where $e_j = (v_j, v_{j+1})$. On the q-nary graph with q^m vertices a path of length l is labeled by a word $w = a_1, \dots, a_{l+m}$ where the connected vertices on the path are obtained by reading off consecutive subwords of m letters; so the first vertex is labeled by $a_1, \dots, a_m$ the second by $a_2, \dots, a_{m+1}$ and so on. Clearly every q-nary graph is connected as any vertex can be reached from any other vertex by a path of at most m edges. On the other hand, a *periodic orbit* $\gamma = (v_1, \dots, v_l, v_1)$ of $E_\gamma = l$ edges, which is a closed path on $\mathcal{G}$, is labeled by a word $w = a_1, \dots, a_l$ of length l, where to obtain all the l subwords of length m the letters of w are rotated cyclically. For example, in Fig. 1 the periodic orbit of topological length 1 denoted by 0 corresponds to the loop 0000 joining vertex 000 to itself. Alternatively 0001 is the periodic orbit of topological length 4,

$$000 \to 001 \to 010 \to 100 \to 000 \; .$$

Clearly the number of periodic orbits of length l on a q-nary graph is q^l. A *primitive periodic orbit* is a periodic orbit that is not a repetition of a shorter periodic orbit. We observe that there is a bijection between the primitive periodic orbits and Lyndon words. Indeed, a Lyndon word serves as a representative of its conjugacy class and by definition cannot be a repetition of a shorter word (see Section 2).

A *pseudo orbit* $\tilde{\gamma} = \{\gamma_1, \dots, \gamma_M\}$ on $\mathcal{G}$ is a set of periodic orbits. We will use $m_{\tilde{\gamma}} = M$ to denote the number of periodic orbits in the pseudo orbit. The topological length of the pseudo orbit is

$$E_{\bar{\gamma}} = \sum_{j=1}^{M} E_{\gamma_j} \ . \tag{25}$$

A *primitive pseudo orbit* $\bar{\gamma} = \{\gamma_1, \dots, \gamma_M\}$ is a set of primitive periodic orbits in which no periodic orbit appears more than once; so primitive pseudo orbits omit repetitions of periodic orbits both in the collection of periodic orbits and inside each periodic orbit that makes up the pseudo orbit.

We can now see that there is a bijection between primitive pseudo orbits and words whose standard decomposition does not contain any Lyndon word more than once so that they are strictly decreasing. Thus, we can apply Theorem 2 to count primitive pseudo orbits on q-nary graphs.

Corollary 1. *The number of primitive pseudo orbits of topological length n on a q-nary graph of order m is $(q-1)q^{n-1}$.*

5. The characteristic polynomial of a quantum graph

Quantum graphs were introduced as a model system in which to study spectral properties when the corresponding classical dynamics is chaotic by Kottos and Smilansky [9,10]. Spectral properties of quantum binary graphs (q-nary graphs with $q = 2$) were investigated by Tanner in Ref. [15].

A discrete graph can be turned into a metric graph by associating a length $l_e > 0$ to each edge $e \in \mathcal{E}$. There are two main approaches to quantize a metric graph which are closely related (see Refs. [2,6]). We describe the approach adopted here. Given an arbitrary directed metric graph, where each vertex has q incoming and q outgoing edges, we equip each vertex, $v \in \mathcal{V}$ with a prescribed unitary $q \times q$ matrix. We call this matrix a vertex scattering matrix and denote it by $\sigma^{(v)}$. Each entry of this matrix $\sigma^{(v)}_{e,e'}$ is a scattering transmission amplitude from edge e' to edge e. Hence, the entries, $\sigma^{(v)}_{e,e'}$ are indexed such that e' is an edge directed towards the vertex v and e is directed out of it, so $v = t(e') = o(e)$.

In particular we consider $q \times q$ vertex scattering matrices of the form,

$$\sigma^{(v)}_{e,e'} = \frac{1}{\sqrt{q}} \begin{pmatrix} 1 & 1 & 1 & \dots & 1 \\ 1 & \omega & \omega^2 & \dots & \omega^{q-1} \\ 1 & \omega^2 & \omega^4 & \dots & \omega^{2(q-1)} \\ \vdots & \vdots & \vdots & \ddots & \vdots \\ 1 & \omega^{k-1} & \omega^{2(k-1)} & \dots & \omega^{(q-1)(q-1)} \end{pmatrix} , \tag{26}$$

where $\omega = \mathrm{e}^{\frac{2\pi \mathrm{i}}{q}}$ is a primitive q-th root of unity. This matrix is the Discrete Fourier Transform (DFT) matrix. Such vertex scattering matrices have the advantage of being democratic, in the sense that the transmission probability $|\sigma^{(v)}_{e,e'}|^2 = 1/q$ for every outgoing edge e. Consequently graphs with the DFT vertex scattering matrices are a well studied model of quantum chaos for which spectral properties are seen to converge rapidly to the predictions of random matrix theory [16].

All the vertex scattering matrices $\sigma^{(v)}$ can be combined into a single $E \times E$ unitary matrix in the following way. Fixing an arbitrary order for the E graph edges we compose an $E \times E$ matrix, Σ, whose entries are indexed by the graph edges and set

$$\Sigma_{e,e'} = \begin{cases} \sigma^{(v)}_{e,e'} & v = t(e') = o(e) \\ 0 & \text{otherwise} \end{cases} ,$$

where $t(e')$ marks the terminal vertex of e' and $o(e)$ marks the origin vertex of e.

Next we define $L = \mathrm{diag}\{l_1, \dots, l_E\}$ to be a diagonal matrix of all edge lengths and set $U(k) = \mathrm{e}^{\mathrm{i}kL}\Sigma$, which is called the unitary (or quantum) evolution operator. The graph spectrum is then defined as

$$\left\{ k^2 \middle| \det\left(\mathrm{I} - U\left(k\right)\right) = 0 \right\} \ . \tag{27}$$

This is the set of eigenvalues of the negative Laplacian on the metric graph when the vertex scattering matrices are those obtained from a self-adjoint realization of the operator, see e.g. Ref. [2].

The *characteristic polynomial* of $U\left(k\right)$ is,

$$F_\xi\left(k\right) = \det\left(\xi \mathrm{I} - U\left(k\right)\right) = \sum_{n=0}^{2B} a_n \xi^{2B-n} \ , \tag{28}$$

and we note that the graph's eigenvalues are obtained as the zeros of $F_{\xi=1}$. The characteristic polynomial coefficients, a_n, are the spectral quantity which we investigate here. It is shown in Ref. [1] that each a_n may be expressed as a sum over pseudo orbits on the graph in the following way. To each periodic orbit $\gamma = (e_1, \ldots, e_m)$ on the quantum graph it is natural to associate a metric length,

$$l_\gamma = \sum_{j=1}^{m} l_{e_j} \tag{29}$$

and a stability amplitude, the product of the elements of the scattering matrix around the orbit,

$$A_\gamma = \Sigma_{e_2 e_1} \Sigma_{e_3 e_2} \ldots \Sigma_{e_n e_{n-1}} \Sigma_{e_1 e_m} \ . \tag{30}$$

Then a pseudo orbit $\tilde{\gamma} = \{\gamma_1, \ldots, \gamma_M\}$ acquires a metric length and stability amplitude,

$$l_{\tilde{\gamma}} = \sum_{j=1}^{M} l_{\gamma_j} \ , \tag{31}$$

$$A_{\tilde{\gamma}} = \prod_{j=1}^{M} A_{\gamma_j} \ . \tag{32}$$

In Ref. [1] the authors prove the following theorem.

Theorem 3. *The coefficients of the characteristic polynomial $F_\xi\left(k\right)$ are given by*

$$a_n = \sum_{\bar{\gamma} |\ E_{\bar{\gamma}} = n} (-1)^{m_{\bar{\gamma}}} A_{\bar{\gamma}}\left(k\right) \exp\left(\mathrm{i} k l_{\bar{\gamma}}\right) \ , \tag{33}$$

where the (finite) sum is over all the primitive pseudo orbits of topological length n.

In Ref. [1] Theorem 3 is used to express the secular function, zeta function and spectral determinant in terms of the dynamical properties of finite numbers of pseudo orbits. In the final section we present results on the second moment of the coefficients.

6. Variance of coefficients of the characteristic polynomial

Typically, spectral properties of quantum chaotic systems can be modeled by the spectrum of a corresponding ensemble of random matrices according to the conjecture of Bohigas, Giannoni and Schmidt [4]. The variance of the coefficients of the characteristic polynomial of an $E \times E$ random scattering matrix from the Circular Orthogonal Ensemble (COE) and Circular Unitary Ensemble (CUE) [7] are,

$$\langle |a_n|^2 \rangle_{\mathrm{COE}} = 1 + \frac{n(E-n)}{E+1} \ , \tag{34}$$

$$\langle |a_n|^2 \rangle_{\mathrm{CUE}} = 1 \ . \tag{35}$$

These correspond to predictions for quantum chaotic systems with and without time-reversal symmetry respectively. In our case the directed scattering matrices break time-reversal symmetry. Hence directed q-nary graphs would be in the class of systems to be modeled by the CUE. However, as is shown in the following, the coefficients of the characteristic polynomial of a quantum graph are seen to deviate from the random matrix predictions even when other spectral-statistics match the corresponding random matrix ensemble.

Starting from (33), we note that $a_0 = 1$ and averaging over k the other coefficients have mean value zero, as the average over k of $\mathrm{e}^{\mathrm{i}kl_{\bar{\gamma}}}$ is zero for pseudo orbits of topological length $n \geq 1$. The *variance* of coefficients of the characteristic polynomial was investigated numerically for the complete graph with four vertices in Ref. [10] and also for binary graphs numerically and theoretically in Refs. [15,16]. The approach we take here extends this discussion to the families of q-nary graphs, for which we obtain analytic results. Following (33) we write the variance of the coefficients of the characteristic polynomial as a sum over pairs of primitive pseudo orbits $\bar{\gamma}, \bar{\gamma}'$ of the same metric length,

$$\langle |a_n|^2 \rangle_k = \sum_{\bar{\gamma},\bar{\gamma}' | E_{\bar{\gamma}} = E_{\bar{\gamma}'} = n} (-1)^{m_{\bar{\gamma}} + m_{\bar{\gamma}'}} A_{\bar{\gamma}} \bar{A}_{\bar{\gamma}'} \lim_{K \to \infty} \frac{1}{K} \int_0^K \mathrm{e}^{\mathrm{i}k(l_{\bar{\gamma}} - l_{\bar{\gamma}'})} \mathrm{d}k \tag{36}$$

$$= \sum_{\bar{\gamma},\bar{\gamma}' | E_{\bar{\gamma}} = E_{\bar{\gamma}'} = n} (-1)^{m_{\bar{\gamma}} + m_{\bar{\gamma}'}} A_{\bar{\gamma}} \bar{A}_{\bar{\gamma}'} \, \delta_{l_{\bar{\gamma}}, l_{\bar{\gamma}'}} \ . \tag{37}$$

When the set of edge lengths is incommensurate, i.e. linearly independent as real numbers over the rationals, the condition that the metric lengths of the pseudo orbits be equal requires that $\bar{\gamma}$ and $\bar{\gamma}'$ traverse the same edges the same number of times. Then, in the absence of time-reversal symmetry, the first order contribution to the variance is generated by pairing an pseudo orbit with itself, $\bar{\gamma}' = \bar{\gamma}$, as in the diagonal approximation of Berry [3]. We thus define

$$\langle |a_n|^2 \rangle_{\mathrm{diag}} = \sum_{\bar{\gamma} | E_{\bar{\gamma}} = n} |A_{\bar{\gamma}}|^2 \ . \tag{38}$$

From (26) we have that the transition probability from any incoming edge e' to any outgoing edge e is always,

$$|\sigma^{(v)}_{e,e'}|^2 = \frac{1}{q} \tag{39}$$

and substituting in (38) produces,

$$\langle |a_n|^2 \rangle_{\mathrm{diag}} = \sum_{\bar{\gamma} | E_{\bar{\gamma}} = n} \frac{1}{q^n} \ . \tag{40}$$

Evaluating this amounts to counting the number of primitive pseudo orbits of topological length n. Then applying Corollary 1 we see the diagonal approximation to the coefficients of the characteristic polynomial of families of q-nary graphs is,

$$\langle |a_n|^2 \rangle_{\mathrm{diag}} = \frac{(q-1)}{q} \ . \tag{41}$$

According to the Bohigas–Giannoni–Schmidt conjecture one might expect, in the absence of time-reversal symmetry, the random matrix result $\langle |a_n|^2 \rangle_{\mathrm{CUE}} = 1$. Hence the diagonal approximation deviates from this result for each family of q-nary graphs in the semiclassical limit, which for graphs is the limit of large graphs, i.e. fixing q and taking the length of the words to infinity. However, the discrepancy is consistent with the results for binary graphs obtained by Tanner [17]. There $\langle |a_n|^2 \rangle_k$ is seen to converge numerically to a constant value of 0.5 independent of n. The diagonal approximation considered here reproduces this result. To avoid the approximation, higher order contributions to the variance of the coefficients would come from correlations between pseudo orbits of the same length with self-intersections such as the figure of eight periodic orbits considered by Seiber and Richter [13,14].

To summarize, the diagonal approximation for the pseudo orbit expansion shows a deviation from random matrix theory which does not disappear in the semi-classical limit for fixed q. However, this deviation would vanish for a sequence of quantum graphs with increasing degree, i.e. increasing q, which is another way of approaching the semi-classical limit. This suggests that random matrix results for the coefficients of the characteristic polynomial may be recovered for sequences of quantum graphs although under stronger conditions than those typically required for other spectral statistics such as the form factor.

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References

[1] R. Band, J.M. Harrison, C.H. Joyner, Finite pseudo orbit expansions for spectral quantities of quantum graphs, J. Phys. A: Math. Theor. 45 (2012) 325204.
[2] G. Berkolaiko, P. Kuchment, Introduction to Quantum Graphs, Mathematical Surveys and Monographs, vol. 186, AMS, Providence, RI, 2013.
[3] M.V. Berry, Semiclassical theory of spectral rigidity, Proc. R. Soc. Lond. A 400 (1985) 229–251.
[4] O. Bohigas, M.-J. Giannoni, C. Schmit, Characterization of chaotic quantum spectra and universality of level fluctuation laws, Phys. Rev. Lett. 52 (1984) 1.
[5] K.-T. Chen, R.H. Fox, R.C. Lyndon, Free differential calculus, IV, Ann. Math. 68 (1958) 81–95.
[6] S. Gnutzmann, U. Smilansky, Quantum graphs: applications to quantum chaos and universal spectral statistics, Adv. Phys. 55 (2006) 527–625.
[7] F. Haake, M. Kuś, H.-J. Sommers, H. Schomerus, K. Życzkowski, Secular determinants of random unitary matrices, J. Phys. A: Math. Gen. 29 (1996) 3641–3658.
[8] M. Hazewinkel, The algebra of quasi-symmetric functions is free over the integers, Adv. Math. 164 (2001) 283–300.
[9] T. Kottos, U. Smilansky, Quantum chaos on graphs, Phys. Rev. Lett. 79 (1997) 4794.
[10] T. Kottos, U. Smilansky, Periodic orbit theory and spectral statistics for quantum graphs, Ann. Phys. 274 (1999) 76.
[11] M. Lothaire (Ed.), Combinatorics on Words, Addison–Wesley, Reading, Massachusetts, 1983.
[12] S. Mantaci, A. Restivo, G. Rosone, M. Sciortino, Sorting suffixes of a text via its Lyndon factorization, in: J. Holub, J. Zdárek (Eds.), Proceedings of the Prague Stringology Conference 2013, 2013, pp. 119–127.
[13] M. Sieber, Leading off-diagonal approximation for the spectral form factor for uniformly hyperbolic systems, J. Phys. A: Math. Gen. 35 (2002) L613–L619.
[14] M. Sieber, K. Richter, Correlations between periodic orbits and their role in spectral statistics, Phys. Scr. 2001 (2001) 128.
[15] G. Tanner, Spectral statistics for unitary transfer matrices of binary graphs, J. Phys. A: Math. Gen. 33 (2000) 3567–3585.
[16] G. Tanner, Unitary-stochastic matrix ensembles and spectral statistics, J. Phys. A: Math. Gen. 34 (2001) 8485–8500.
[17] G. Tanner, The autocorrelation function for spectral determinants of quantum graphs, J. Phys. A: Math. Gen. 35 (2002) 5985.