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Families of Line-Graphs and Their Quantization

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Any directed graph G with N vertices and J edges has an associated line-graph $L(G)$ where the J edges form the vertices of $L(G)$. We show that the non-zero eigenvalues of the adjacency matrices are the same for all graphs of such a family $L^n(G)$. We give necessary and sufficient conditions for a line-graph to be quantisable and demonstrate that the spectra of associated quantum propagators follow the predictions of random matrices under very general conditions. Line-graphs may therefore serve as models to study the semiclassical limit (of large matrix size) of a quantum dynamics on graphs with fixed classical behaviour.

KEY WORDS: Quantum graphs; line-graph; spectral statistics; semiclassical limit.

1. INTRODUCTION

Spectra of quantum graphs display in general universal statistics characteristic for ensembles of random unitary matrices. This observation by Kottos and Smilansky[1, 2] has led to a variety of studies in this direction.[3–11] It has became clear that the quantisation scheme of Kottos and Smilansky can be considerably generalised to be applicable also for directed graphs (digraphs).[12–14] One of the main points of interest is to understand under which circumstances the quantisation of a graph generates a spectrum which follows random matrix theory (RMT) and when to expect deviations thereof. General statements can, however, only be made in the limit of

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large matrices and we thus face the problem of constructing larger and larger graphs representing the same classical dynamics at least in the limit of infinite network size. We will offer a simple and straightforward way to define such families of graphs in this paper.

We thereby consider families of graphs generated from an arbitrary initial graph by using the concept of *line-graphs*[15,16] (also called *edge-graphs*). Consider any initial directed graph G with N vertices and J bonds (edges). The line-graph $L(G)$ obtained from G consists of J vertices which are the edges of its ancestor G. Iterating this procedure we construct an infinite family of digraphs $L^n(G)$ with in general increasing number of vertices. We will show that all graphs in a given family defined in this way have the same topological and metric properties. In particular, the sets of periodic orbits and the non-zero eigenvalues of the adjacency and transition matrices are identical for digraphs of such a family. We will give necessary and sufficient conditions for a line-graph to be quantisable.

Line-graph families thus form a set of graphs whose size increases with n but whose "classical" dynamics is fixed. The semiclassical limit of the system is then obtained by increasing the index n. The entire family of graphs, corresponding to the same classical dynamics, is uniquely determined by a given initial graph. This approach to the semiclassical limit for quantum graphs offers an alternative to the previous method based on transition matrices representing Markov chains associated with certain piecewise linear 1D dynamical systems.[14]

Our paper is organized as follows. In Section 2 we recall the definition of a line-graph and present an example of a family of digraphs. Sections 3 and 4 contain the main results of this work: a proof that all graphs belonging to a given family of line-graphs represent the same dynamics and conditions for the quantisability of line-graphs. Section 5 is devoted to examples of quantisable line-graph families. We analyze in particular the statistical properties of the spectra of the unitary matrices obtained when quantising the graph. Concluding remarks are presented in Section 6.

2. LINE-GRAPHS-DEFINITIONS AND BASIC PROPERTIES

Consider a directed graph G with N vertices and J edges (called also bonds or arcs). We denote the set of vertices $V(G) = \{v_1,\dots, v_N\}$ and the set of edges by $E(G) = \{(v_i v_j) : G$ has an edge leading from v_i to $v_j\}$. To simplify the notation, we will only consider graphs with at most one edge going from a vertex v_i to a vertex v_j. All the results in this paper apply, however, also for directed multi-graphs G, i.e., for graphs with two or more edges connecting two vertices in the same direction. We will use the ordered pair (ij) to represent a directed edge. A digraph G may have loops, i.e., edges starting and ending at the same vertex. A *line-graph* $L(G)$ is constructed from a graph G by considering the edges as vertices, that is,

$$V(L(G)) = E(G), \tag{1}$$

and vertices in $L(G)$ are adjacent if the edges in G are. It is clear from the definition that $L(G)$ does not have multi-edges even if G does; one obtains

$$E(L(G)) = \{((ij), (jk)) : (ij) \in E(G), (jk) \in E(G)\}. \tag{2}$$

We will be interested in families of digraphs obtained from G by iterating the line-graph procedure. The *nth generation line-graph* $L^n(G)$ of G is thereby defined as $L^n(G) = L(L^{n-1}(G))$. We will call the graph $L^{n-1}(G)$ the *ancestor* of the line-graph $L^n(G)$ and G the *initial graph* of the family.

In what follows, we will need the set of vertices which can be reached from a vertex v_i in n steps. We define the *n-step out-neighbourhood* of v_i as

$$N_+^{(n)}(v_i) = \{v_j \in V(G) : v_j \text{ can be reached from } v_i \text{ in } n \text{ steps}\}; \tag{3}$$

equivalently, we define the *n-step in-neighbourhood* of v_i as

$$N_-^{(n)}(v_i) = \{v_j \in V(G) : v_i \text{ can be reached from } v_j \text{ in } n \text{ steps}\}. \tag{4}$$

The cardinality (i.e., the number of elements) of $N_\pm^{(1)}(v_i)$ is often called the *out/in-degree*, $d^\pm(v_i)$, of v_i corresponding to the number of vertices adjacent to v_i with respect to outgoing or incoming edges.

The topology of a digraph G is most conveniently described in terms of its *connectivity* or *adjacency matrix* A^G of size N with

$$A_{ij}^G = \begin{cases} 1 & (ij) \in E(G) \\ 0 & (ij) \notin E(G) \end{cases} \qquad i, j = 1 \cdots N. \tag{5}$$

The degree of a vertex v_i is then given as

$$d^+(v_i) = \sum_{j=1}^{N} A_{ij}^G \qquad \text{and} \qquad d^-(v_j) = \sum_{i=1}^{N} A_{ij}^G. \tag{6}$$

The adjacency matrix of the line-graph $L(G)$ of G may be expressed as

$$A_{ij,kl}^{L(G)} = A_{ij}^G \, \delta_{jk} \, A_{kl}^G. \tag{7}$$

In fact if we define $A^{L(G)}$ as the adjacency matrix of dimension J including only the relevant index pairs $(ij), (kl) \in E(G)$ then $A_{ij,kl}^{L(G)} = \delta_{jk}$.

A stochastic Markov-process on the graph G is defined in terms of a transition matrix T^G with $T^G_{ij} \geqslant 0$ representing the probability of going from vertices i to j. We demand that T^G has the same zero-pattern as A^G, that is $A^G_{ij} \neq 0$ iff $T^G_{ij} \neq 0$ for all $i, j = 1, \ldots, N$; furthermore stochasticity of T^G implies that $\sum_j T^G_{ij} = 1$. We define the transition matrix $T^{L(G)}$ of the stochastic process induced by T^G on the line-graph of G by

$$T^{L(G)}_{ij,\,kl} = A^G_{ij}\, \delta_{jk}\, T^G_{kl}. \tag{8}$$

It is obvious from the definition that $T^{L(G)}$ is a stochastic matrix which has the same zero-pattern as $A^{L(G)}$.

Before moving on to general results on line-graph families, we will discuss a particular example to see how this construction works. Consider first a directed cycle digraph C_M (see Fig. 1) consisting of M vertices connected by M bonds. Such a graph is strongly connected, that is, there exists at least one directed path leading from a vertex v_i to v_j for all $i, j = 1, \ldots, M$. The line-graph $L(C_M)$ is isomorphic to C_M (see Fig. 1), so all cycles C_M are fixed points of the line-graph construction, $L(C_M) = C_M$.

Let us discuss next a family of digraphs generated by the initial graph F defined as

$$V(F) = \{v_1, v_2\}, \qquad E(F) = \{(v_1 v_1), (v_1 v_2), (v_2 v_1)\} = \{(11), (12), (21)\}\cdot \tag{9}$$

Fig. 2 shows the first four graphs of this family. Their adjacency matrices are

$$C^F = \begin{pmatrix} 1 & 1 \\ 1 & 0 \end{pmatrix}, \quad C^{L(F)} = \begin{pmatrix} 1 & 1 & \cdot \\ \cdot & \cdot & 1 \\ 1 & 1 & \cdot \end{pmatrix}, \quad C^{L^2(F)} = \begin{pmatrix} 1 & 1 & \cdot & \cdot & \cdot \\ \cdot & \cdot & 1 & \cdot & \cdot \\ \cdot & \cdot & \cdot & 1 & 1 \\ 1 & 1 & \cdot & \cdot & \cdot \\ \cdot & \cdot & 1 & \cdot & \cdot \end{pmatrix},$$

$$C^{L^3(F)} = \begin{pmatrix} 1 & 1 & \cdot & \cdot & \cdot & \cdot & \cdot & \cdot \\ \cdot & \cdot & 1 & \cdot & \cdot & \cdot & \cdot & \cdot \\ \cdot & \cdot & \cdot & 1 & 1 & \cdot & \cdot & \cdot \\ \cdot & \cdot & \cdot & \cdot & \cdot & 1 & 1 & \cdot \\ \cdot & \cdot & \cdot & \cdot & \cdot & \cdot & \cdot & 1 \\ 1 & 1 & \cdot & \cdot & \cdot & \cdot & \cdot & \cdot \\ \cdot & \cdot & 1 & \cdot & \cdot & \cdot & \cdot & \cdot \\ \cdot & \cdot & \cdot & 1 & 1 & \cdot & \cdot & \cdot \end{pmatrix}; \tag{10}$$

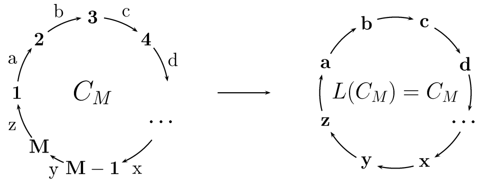

Fig. 1. Directed cycle digraph C_M, its line-graph $L(C_M)$ is isomorphic to it.

the dots represent here entries being equal to zero. To introduce a stochastic process on F we may choose equal probabilities of staying at vertex 1 and of going from 1 to 2. This corresponds to the transition matrix

$$T^F = \frac{1}{2}\begin{pmatrix} 1 & 1 \\ 2 & 0 \end{pmatrix}. \tag{11}$$

The transition matrices $T^{L^n(F)}$ can be obtained from $A^{L^n(F)}$ by replacing 1's by $\frac{1}{2}$'s in all rows in which there are two entries equal to unity. The resulting matrices are stochastic. Let N_G denote the number of vertices of a digraph G. Then the numbers of vertices of the digraphs $L^n(F)$ fulfill the Fibonacci relation

$$N_{L^n(F)} = N_{L^{n-1}(F)} + N_{L^{n-2}(F)}, \tag{12}$$

for $n > 1$ with $N_F = 2$ and $N_{L(F)} = 3$.

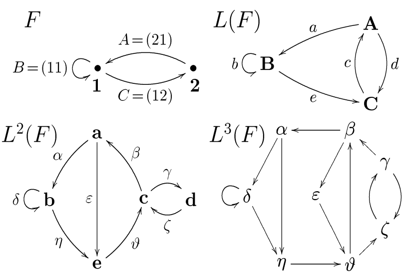

Fig. 2. Fibonacci family of line-graphs; the initial graph F, and next three members of the line-graph family consisting of 2, 3, 5 and 8 vertices, respectively, are shown.

3. LINE-GRAPH FAMILIES $L^n(G)$–STOCHASTIC DYNAMICS

We shall start this section by stating basic properties of the line-digraph construction. If G is a strongly connected digraph not isomorphic to a cycle, then the number of its bonds is larger than the number of its vertices, so

$$N_{L(G)} > N_G \,. \tag{13}$$

Observe that $L(G)$ is also a strongly connected digraph different from a cycle. The above statements allow us to draw an important conclusion:

Corollary 1. For any strongly connected digraph G, not isomorphic to a cycle, its line-graph family $L^n(G)$ contains infinite number of different digraphs and

$$\lim_{n\to\infty} N_{L^n(G)} = \infty \,. \tag{14}$$

In the following we analyze topological and dynamical properties of line-graph families $L^n(G)$ with associate stochastic Markov processes. We start by introducing periodic orbits on a digraph.

Definition 2. A sequence of p vertices $\gamma = v_{i_1} v_{i_2} \cdots v_{i_p}$ such, that $v_{i_j} \in V(G), j = 1 \cdots p$ and $(v_{i_j} v_{i_{j+1}}) \in E(G), j = 1 \cdots p-1, (v_{i_p} v_{i_1}) \in E(G)$ is called a periodic orbit of period p on the digraph G. The set of periodic orbits on G is denoted by $PO(G)$.

A periodic orbit is called *primitive*, if it is not a repetition of another periodic orbit. It is obvious from the definition of a line-graph that there is a one-to-one relation between periodic orbits of G and $L(G)$, that is, $\gamma = v_{i_1} v_{i_2} \cdots v_{i_p} \in PO(G)$ iff $\eta = (v_{i_1} v_{i_2})(v_{i_2} v_{i_3}) \cdots (v_{i_{p-1}} v_{i_p})(v_{i_p} v_{i_1}) \in PO(L(G))$. The set of periodic orbits $PO(L^n(G))$ is thus isomorphic to $PO(G)$ and the map

$$\Theta \colon PO(G) \to PO(L(G)) \tag{15}$$

between periodic orbits of G and $L(G)$ is bijective and conserves the period of the orbit. This implies that the topological entropy measuring the exponential of growth of the number of periodic orbits with their period p is the same for all generations of the line-graph family. The four graphs presented in Fig. 2 may serve as an example. All the graphs $L^n(F)$ have only one primitive orbit of periods one to four.

Next, we define the *stability factor* or *amplitude* of a periodic orbit, $\gamma = v_{i_1} v_{i_2} \cdots v_{i_p} \in PO(G)$ of a graph G with associated stochastic process T^G as

$$a_\gamma^G = T^G_{i_1 i_2} \cdot T^G_{i_2 i_3} \cdot \cdots \cdot T^G_{i_p i_1} . \tag{16}$$

The amplitude a_γ^G is the probability of staying on the orbit γ after p iterations of the stochastic process, where p is the period of γ. One obtains for the stability factor of periodic orbits on the line-graph

$$\begin{aligned} a^{L(G)}_{\Theta(\gamma)} &= T^{L(G)}_{i_1 i_2, i_2 i_3} \cdot T^{L(G)}_{i_2 i_3, i_3 i_4} \cdot \cdots \cdot T^{L(G)}_{i_p i_1, i_1 i_2} \\ &= A^G_{i_1 i_2} T^G_{i_2 i_3} \cdot A^G_{i_2 i_3} T^G_{i_3 i_4} \cdot \cdots \cdot A^G_{i_p i_1} T^G_{i_1 i_2} = a_\gamma^G , \end{aligned} \tag{17}$$

and the last identity follows from

$$A^G_{ij} \cdot T^G_{ij} = T^G_{ij} . \tag{18}$$

We thus obtain that the mapping Θ leaves the stability factors of periodic orbits invariant, that is,

$$a^{L(G)}_{\Theta(\gamma)} = a_\gamma^G . \tag{19}$$

The observations made above on the invariance of topological and dynamical properties under the line-graph construction can be put in a more general form. The topological entropy of a graph may be determined by the logarithm of the largest modulus of eigenvalue of the adjacency matrix of the graph. Denoting the characteristic polynomial of the adjacency matrix by

$$P^G(\lambda) = \det(A^G - \lambda \mathbf{1}) \tag{20}$$

one obtains:

Theorem 3. The spectrum of the adjacency matrix of the line-graph, $A^{L(G)}$, is identical to the spectrum of A^G and an appropriate number of eigenvalues equal to zero, that is,

$$P^{L(G)}(\lambda) = P^G(\lambda) \cdot (-\lambda)^{N_{L(G)} - N_G} . \tag{21}$$

Proof. We start by the following lemma.

Lemma 4. The traces of powers of the adjacency matrix of a line-graph, $A^{L(G)}$, are equal to the trace of the same power of A^G, that is,

$$\mathrm{Tr}(A^{L(G)})^n = \mathrm{Tr}(A^G)^n \qquad \text{for all} \quad n. \tag{22}$$

Since all entries of any adjacency matrix are equal to 0 or to 1 we have $A^G_{ij} \cdot A^G_{ij} = A^G_{ij}$. One thus obtains

$$\begin{aligned}
\mathrm{Tr}(A^{L(G)})^n &= \sum_{(i_1 j_1)(i_2 j_2)\cdots(i_n j_n) \in E(G)} A^{L(G)}_{i_1 j_1,\, i_2 j_2} A^{L(G)}_{i_2 j_2,\, i_3 j_3} \cdots A^{L(G)}_{i_n j_n,\, i_1 j_1} \\
&= \sum_{i_1 \cdots i_n j_1 \cdots j_n \in V(G)} (A^G_{i_1 j_1} \delta_{j_1 i_2} A^G_{i_2 j_2})(A^G_{i_2 j_2} \delta_{j_2 i_3} A^G_{i_3 j_3}) \cdots (A^G_{i_n j_n} \delta_{j_n i_1} A^G_{i_1 j_1}) \\
&= \sum_{i_1 \cdots i_n \in V(G)} A^G_{i_1 i_2} A^G_{i_2 i_3} A^G_{i_3 i_4} \cdots A^G_{i_n i_1} = \mathrm{Tr}(A^G)^n. \qquad (23)
\end{aligned}$$

Let τ_k denote the coefficients of the characteristic polynomial of A^G in the descending order

$$P^G(\lambda) = (-\lambda)^{N_G} - \tau_1(-\lambda)^{N_G - 1} + \tau_2(-\lambda)^{N_G - 2} - \cdots (-1)^{N_G} \tau_{N_G}. \qquad (24)$$

By means of the Newton formulas the coefficients τ_k may be expressed in terms of the traces $D_n := \mathrm{Tr}(A^G)^n$ as[17]

$$\tau_k = \frac{1}{k!} \begin{vmatrix} D_1 & 1 & 0 & \cdots & 0 \\ D_2 & D_1 & 2 & \cdots & 0 \\ D_3 & D_2 & D_1 & \cdots & 0 \\ \vdots & \vdots & \vdots & \vdots & \vdots \\ D_k & D_{k-1} & D_{k-2} & \cdots & D_1 \end{vmatrix}. \qquad (25)$$

Lemma 4 shows that the first N_G coefficients of the polynomial $P^{L(G)}$ in front of the largest powers of λ are equal to those of P^G. The rest of the coefficients of $P^{L(G)}$ vanish, the characteristic polynomials of $A^{L(G)}$ and A^G differ thus only by a factor $(-\lambda)^{N_{L(G)} - N_G}$; this completes the proof of the Theorem 3.

A relation similar to (20) holds for the characteristic polynomial of T^G

$$R^G(\lambda) = \det(T^G - \lambda \mathbf{1}). \qquad (26)$$

One obtains:

Theorem 5. The spectrum of the transition matrix of a line-graph, $T^{L(G)}$ consists of the spectrum of T^G and an appropriate number of eigenvalues equal to zero, so

$$R^{L(G)}(\lambda) = R^G(\lambda) \cdot (-\lambda)^{N_{L(G)} - N_G}. \qquad (27)$$

Proof is analogous to this of the Theorem 3, since a lemma equivalent to the Lemma 4 holds:

Lemma 6. Traces of any power of the transition matrix of a line-graph $T^{L(G)}$ are equal to the trace of the same power of T^G, that is

$$\mathrm{Tr}(T^{L(G)})^n = \mathrm{Tr}(T^G)^n. \tag{28}$$

The derivation follows the arguments in the proof of Lemma 4 using the property (18) instead.

Theorem 5 demonstrates that the stochastic dynamics on the line-graph $L(G)$ is equivalent to the original Markov process on G. We would therefore expect that dynamical quantities like the metric entropy of the stochastic process are invariant under the line-graph iteration as well. The metric entropy depends on the choice of the invariant measure, so we need to consider invariant measures first. The action of T^G on left vectors represents the evolution of measures. One obtains

Lemma 7. If ρ_i is a left eigenvector of T^G corresponding to the eigenvalue λ, then $(\rho_i T^G_{ij})$ is the left eigenvector of $T^{L(G)}$ to the same eigenvalue.

Proof. Let us calculate

$$\sum_{(ij)\in E(G)} (\rho_i T^G_{ij})\, T^{L(G)}_{ij,kl} = \sum_{i,j\in V(G)} \rho_i T^G_{ij} A^G_{ij} \delta_{jk} T^G_{kl} = \sum_{i\in V(G)} \rho_i T^G_{ik} T^G_{kl} = \lambda(\rho_k T^G_{kl}), \tag{29}$$

where we have used (18) and the fact that ρ_i is the left eigenvector of T^G,

$$\sum_{i\in V(G)} \rho_i T^G_{ij} = \lambda \rho_j. \tag{30}$$

The invariant measures of a Markov chain on G is given by the left eigenvectors of T^G with eigenvalue 1. According to Lemma 7 each invariant measure of T^G defines the corresponding invariant measure of $T^{L(G)}$. Assuming that ρ^G is an invariant measure of T^G, the metric entropy of the corresponding Markov process[18] reads

$$H^G_{\mathrm{metric}} = -\sum_{i\in V(G)} \rho^G_i \sum_{j\in V(G)} T^G_{ij} \ln T^G_{ij}. \tag{31}$$

The metric entropy of the Markov process on $L(G)$ with respect to the corresponding invariant measure $\rho_{ij}^{L(G)} = \rho_i^G T_{ij}^G$ is then given as (see Lemma 7)

$$
\begin{aligned}
H_{\text{metric}}^{L(G)} &= -\sum_{(ij) \in E(G)} \rho_{ij}^{L(G)} \sum_{(kl) \in E(G)} T_{ij,kl}^{L(G)} \ln T_{ij,kl}^{L(G)} \\
&= -\sum_{ijkl \in V(G)} \rho_i^G T_{ij}^G A_{ij}^G \delta_{jk} T_{kl}^G \ln A_{ij}^G \delta_{jk} T_{kl}^G \\
&= -\sum_{ijl \in V(G)} \rho_i^G T_{ij}^G T_{jl}^G (\ln A_{ij}^G + \ln T_{jl}^G) = -\sum_{jl \in V(G)} \rho_j^G T_{jl}^G \ln T_{jl}^G. \qquad (32)
\end{aligned}
$$

We thus find that the metric entropy of a stochastic process defined by $T^{L(G)}$ based on the invariant measure $\rho^{L(G)}$ is indeed identical to the metric entropy of a process T^G based on the invariant measure ρ^G, that is,

$$H_{\text{metric}}^{L(G)} = H_{\text{metric}}^{G}. \qquad (33)$$

The results stated in this section show that the topological and metric properties of the dynamics on a given graph G and the corresponding line-graph $L(G)$ are identical. In fact we have proven by recurrence that all digraphs in the family $L^n(G)$ have the same set of periodic orbits, the same non-vanishing spectrum of the adjacency matrices $A^{L^n(G)}$ and of the transition matrices $T^{L^n(G)}$, as well as the same topological and metric entropy.

4. THE QUANTISATION OF LINE-GRAPH FAMILIES

4.1. Unitary Propagation on Graphs

So far we have considered stochastic processes on digraphs defined by a transition matrix T^G. Recently, Kottos and Smilansky[1] proposed to study unitary propagation on graphs and to link the spectral properties of the unitary dynamics to an underlying Markov process on this graph. Generalising their approach we may consider the following definition of quantising a Markov chain:

Definition 8

(a) A digraph G is called *quantisable* if there exists a unitary matrix U^G with the same zero-pattern as the adjacency matrix A^G.

(b) A stochastic transition matrix T^G is called *quantisable* if there exists a unitary matrix U^G such that

$$T_{ij}^G = |U_{ij}^G|^2. \qquad (34)$$

The matrix U^G represents a one-step propagator, which describes unitary time evolution in a finite Hilbert space of dimension N_G. Note that not all stochastic matrices T^G can be quantised in the sense described above. The stochastic matrices, for which a unitary matrix exists fulfilling Eq. (34) are called *unistochastic*.[19] The matrix T^G in (34) is by construction bistochastic, that is, the sum over the matrix elements in each row and column of T^G equals 1. However, for $N_G > 2$ bistochasticity is not a sufficient condition for unistochasticity (see, e.g., refs. 19–21 and 14), and it is in general hard to decide whether a given bistochastic matrix is unistochastic or not. Even necessary and sufficient conditions for the pattern of unitary matrices are not known, see ref. 22 for some necessary conditions.

On the other hand, the quantisation of a unistochastic matrix T^G is not unique. For every matrix U^G fulfilling (34), the set of unitary matrices of the form

$$\tilde{U}^G = D_1 U^G D_2, \tag{35}$$

with D_1 and D_2 being diagonal unitary matrices, are also quantisations of T^G. One can therefore introduce a $2N_G - 1$ parameter family of unitary matrices corresponding to the same classical stochastic process defined by T^G. By choosing the phases in D_1 and D_2 randomly with respect to the uniform measure on the interval $[0, 2\pi)$ one can define an ensemble of unitary matrices linked to the transition matrix T^G as proposed in ref. 13, also called a *unitary stochastic ensemble* (*USE*) of T^G. The transition matrix T^G is stochastic and its largest eigenvalue λ_1 is equal to unity.[19] It was conjectured in ref. 13 that the statistical properties of spectra of unitary matrices in a given *USE* after ensemble average are linked to the *spectral gap* $\Delta_{T^G} = 1 - |\lambda_2|$ of T^G, where λ_2 is the subleading eigenvalue of T^G. The conjecture in ref. 13 implies in particular the following

Conjecture 9. Let $T(N)$ be a family of unistochastic transition matrices of dimension N; the corresponding unitary stochastic ensembles follow random matrix theory (RMT) in the limit $N \to \infty$ if the spectral gap is bounded from below, that is, if $\Delta_{T(N)} \geqslant c > 0$ in this limit.

It has been shown in the last section, that the spectral gap remains constant for stochastic processes generated by line-graph iterations. The conjecture thus implies that unistochastic ensembles derived from quantisable line-graph families $L^n(G)$ follow RMT in the limit $n \to \infty$ (assuming G is a strongly connected digraph not isomorphic to a cycle) if the spectral gap of the Markov chain on the initial graph $\Delta_{T(G)} > 0$. As mentioned above not all stochastic processes on digraphs are quantisable in the sense above and it is in general hard to decide whether a given bistochastic transition matrix is unistochastic or not or even whether a given graph G is quantisable. Surprisingly, life becomes much easier when considering line-graphs. Necessary and sufficient conditions for the quantisability of $L^n(G)$ can actually be given and will be discussed in the next section.

4.2. Quantisable Line-Graphs

We start by giving an answer to the question whether a given graph H is the line-graph of another graph. The following are necessary and sufficient conditions given by Richards,[23] see ref. 24 for a comprehensive overview over other equivalent statements.

Theorem 10. Let H be a digraph and A^H be its adjacency matrix. The following statements are equivalent:

(i) H is a line-digraph;

(ii) any two rows of A^H are either identical or orthogonal;

(iii) any two columns of A^H are either identical or orthogonal.

It should be noted that a line-graph does in general not specify uniquely its ancestor graph. This non-uniqueness is caused by sources and sinks, (that is vertices with only outgoing or incoming edges) or isolated vertices in the line-graph, see ref. 24. This problem is less relevant for quantisable line-graphs as will be shown later, we will therefore not consider it here further.

An immediate consequence of Theorem 10 is the following necessary and sufficient condition for a line-graph to be quantisable:

Corollary 11. Let H be a digraph with N vertices and A^H be its adjacency matrix. Then H is a quantisable line-digraph iff there exist permutation matrices P and Q such that PA^HQ is block-diagonal of the form

$$PA^HQ = \begin{pmatrix} J_{n_1} & & & \\ & J_{n_2} & & \\ & & \cdots & \\ & & & J_{n_k} \end{pmatrix} \tag{36}$$

where J_n is the square matrix of dimension n containing only 1's and

$$\sum_{i=1}^{k} n_i = N. \tag{37}$$

Proof. Follows directly from Theorem 10. The identical rows (and columns) of A^H form submatrices of A^H containing only 1's. These submatrices have to be square matrices in order to have the same pattern as a unitary matrix. The last condition (37) follows from the fact that a unitary matrix can not have a zero row or column.

The number of submatrices k in (36) is equal to the number of vertices in the ancestor graph and n_i corresponds to the number of incoming and outgoing edges at a vertex v_i of the ancestor graph. The Corollary 11 is thus equivalent to the statement

Corollary 12. A graph G has a quantisable line-graph $L(G)$ iff for every vertex v_i in $V(G)$ the number of outgoing edges equals the number of incoming edges, that is, $d^+(v_i) = d^-(v_i)$.

The number of incoming and outgoing edges may of course vary from vertex to vertex.

Quantisability of a line-graph turns out to be a rather strong condition. Disregarding possible isolated vertices in the ancestor graph, we can make the following statements about the ancestor graph of a quantisable line-graph:

Corollary 13. Let H be a quantisable line-graph and G the ancestor of H; this implies

(i) the ancestor graph G is uniquely defined by H up to graph isomorphism;

(ii) G is either strongly connected or disconnected; if it is disconnected, then each of the disconnected components is strongly connected.

4.3. Quantisable Families of Line-Graphs

We now turn to the question, whether a given graph G has a quantisable nth generation line-graph $L^n(G)$. A necessary and sufficient condition is given by the following theorem

Theorem 14. A graph G has a quantisable nth generation line-graph $L^n(G)$ iff for every vertex $v_i \in V(G)$ and every $v_j \in N_+^{(n-1)}(v_i)$, that is, for every vertex v_j which can be reached from v_i in $n-1$ steps, one finds

$$d^-(v_i) = d^+(v_j). \tag{38}$$

Equivalently, one can write the condition above in terms of the $(n-1)$-step in-neighbourhood $N_-^{(n-1)}$ of the vertices of G.

Proof. Let us start by giving the condition for the $(n+1)$-st generation line-graph to be quantisable; from Corollary 12 one obtains that $L^{n+1}(G)$ is quantisable, iff every vertex $v_i^{(n)} \in V(L^n(G))$ has as many incoming as outgoing edges. We may thus write

$$\sum_j A_{ji}^{L^n(G)} = \sum_k A_{ik}^{L^n(G)} \qquad \text{for all} \quad i, \tag{39}$$

and the sum runs over all possible vertices of $L^n(G)$. A vertex $v_i^{(n)} \in V(L^n(G))$ can be written in terms of n-step paths in the original graph G, that is,

$$v_i^{(n)} \equiv (v_{i_0}, v_{i_1}, \dots, v_{i_n}) \qquad \text{for a set of vertices with} \quad A^G_{i_0 i_1} \cdot A^G_{i_1 i_2} \cdots A^G_{i_{n-1} i_n} \neq 0 \tag{40}$$

We now write Eq. (39) in the form

$$\sum_i A_{ij}^{L^n(G)} = \sum_{i_0} A^{L^n(G)}_{i_0 \cdots i_n,\, i_1 \cdots i_{n+1}} = A^G_{i_1 i_2} \cdot A^G_{i_2 i_3} \cdot \cdots \cdot A^G_{i_n i_{n+1}} \sum_{i_0} A^G_{i_0 i_1} \tag{41}$$

and

$$\sum_i A_{ji}^{L^n(G)} = \sum_{i_{n+2}} A^{L^n(G)}_{i_1 \cdots i_{n+1},\, i_2 \cdots i_{n+2}} = A^G_{i_1 i_2} \cdot A^G_{i_2 i_3} \cdot \cdots \cdot A^G_{i_n i_{n+1}} \sum_{i_{n+2}} A^G_{i_{n+1} i_{n+2}} . \tag{42}$$

We thus obtain the condition

$$d^-(v_{i_1}) = \sum_{i=1}^N A^G_{i i_1} = \sum_{i=1}^N A^G_{i_{n+1} i} = d^+(v_{i_{n+1}}) \qquad \text{if} \quad A^G_{i_1 i_2} \cdot A^G_{i_2 i_3} \cdot \cdots \cdot A^G_{i_n i_{n+1}} \neq 0, \tag{43}$$

that is, if there exists a path to reach $v_{i_{n+1}}$ from v_{i_1} in n steps; this completes the proof of the theorem.

Equivalently, Theorem 14 may be expressed as

Corollary 15. A graph G with adjacency matrix A^G has a quantisable nth generation line-graph $L^n(G)$ iff for every pair of vertices $v_i, v_j \in V(G)$

$$d^-(v_i) = d^+(v_j) \quad \text{whenever} \quad ((A^G)^{n-1})_{ij} \neq 0, \tag{44}$$

where $(A^G)^{n-1}$ denotes the $(n-1)$st power of the matrix A^G.

It is clear from the conditions above that more and more restrictions are imposed on G if one wants to construct families of line-graphs with an increasing number of quantisable line-graph generations. In the following we give a couple of general statements on line-graph families. We assume here that the ancestor graph G is connected; a generalisation to disconnected line-graphs is obvious in the light of Corollary 13.

Corollary 16. Let G be a digraph and $L^n(G)$ its family of line-graphs;

(i) $L^n(G)$ is quantisable for all n iff G is regular, that is, iff for every pair of vertices $v_i, v_j \in V(G)$, $d^+(v_i) = d^+(v_j) = d^-(v_i) = d^-(v_j)$.

(ii) Let G be a graph with a primitive adjacency matrix A^G, that is, there exists an integer k such that $(A^G)^k$ has all matrix elements strictly positive. Then $L^n(G)$ is quantisable for $n \geqslant k$ iff G is regular.

(iii) A graph of order N is called bipartite, denoted K_{N_1, N_2}, if there exist two distinct sets of vertices V_1 and V_2 with N_1 and N_2 elements, respectively, $N_1 + N_2 = N$, such that every vertex in V_1 is connected to every vertex in V_2 but not to any vertex in V_1 and *vice versa*. For $N_1 \neq N_2$ we have: A line-graph $L^n(K_{N_1, N_2})$ is quantisable iff n is an odd integer.

(iv) An r-partite graph $K_{N_1, N_2, \ldots, N_r}$ is defined in analogy to a bipartite graph. For $r \geqslant 3$ and whenever at least two of the r vertex sets contain a different number of vertices one obtains: the line-graph generations are quantisable for $n = 1$ only.

(v) The first generation line-graph of an undirected graph without isolated vertices is quantisable.

The above list is only a small selection of possible conclusions following directly from Theorem 14 for some important classes of graphs. Many more could be formulated here. It becomes clear from the examples that quantisability is a very restrictive condition. Especially point 2 in Corollary 16 is important in connection with Corollary 13. Strongly connected graphs are typically primitive; only graphs with additional structure like bipartite graphs do not fall into this class. Line-graph families with infinitely many members being quantisable thus implies a high degree of regularity in the graph.

In the next section we will discuss some examples of quantisable line-graph families and study the spectral properties of matrices of the associated unitary stochastic ensembles.

5. EXAMPLES

5.1. De Bruijn Graph Families

The aim of this section is to present the statistical properties of ensembles of unitary matrices corresponding to quantisable line-graph families of regular initial graphs G. One set of such families consists of de Bruijn graphs of Mth order.[16] They are obtained as the line-graph families of fully connected initial digraphs K_M with $A^{K_M} = J_M$, that is,

$$V(K_M) = \{1,..., M\}, \qquad E(K_M) = \{(ij) : i, j \in V(K_M)\}. \tag{45}$$

The graphs K_M have M vertices and M^2 bonds connecting each vertex with all other including itself, so they have M loops. The line-graph families $L^n(K_M)$ have accordingly M^{n+1} vertices and M^{n+2} edges with M incoming and outgoing edges at each vertex, that is, the $L^n(K_M)$ are all M-regular. The family $L^n(K_2)$ are the family of binary graphs studied in ref. 12.

In the following, we will consider stochastic transition matrices T^{K_M} on the initial graph K_M with constant transition probabilities $1/M$ between all vertices, that is, $T^{K_M} = \frac{1}{M} J_M$. These matrices saturate the well known van der Waerden inequality concerning permanents of bistochastic matrices, i.e., $\mathrm{per}(T) \geqslant M!/M^M$.[19] It is easy to see that the $T^{L^n(K_M)}$ are unistochastic, since related unitary matrices (34) may be constructed out of discrete Fourier transforms of size M, $\mathscr{F}^{(M)}_{ml} = \frac{1}{\sqrt{M}} e^{2\pi i\, ml/M}$. The graphs $L^n(K_M)$ have topological entropy equal to $\ln M$. The metric entropy of the process defined by $T^{L^n(K_M)}$ is also equal to $\ln M$.

The adjacency (and transition) matrices for the stochastic process on de Bruijn graphs represent a discrete generalization of the Bernoulli shift. Three matrices from the family $L^n(K_4)$ are depicted in Fig. 3. The non-zero elements are marked as black squares, they are placed along four lines. In the limit of large n the structure of the matrices approaches the graph of the function $4x|_{\mathrm{mod}\,1}$ (Renyi map) rotated clockwise by angle $\pi/2$. Such

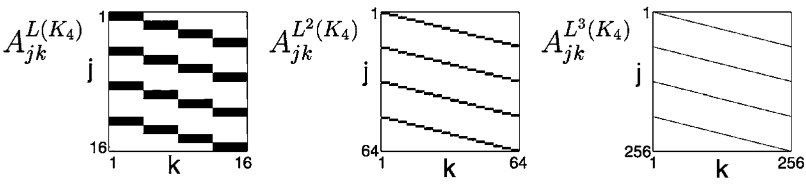

Fig. 3. Adjacency matrices $A^{L^n(K_4)}$ of 4th-order de Bruijn graphs generated as the line-graphs of the fully connected graph K_4, for $n = 1$, $n = 2$ and $n = 3$. Nonzero entries are denoted as black squares. The matrix size equals 16, 64, and 256 respectively.

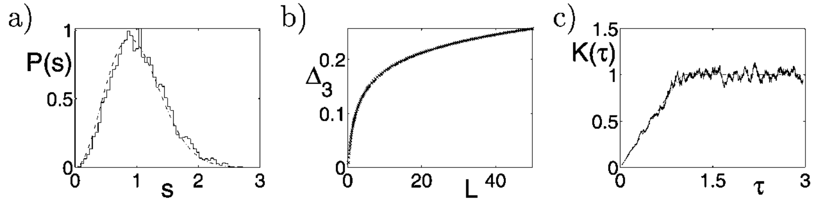

Fig. 4. Spectral statistics of a single unitary matrix of size $N = 4096$ corresponding to the de Bruijn graph $L^5(K_4)$: (a) level spacing distribution $P(s)$, (b) spectral rigidity $\Delta_3(L)$ and (c) spectral form factor $K(\tau)$ (with $\Delta\tau = 0.07$). CUE predictions (coinciding with numerical data in panel (b)) are represented by dot-dashed lines.

a correspondence between digraphs and classical dynamical systems has been recently pointed out in ref. 14.

We are interested in the spectral properties of a generic quantum propagator $U^{L^n(K_M)}$ corresponding to the Markov process on a de Bruijn graph. By means of the discrete Fourier transform $\mathscr{F}$ we constructed a unitary propagator associated with the stochastic transition matrix T^{K_M}. By multiplying with random diagonal unitary matrices D_1 and D_2 we obtain a typical element $\tilde{U}$ of the ensemble (35). Fig. 4 shows the spectral statistics received from eigenphases of a single unitary matrix of size $N = 4096$ from the ensemble, $U^{L^5(K_4)}$. The level spacing distribution $P(s)$, the spectral rigidity $\Delta_3(L)$[25] and the spectral form factor $K(\tau)$ (the Fourier transform of the two point correlation function)[26] are plotted. The statistics coincides well with the predictions of random matrices for the Circular Unitary Ensemble (CUE),[27] although it is only the fifth iteration of the line-graph construction. The spectral form factor $K(\tau)$ was averaged over a parameter window $\Delta\tau$. We have also obtained qualitatively similar results averaging $K(\tau)$ over a unitary stochastic ensemble as defined in (35) consisting of 10^3 unitary matrices $\tilde{U}$ of size 64.

5.2. Symmetric Cycle Graph Family

Next we consider a family of quantisable line-graphs which are constructed from symmetric cycle digraphs. A M-symmetric cycle graph G_M is an undirected graph with M vertices placed on a circle each vertex connected with its two neighbors only see Fig. 5. More formally,

$$\begin{aligned} V(G_M) &= \{1,\dots, M\}, \\ E(G_M) &= \{(1M), (M1)\} \cup \{(i\,i+1), (i+1\,i) : i = 1 \cdots M-1\}. \end{aligned} \tag{46}$$

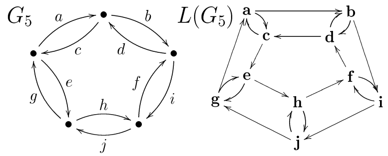

Fig. 5. Cycle graph family: G_5 and its line-graph $L(G_5)$.

The initial digraph G_M is a 2-regular graph which implies that its line-graphs $L^n(G_M)$ are all quantisable following Corollary 16. The nth line-graph generation has $M \cdot 2^n$ vertices, see Fig. 5. Next, we choose a stochastic process with equal probabilities, 1/2, to move from a given vertex to one of its neighbors. The topological and metric entropies are both equal to ln 2 in this case. The non-zero matrix elements of the adjacency matrices in the family have the same structure for any fixed M, see Fig. 6 for the family $L^n(G_5)$. Cycle graphs and their quantisation play an important role in the study of Anderson-type localisation in one-dimensional diffusive systems. A full description of localisation in terms of return probabilities on infinite chains has been given by Schanz and Smilansky,[5] cycle graphs have also been discussed in ref. 13 in connection with the spectral gap of the corresponding Markov process. One finds

$$\Delta_{T^{G_M}} \sim M^{-2} \tag{47}$$

that is, the spectral gap vanishes for large M. We may now consider two limits: by fixing the generation n of the line-graph $L^n(G_M)$ and looking at the limit $M \to \infty$ one indeed finds deviation from RMT due to localisation;[13] we may on the other hand fix M and increase n which produces line-graphs with an increasing number of vertices but constant spectral gap and we expect RMT-behaviour in this limit.

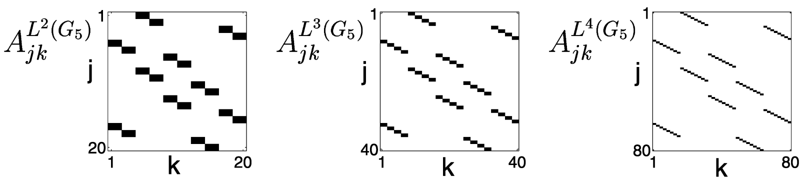

Fig. 6. Structure of the adjacency matrices of line-graphs family $L^n(G_5)$ obtained from the symmetric cycle graph G_5 with $n = 2$, $n = 3$ and $n = 4$ with matrix size $N = 20$, 40, 80, respectively.

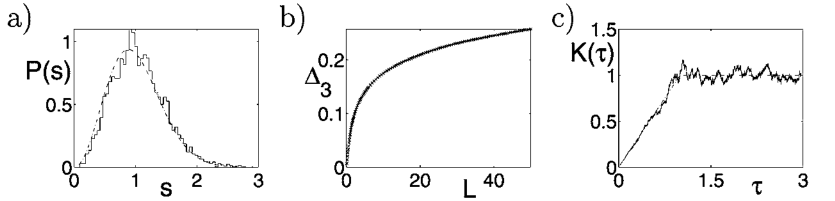

Fig. 7. As in Fig. 4 for a single random unitary matrix of size 5120 associated with the digraph $L^{10}(G_5)$.

This is indeed what is observed; in Fig. 7 the statistics obtained from a quantum propagator $U^{L^{10}(G_5)}$, with randomly chosen phases conforms well with the prediction of CUE.

5.3. Bipartite Graph Family $L^n(K_{2,M})$

As a last example we will have a look at bipartite digraphs K_{N_1,N_2}, see Corollary 16(iii). In terms of its vertex and edge set, K_{N_1,N_2} is defined as

$$\begin{aligned} V(K_{N_1,N_2}) &= V_1 \cap V_2, \quad V_i = \{1,\ldots, N_i\}, \\ E(K_{N_1,N_2}) &= \{(ij), (ji) : i \in V_1, j \in V_2\}. \end{aligned} \tag{48}$$

A class of bipartite graphs, which has been studied recently in the context of spectral statistics of quantum graphs are so-called star graphs $K_{1,M}$ which have one central vertex and M arms.[2, 20, 13] Using the quantisation condition employed by Kottos and Smilansky[2] leads to quantum propagation with an associate transition matrix with spectral gap scaling like $\Delta_M \sim 1/M$; again one finds deviations of the spectral statistics from RMT persisting in the large M limit. By fixing M and considering the line-graph family $L^n(K_{1,M})$, which is quantisable for n odd, see Corollary 16, we can again achieve a large matrix limit with non-vanishing spectral gap. We indeed find convergence to the RMT - statistics to a degree very similar to Figs. 4 and 7. We also studied bipartite graphs $K_{2,M}$ and its line-graphs. An example of such a graph is plotted in Fig. 8. The graphs in the family

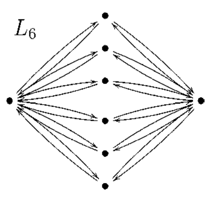

Fig. 8. Bipartite digraph $K_{2,6}$ — the initial digraph in the bipartite graph family $L^n(K_{2,6})$.

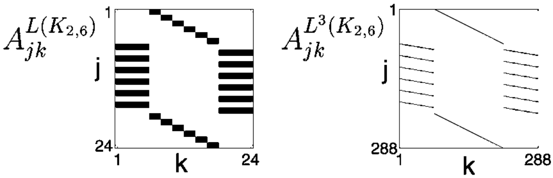

Fig. 9. Structure of the adjacency matrices for line-graphs of bipartite graphs $L^n(K_{2,6})$ for $n = 1$ and $n = 3$; the corresponding matrix sizes are $N = 24$ and $N = 288$.

$L^n(K_{2,M})$ have vertices with either 2 or M outgoing edges and are again quantisable for n odd. A unistochastic transition matrix may be constructed choosing probabilities $1/2$ for vertices with 2 outgoing bonds and $1/M$ otherwise. Figure 9 shows the structure of the non-zero elements of transition matrices for $L(K_{2,6})$ and $L^3(K_{2,6})$.

The construction of a unitary quantum map may be achieved by means of the discrete Fourier transform. As for the previous examples, the spectral statistics of eigenphases of $U^{L^n(K_{2,6})}$ follows CUE to the same degree as shown in Figs. 4 and 7 for $n \geqslant 5$.

6. CONCLUSIONS

By constructing directed line-graphs from an arbitrary initial digraph G one obtains a family of graphs with in general increasing number of vertices but identical topological and metric properties. We showed that all digraphs in such a family indeed have the same set of periodic orbits and that furthermore the non-zero eigenvalues of the adjacency matrices of graphs from the same family are identical. Next we considered stochastic Markov processes on a digraph and defined the corresponding process on its line-graph. We demonstrated that both processes have the same metric entropy and the transition matrices describing the processes have the same non-zero eigenvalues. The construction of the line-graph family is in fact a method to translate a finite Markov processes to a larger space preserving its topological and metric properties.

We gave necessary and sufficient conditions for a line-graph to be quantisable and gave examples of line-graph families $L^n(G)$ which can be quantised for infinitely many n. The line-graph construction thus makes it possible to consider a semiclassical limit of large matrix size for unitary ensembles on graphs with fixed "classical," i.e., stochastic dynamics. This method complements an idea developed in a previous paper,[14] in which a semiclassical limit was considered by looking for a specific dynamical system associated with an initial graph.

We would like to stress again that the problem of finding necessary and sufficient conditions for a general bistochastic matrix T to be unistochastic is still open.[21] Such conditions can, however, be given for line-graphs and turn out to be very restrictive. One way to enlarge the number of graph families with well defined classical limit is to consider unitary matrices U^n and associated transition matrices $T^{(n)}$ for which topological and metric properties converge to fixed values in the limit of large matrix sizes.

Quantum maps generated from Markov processes on families of line-graphs considered here all display CUE statistics in their spectral fluctuations. These results were observed for families originating from fully connected digraphs (de Bruijn), symmetric cycles and bipartite digraphs of the form $K_{1,M}$ and $K_{2,M}$. This behaviour is attributed to the fact that the spectral gap is positive and constant under the line-graph iteration in all cases whereas the number of vertices increases with n. The results thus confirm the Conjecture 9, which relates the size of the spectral gap of the classical transition matrix and the spectral statistics of the associated ensemble of random unitary matrices.

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