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Unitary-stochastic matrix ensembles and spectral statistics

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Abstract

We propose to study unitary matrix ensembles defined in terms of unitary-stochastic transition matrices associated with Markov processes on graphs. We argue that the spectral statistics of such an ensemble (after ensemble averaging) depends crucially on the spectral gap between the leading and subleading eigenvalue of the underlying transition matrix. It is conjectured that unitary-stochastic ensembles follow one of the three standard ensembles of random matrix theory in the limit of infinite matrix size $N \to \infty$ if the spectral gap of the corresponding transition matrices closes slower than $1/N$. The hypothesis is tested by considering several model systems ranging from binary graphs to uniformly and non-uniformly connected star graphs and diffusive networks in arbitrary dimensions.

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1. Introduction

The study of quantum mechanics on graphs has become an important tool for investigating the influence of classical dynamics on spectra, wavefunctions and transport properties of quantum systems. Quantum networks have been used with great success to model quantum phenomena observed in disordered metals and mesoscopic systems (Shapiro 1982, Chalker and Coddington 1988); typical behaviour found in extended, diffusive systems such as localization–delocalization transitions (Freche *et al* 1999), multifractal properties of wavefunctions at the transition point (Klesse and Metzler 1995, Huckestein and Klesse 1999), transport properties (Pascaud and Montambaux 1999, Huckestein *et al* 2000) and the statistical properties of quantum spectra (Klesse and Metzler 1997) have been studied on graphs in the limit of infinite network size. Recently, Kottos and Smilansky (1997, 1999) proposed to study quantum spectra of non-diffusive graphs with only relatively few vertices or nodes. This work was motivated by understanding how the topology of the graph as well as the boundary conditions imposed at the vertices influence the statistical properties of the eigenvalue spectrum. A closed expression for the level spacing distribution of quantum graphs has recently been given by Barra and Gaspard (2000).

The statistical properties of general quantum systems have been studied intensively over the last two decades or so. Numerical evidence suggests that the eigenvalue spectrum of a quantum system whose classical limit is chaotic follows one of the three standard ensembles in random matrix theory (RMT) (Mehta 1991) after suitable energy averaging. Quantum systems, whose classical limits show mixed or integrable classical dynamics, deviate from the RMT results. Little progress has been made from a theoretical point of view since the connection between quantum spectra and RMT was first noted by Bohigas *et al* (1984), Berry (1985) and others. Universality in the long-range spectral correlations could be attributed to classical sum-rules (Berry 1985). Led by supersymmetric arguments, Agam *et al* (1995) and Andreev and Altshuler (1995) linked the existence of universal statistics to the decay of correlation in the classical dynamics. This result was supported by semiclassical arguments given by Bogomolny and Keating (1996). Zirnbauer (1999) considered ensembles of possible quantizations of a given classical system and reformulated the original random matrix conjectures by suggesting that the ensemble of quantum spectra corresponding to quantizations of a classical chaotic dynamics follow RMT on average.

The approach taken in the following is in the spirit of Zirnbauer's averaging over quantizations. We make a connection between certain unitary matrix ensembles and classical Markov processes on a graph. It is argued that the statistical properties of an ensemble after ensemble averaging depend crucially on the spectrum of the transition matrix of the corresponding Markov process. Convergence of the ensemble average towards one of the three generic unitary matrix ensembles, the circular-unitary, circular-orthogonal or circular-symplectic ensembles (CUE, COE or CSE) in the limit of infinite matrix size, is conjectured to hold only if correlations in the stochastic Markov process decay fast enough in this limit.

Before introducing these concepts in the following sections, we briefly recapitulate the main ideas behind the quantization of graphs. A quantum graph is essentially a network of vibrating strings fulfilling certain boundary conditions at the vertices. (In the usual notation of graph theory, we call a directed bond between a vertex i and a vertex j of the graph an edge (ij).) Wave propagation on the graph is written in terms of one-dimensional plane waves moving in both directions along undirected edges, and one therefore considers *undirected* graphs in general. Following the notation of Kottos and Smilansky (1997), a quantum graph is characterized by an N-dimensional, unitary matrix $\boldsymbol{S}_B(k)$ with k being the wavenumber and N corresponds to the number of *directed* edges. It may be written in the form

$$\boldsymbol{S}_B(k) = \boldsymbol{D}(k)\boldsymbol{V}(k). \tag{1}$$

Here, $\boldsymbol{D}$ is a diagonal matrix with diagonal elements $d_{ii} = \exp(\mathrm{i}kL_i)$ where L_i is associated with the length of the edge i. The matrix elements of $\boldsymbol{V}$ contain the reflection and transmission coefficients for edge–edge transitions at vertices which depend on the boundary conditions chosen, see Kottos and Smilansky (1997, 1999) as well as Akkermans *et al* (2000) for details. The matrix $\boldsymbol{S}_B$ is a discrete quantum propagator evolving N-dimensional complex wave vectors Ψ between edges according to $\Psi_{n+1} = \boldsymbol{S}_B(k)\Psi_n$. The eigenfrequencies of the system are the wavenumbers k_n at which stationary solutions exist, i.e. $\boldsymbol{S}(k_n)$ has an eigenvalue one.

When studying the connection between the quantum and classical behaviours on graphs, we have to define first what we mean by a 'classical' dynamics on a finite network and second what constitutes the classical or thermodynamic limit when letting the size of the network go to infinity. Defining a classical deterministic dynamics on a graph which consists of a finite number of vertices acting as branching points of the dynamics does indeed not make sense in general (Barra and Gaspard 2001). Instead, one may link the probabilistic dynamics of a Markov process defined on the same network with the quantum evolution described by the unitary matrix $\boldsymbol{S}_B$. Kottos and Smilansky (1997) suggested considering the Markov process defined by the transition matrix $\boldsymbol{T}$ with matrix elements given by the relation $t_{ij} = |S_{Bij}|^2$. The stochastic matrix $\boldsymbol{T}$ is itself a propagator describing the time evolution of a probability distribution of particles moving stochastically through the network with transition probabilities between adjacent edges given by the matrix elements of $\boldsymbol{T}$. The degree of chaos found in such a stochastic dynamics is characterized by the decay of correlation of an initial probability distribution and thus by the spectrum of $\boldsymbol{T}$. Note that the classical Markov process depends on the structure of the graph as well as on the boundary conditions via $\boldsymbol{V}$ but not on metric properties of the graph entering through the phases L_i; this is in contrast to the stochastic dynamics introduced by Barra and Gaspard (2001). Note also that the transition matrices $\boldsymbol{T}$ as defined above describe transitions between the edges of the graph, not between vertices.

In the following we generalize this approach by making a connection between arbitrary unitary matrices and their associated stochastic transition matrices. In section 2, we briefly discuss the possible Markov processes which may be associated with unitary evolution on finite graphs and we specify an ensemble of unitary matrices linked to a given transition matrix. In section 3 we introduce the spectral form factor which is the statistical quantity considered throughout the paper, and we define a classical limit for networks and formulate a random matrix conjecture for unitary matrix ensembles in the limit of infinite network size. Some model systems are studied in more detail in section 4.

2. Unitary matrices and associated transition matrices

Any unitary matrix $\boldsymbol{U}$ of dimension N can naturally be linked to a stochastic transition matrix $\boldsymbol{T}$ of a finite Markov process with time-independent transition probabilities by making the following connection between matrix elements of $\boldsymbol{U}$ and $\boldsymbol{T}$, i.e.

$$u_{ij} = r_{ij}\mathrm{e}^{\mathrm{i}\phi_{ij}} \longrightarrow t_{ij} = |u_{ij}|^2 = r_{ij}^2. \tag{2}$$

The matrix $\boldsymbol{T}$ is clearly a stochastic matrix due to the unitarity of $\boldsymbol{U}$; that is, $\boldsymbol{T}$ fulfils

$$\begin{aligned} &t_{ij} \geqslant 0 && \text{for all} \quad i, j = 1, \ldots, N \\ &\sum_{j=1}^{N} t_{ij} = 1 && \text{for all} \quad i = 1, \ldots, N. \end{aligned} \tag{3}$$

This implies that one is an eigenvalue of $\boldsymbol{T}$, all other eigenvalues have a modulus less than or equal to one. The matrix elements t_{ij} can be interpreted as probabilities for making a transition from a vertex i to a vertex j on a graph of N vertices. The structure of the corresponding graph is explicitly defined through $\boldsymbol{T}$ and thus $\boldsymbol{U}$, i.e. an edge (ij) exists if and only if $t_{ij} > 0$. The connection (2) therefore provides a natural link between a unitary 'quantum' evolution and a stochastic 'classical' dynamics in the form

$$\begin{array}{cc} \text{quantum} & \text{classical} \\ \Psi_{n+1} = \boldsymbol{U}^{\dagger}\Psi_n & p_{n+1} = \boldsymbol{T}^{\dagger} p_n. \end{array} \tag{4}$$

Here, Ψ_n is a complex N-dimensional wave vector propagating through the network and p_n is a probability distribution; its ith component corresponds to the probability of finding a particle at vertex i at time n after having wandered stochastically through the network starting with a probability distribution p_0 at time $n = 0$ (Berman and Plemmons 1979). Note that, in contrast to the quantum graphs briefly described in section 1, the graphs defined through general unitary matrices may be directed. The dynamics on the graph is now defined with respect to the vertices of the graph, not with respect to the edges.

It is conjectured that statistical properties of generic quantum spectra are strongly influenced by how fast correlations in the corresponding classical dynamics decay (Bohigas *et al* 1984, Berry 1985). We may thus expect that the statistical properties of the spectrum of a unitary matrix $\boldsymbol{U}$ are linked to the properties of the stochastic dynamics generated by the associated transition matrix $\boldsymbol{T}$. Before discussing this further in section 3, we explore the link between unitary and stochastic matrices in more detail.

2.1. Unitary-stochastic matrices

Not every stochastic matrix $\boldsymbol{T}$ fulfilling the conditions (3) can be associated with a unitary matrix as defined in (2). Indeed, unitarity requires that besides (3), also the condition

$$\sum_{i=1}^{N} t_{ij} = 1 \qquad \text{for all} \quad j \tag{5}$$

holds; that is, $\boldsymbol{T}$ must be *doubly stochastic* (Marshall and Olkin 1979). One deduces immediately that the vector $\tilde{p}$ with components $\tilde{p}_i = 1/N$ for all $i = 1, \ldots, N$ is a stationary state, i.e. it is the left eigenvector of $\boldsymbol{T}$ with eigenvalue 1. (Of course, it is also the right eigenvalue of $\boldsymbol{T}$ as for all stochastic matrices.) This in turn implies that the Markov process is ergodic or irreducible (Berman and Plemmons 1979) if the graph is connected, that is, if it is not possible to decompose the underlying graph into disconnected subgraphs. A general stochastic matrix is called primitive if $\boldsymbol{T}^k$ is positive for some $k \geqslant 0$, that is $t_{ij}^{(k)} > 0$ for all i and j (Berman and Plemmons 1979). This implies that the spectrum of $\boldsymbol{T}$ given in terms of the eigenvalues $\{\Lambda_0, \ldots, \Lambda_{N-1}\}$ with $|\Lambda_i| \leqslant |\Lambda_j|$ for $i > j$ or in terms of the eigenexponents $\{\lambda_i = -\log|\Lambda_i|\}$ has a finite gap between the leading exponent $\lambda_0 = 0$ and the next-to-leading exponents, i.e.

$$\Delta = \lambda_1 - \lambda_0 = \lambda_1 > 0. \tag{6}$$

A doubly-stochastic matrix is primitive if the graphs corresponding to $\boldsymbol{T}^n$ are connected for all n. A finite gap in the spectrum means that initial probability distributions p_0 on the network decay exponentially towards the equilibrium distribution $\tilde{p}$ with decay rate λ_1.

Without going further into the theory of doubly-stochastic matrices we note that a doubly-stochastic matrix can be written in terms of $(N-1)^2$ independent parameters, say the matrix elements in the first $N-1$ rows and columns. These matrix elements are constrained by the inequalities

$$\begin{array}{ll} \displaystyle\sum_{i=1}^{N-1} t_{ij} \leqslant 1 \qquad \text{for all} \quad j & \displaystyle\sum_{j=1}^{N-1} t_{ij} \leqslant 1 \qquad \text{for all} \quad i \\ \displaystyle\sum_{i,j=1}^{N-1} t_{ij} \geqslant N-2 & t_{ij} \geqslant 0 \qquad \text{for all} \quad i, j \end{array} \tag{7}$$

and thus correspond to a finite domain in the $(N-1)^2$-dimensional parameter space.

Not every doubly-stochastic matrix can be associated with a unitary matrix as defined in equation (2). The rows and columns of a unitary matrix have to obey orthogonality conditions which impose further restrictions on the matrix elements t_{ij}. One therefore defines the subset of doubly-stochastic matrices $\boldsymbol{T}$ which fulfil $t_{ij} = |u_{ij}|^2$ for some unitary matrix $\boldsymbol{U}$ as *unitary-stochastic* transition matrices (Marshall and Olkin 1979). The dimension of the parameter space for unitarity-stochastic matrices is $(N-1)^2$ as for doubly-stochastic matrices; the parameter space covered by unitary-stochastic matrices is, however, in general smaller than the domain specified in equation (7). To get precise bounds for the possible parameters for unitary-stochastic matrices is a non-trivial problem in general and is beyond the scope of this paper (see also Pakoński *et al* (2001) for details).

2.2. Unitary-stochastic ensembles

Next we focus on the space of unitary matrices related to a given unitary-stochastic matrix $\boldsymbol{T}$. This space, together with a probability measure specified later, forms an ensemble which we call a *unitary-stochastic ensemble* $U(N, \boldsymbol{T})$. These ensembles have a surprisingly simple structure. The number of independent parameters determining a unitary matrix uniquely is N^2. Of these, $(N-1)^2$ parameters are fixed by the unitary-stochastic matrix $\boldsymbol{T}$, namely the amplitudes $r_{ij} = \sqrt{t_{ij}}$. After decomposing $\boldsymbol{U} \in U(N, \boldsymbol{T})$ in the form

$$\boldsymbol{U} = \boldsymbol{D}_1 \tilde{\boldsymbol{U}} \boldsymbol{D}_2 = \begin{pmatrix} e^{i\varphi_1} & & & \\ & e^{i\varphi_2} & & \\ & & \ddots & \\ & & & e^{i\varphi_N} \end{pmatrix} \begin{pmatrix} r_{11} & r_{12} & \dots & r_{1N} \\ r_{21} & & & \\ \vdots & & \boldsymbol{W} & \\ r_{N1} & & & \end{pmatrix} \begin{pmatrix} 1 & & & \\ & e^{i\varphi_{N+1}} & & \\ & & \ddots & \\ & & & e^{i\varphi_{2N-1}} \end{pmatrix} \tag{8}$$

one finds that the remaining $2N-1$ independent parameters are the phases φ_i which can take any values in $[0, 2\pi]$. The building block of the ensemble is the unitary matrix $\tilde{\boldsymbol{U}}$ which has been chosen here to have real, positive matrix elements in the first row and column. The phases of $\tilde{\boldsymbol{U}}$, and thus of $\boldsymbol{W}$, are fixed by the $N(N-1)$ orthogonality conditions between the rows (or columns) of $\tilde{\boldsymbol{U}}$. This set of equations has a discrete set of solutions and $\tilde{\boldsymbol{U}}$ is in general not uniquely determined by $\boldsymbol{T}$ for $N \geqslant 3$ (Pakoński *et al* 2001). To find all possible solutions for $\tilde{\boldsymbol{U}}$ is a non-trivial problem in general and is linked to the problem of finding the maximally available parameter space for unitary-stochastic matrices of a given dimension.

The ensemble $U(N, \boldsymbol{T})$ as a whole is parameterized by $2N-1$ phases φ_i at most and has, for fixed $\tilde{\boldsymbol{U}}$, the topology of a $2N-1$-dimensional torus. The symmetry properties of the ensemble are essentially given by the symmetries of $\tilde{\boldsymbol{U}}$; we expect in particular time reversal symmetry if $\tilde{\boldsymbol{U}}$ and thus $\boldsymbol{T}$ are symmetric. The non-uniqueness will play a role only if the possible solutions $\tilde{\boldsymbol{U}}$ belong to different symmetry classes. Assuming that this is not the case, we may treat ensembles for fixed $\boldsymbol{T}$ but different $\tilde{\boldsymbol{U}}$ as equivalent and we therefore disregard the non-uniqueness problem for $\tilde{\boldsymbol{U}}$ in what follows.

Taking the uniform probability measure on the parameter space $\varphi_1, \dots, \varphi_{2N-1}$, we can perform the ensemble average of a function $f(\boldsymbol{U})$ by straightforward integration over the angles φ, that is

$$\langle f \rangle_{U(N,\boldsymbol{T})} = \frac{1}{(2\pi)^{2N-1}} \int_0^{2\pi} d\varphi_1 \dots \int_0^{2\pi} d\varphi_{2N-1}\, f(\varphi_1, \dots, \varphi_{2N-1}; \boldsymbol{T}). \tag{9}$$

The multiple-integral can be reduced to an integral over only the first N phases if f depends on the eigenvalues of $\boldsymbol{U}$ only. The average (9) may be written in terms of a 'time' average over an ergodic path on the torus. After choosing $2N-1$ rationally independent but otherwise arbitrary length segments $L_1, \dots, L_{2N-1}$, one defines the trajectory

$$(\varphi_1, \dots, \varphi_{2N-1})(k) = (kL_1, \dots, kL_{2N-1}) \bmod 2\pi$$

which covers the torus uniformly when letting the fictitious time k go to infinity. The average is now taken over the one-dimensional parameter family

$$\boldsymbol{U}(k) = \boldsymbol{D}_1(k) \tilde{\boldsymbol{U}} \boldsymbol{D}_2(k) \tag{10}$$

where the k-dependence in $\boldsymbol{D}_1$ and $\boldsymbol{D}_2$ enters through the replacement $\varphi_i = kL_i$ in (8). This parameterization is a generalization of the product form in equation (1). The average can now be written as

$$\langle f \rangle_{U(N,\boldsymbol{T})} = \lim_{k_0 \to \infty} \frac{1}{k_0} \int_0^{k_0} dk\, f(\boldsymbol{U}(k)). \tag{11}$$

The importance of choosing rationally independent lengths segments L_i, also stressed by Kottos and Smilansky (1997), becomes obvious. For rationally dependent L_i, only a lower-dimensional subspace of the full parameter space is covered in equation (11) which may lead to averages different from the full ensemble average (9).

3. Spectral statistics for unitary-stochastic ensembles

So far we have proposed to divide the unitary group into unitary-stochastic ensembles (USE) which are defined explicitly through unitary-stochastic matrices $\boldsymbol{T}$. We now argue that the spectral statistics of unitary matrices forming a USE depend strongly on the eigenvalues of $\boldsymbol{T}$.

3.1. The spectral form factor

In the following we identify the spectrum of a unitary matrix $\boldsymbol{U}$ of dimension N with the set of eigenphases $\{\theta_1, \ldots, \theta_N\}$ of $\boldsymbol{U}$. The statistical measure used is the so-called spectral form factor, the Fourier transform of the spectral two-point correlation function

$$R_2(x) = \frac{1}{\overline{d}^2} \left\langle d(\theta) d(\theta + x/\overline{d}) \right\rangle_{U(N,\boldsymbol{T}),\theta} . \qquad (12)$$

Here, $d(\theta, N) = \sum_{i=1}^{N} \delta(\theta - \theta_i)$ denotes the density of states and the mean density $\overline{d}$ is given by $\overline{d} = N/2\pi$ (see, for example, Tanner (1999)). The average is taken over the angle θ and a USE. After averaging out the θ dependence, one recovers the Fourier coefficients in terms of the traces of $\boldsymbol{U}$; i.e., one obtains for the form factor

$$K(\tau) = \left\langle \tfrac{1}{N} |\operatorname{Tr} \boldsymbol{U}^{N\tau}|^2 \right\rangle_{U(N,\boldsymbol{T})} \qquad (13)$$

where $\tau = n/N$ and the average is taken over a USE. The traces of $\boldsymbol{U}^n$ can be written as (Kottos and Smilansky 1997)

$$\operatorname{Tr} \boldsymbol{U}^n = \sum_p^{(n)} A_p \mathrm{e}^{\mathrm{i}L_p} \qquad (14)$$

where the summation is over all periodic or closed paths of length n on the graph. Characterizing a given periodic path by its vertex code $(v_1, v_2 \ldots v_n)$, $v_i \in \{1, 2, \ldots, N\}$ with $(v_i v_{i+1})$ being allowed transitions between vertices, one obtains, following the notation in equation (2):

$$L_p = \sum_{i=1}^{n} \phi_{v_i v_{i+1}} \qquad A_p = \prod_{i=1}^{n} r_{v_i v_{i+1}} . \qquad (15)$$

The form factor can thus be written as a double sum over periodic paths on the graph

$$K(\tau) = \left\langle \frac{1}{N} \sum_{p,p'}^{(n)} A_p A_{p'} \mathrm{e}^{\mathrm{i}(L_p - L_{p'})} \right\rangle_{U(N,\boldsymbol{T})} \qquad (16)$$

$$\approx g \frac{n}{N} \operatorname{Tr} \boldsymbol{T}^n + \left\langle \sum_{p \neq p'}^{(n)} A_p A_{p'} \mathrm{e}^{\mathrm{i}(L_p - L_{p'})} \right\rangle_{U(N,\boldsymbol{T})} . \qquad (17)$$

The first term in (17) is the so-called diagonal term (Berry 1985). It stems from periodic orbit pairs (p, p') related through cyclic permutations of the vertex symbol code, that is, of orbits with vertex codes $(v_1, v_2 \ldots v_n), (v_2, v_3 \ldots v_n, v_1), \ldots, (v_n, v_1 \ldots v_{n-2}, v_{n-1})$; there are typically n orbits related by cyclic permutations and all these orbits have the same amplitude A and phase L. The corresponding periodic orbit pair contributions in (16) are thus equal to A_p^2

which is the classical probability for following a given cycle for one period. Additional periodic orbit degeneracies may occur due to symmetries. For time reversal symmetric dynamics, for example, periodic cycles with symbol code $(v_1, v_2 \ldots v_n)$ and $(v_n, v_{n-1} \ldots v_1)$ have identical phases and amplitudes. This leads to an additional symmetry degeneracy factor g in (17) which is one for non time reversal symmetric dynamics and two for time reversal symmetric dynamics.

The diagonal term constitutes the important connection between the form factor and the stochastic transition matrix $\boldsymbol{T}$. The second term in (17) is a double sum over the remaining periodic orbit pairs. Contributions to this term which survive the ensemble average can be formulated in terms of periodic orbit degeneracy classes and are due to phase correlations imposed by unitarity conditions (Berkolaiko and Keating 1999, Tanner 2000). These contributions are negligible in the limit $\tau \to 0$ after ensemble averaging, but are vital to reproduce the form factor for finite τ values.

Working in the diagonal approximation valid in the asymptotic regime $n \to \infty$ and $n/N = \tau \to 0$, one obtains

$$K(\tau) \approx g\,\tau\ \mathrm{Tr}\,\boldsymbol{T}^n = g\,n\,\overline{P}(n) \tag{18}$$

where we introduce the mean return probability per vertex (Argaman *et al* 1993)

$$\overline{P}(n) = \tfrac{1}{N}\,\mathrm{Tr}\,\boldsymbol{T}^n. \tag{19}$$

We argue that the spectrum of $\boldsymbol{T}$ determines whether or not the statistical behaviour of a USE $U(N, \boldsymbol{T})$ follows RMT in the classical limit $N \to \infty$. Before doing so, we have to specify more precisely what we mean by the classical or thermodynamic limit of a stochastic dynamics on a finite graph.

3.2. The classical limit and a random matrix conjecture for USEs

In what follows we define the classical limit of a family of stochastic Markov processes when letting the number of vertices, and thus the dimension of $\boldsymbol{T}$, go to infinity. We thereby distinguish between *finite* systems on the one hand and *extended* systems on the other. A series of Markov processes approximating the Perron–Frobenius operator of a deterministic system acting on a bounded domain is a typical example of convergence to a finite classical system. The piecewise linear maps on the unit interval considered by Pakoński *et al* (2001) are particularly simple examples where the leading eigenvalues of the Perron–Frobenius operator are recovered already by finite transition matrices. Transition matrices with increasing dimension N resolving the phase space dynamics on finer and finer scales are necessary to capture more and more details of the classical dynamics for generic maps. We distinguish these types of systems from extended systems consisting of networks of connected, equivalent subsystems, as for example the lattices shown in figure 3. Appropriate rescaling with respect to the system size is necessary here to define useful quantities describing the dynamical behaviour per 'unit cell'.

To make the notion of a classical limit precise, we adopt the following definition in what follows. We consider a series of Markov processes given in terms of transition matrices $\{\boldsymbol{T}_i,\ i = 1, \ldots, \infty\}$ with $\dim \boldsymbol{T}_i < \dim \boldsymbol{T}_j$ for $i < j$. We say that such a series has a well-defined classical limit corresponding to

- a finite classical system if the integrated return probability $IP_i(n) = \mathrm{Tr}\,\boldsymbol{T}_i^n$ converges uniformly to a limit function $IP_{\mathrm{cl}}(n)$ in the limit $N_i \to \infty$;
- an extended classical system if the mean return probability per vertex $\overline{P}_i(n) = \mathrm{Tr}\,\boldsymbol{T}_i^n/N_i$ converges uniformly to a limit function $\overline{P}_{\mathrm{cl}}(n)$ in the limit $N_i \to \infty$.

The semiclassical limit for a family of USE is then defined via a family of unitary-stochastic transition matrices $\{T_i\}$ with a well-defined classical limit in the above sense.

We are now able to formulate a random matrix conjecture for a USE in terms of the spectral gap Δ similar to the Bohigas–Giannoni–Schmit conjecture for general quantum systems (Bohigas *et al* 1984). We propose[1]:

The spectral statistics of a family of USEs $\{U(N_i, T_i)\}$ with associated transition matrices T_i having a well-defined classical limit follows one of the three random matrix ensembles CUE, COE or CSE in the semiclassical limit if the spectral gap $\Delta_i = \lambda_1^{(i)} - \lambda_0^{(i)} = \lambda_1^{(i)}$ of T_i decreases slower than $1/N_i$ in the classical limit, that is

$$\lim_{i\to\infty} \frac{\log N_i}{N_i \Delta_i} = 0. \tag{20}$$

This conjecture implies that USEs associated with transition matrices with a non-zero spectral gap and exponential decay of correlation in the classical limit follow RMT statistics. More important is the fact that the bound (20) does not exclude RMT statistics for classical dynamics with a vanishing gap and in general algebraic decay of correlation. We also emphasize that it is the spectral gap which is the crucial quantity in the conjecture. No reference is made to the Kolmogorov–Sinai (KS) entropy or similar measures of chaos as for example in the original conjecture by Bohigas *et al* (1984). We present systems with positive KS entropy not following RMT statistics in the classical limit in section 4.

The $1/N$-threshold condition in (20) is a consequence of the $\tau = n/N$ scaling; rewriting (18) in the form

$$|K(\tau) - g\tau| \approx \left| g\tau \sum_{i=1}^{N-1} \Lambda_i^n \right| \leqslant g\tau(N-1)\mathrm{e}^{-\lambda_1 N\tau}$$

condition (20) implies that the right-hand side vanishes for fixed τ and $N \to \infty$. The logarithmic term in (20) has been added to account for possible degeneracies in the classical spectrum. To prove this conjecture, one has to show that the classical condition (20) implies the RMT result for all τ (as well as for higher-order correlation functions). This problem lies at the heart of many studies conducted in the recent past (Kottos and Smilansky 1999, Berkolaiko and Keating 1999, Schanz and Smilansky 2000a, 2000b, Tanner 2000) and is not addressed further. In the next section, we instead consider a few model systems with spectral gaps below, on and above the critical threshold, and we give numerical results showing that the threshold condition is indeed vital for spectral statistics.

4. Numerical results

4.1. Unitary-stochastic ensembles with non-vanishing spectral gap

We first discuss families of USEs with transition matrices having a non-vanishing spectral gap in the classical limit. We expect these ensembles to follow RMT statistics for $N \to \infty$. Two specific examples are considered: binary graphs with sparsely filled transition matrices and a finite spectral gap, and fully connected graphs with uniform transition amplitudes having an infinitely large spectral gap. In both cases we find power-law convergence of the form factor to one of the three RMT ensembles.

[1] The condition that the family $\{T_i\}$ must have a classical limit can be relaxed. We indeed expect that USEs corresponding to an arbitrary series of transition matrices $\{T_i\}$ fulfilling the condition (20) follow RMT in the limit $N_i \to \infty$. However, the series can then not be linked to a dynamical system in general.

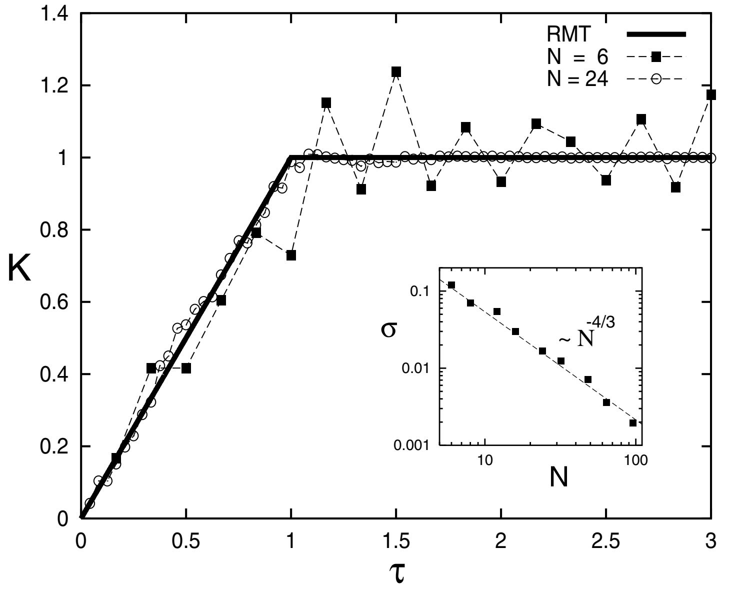

Figure 1. The form factor for binary graphs with $N = 6$ and 24. The inset shows the standard deviation of $K(\tau)$ from the RMT result as a function of N for $N = 6, 8, 12, 16, 24, 32, 48, 64$ and 96.

4.1.1. Binary graphs. We consider a special class of binary graphs with transition matrices

$$t_{ij} = \begin{cases} \frac{1}{2} & \text{if} \quad j = 2\mathrm{i} \mod N \qquad \text{or} \qquad j = (2\mathrm{i}+1) \mod N \\ 0 & \text{otherwise} \end{cases} \tag{21}$$

where the number of vertices N is even (Tanner 2000). Every vertex has two incoming and two outgoing edges and the maximal number of steps to reach every vertex from every other vertex is $\log_2 N$. It is easy to see that binary graphs of dimension $N = 2^k$, $k \in \mathbb{N}$, so-called de Bruijn graphs (Stanley 1999), have a well-defined classical limit as defined in section 3.2 which is the dynamics of the Bernoulli shift map. All eigenvalues of the transition matrices in this family are zero except the leading eigenvalue $\Lambda_0 = 1$; the spectral gap is infinitely large and the return probability $IP(n) = 1$ for all $N = 2^k$.

Furthermore it can be shown that every family of binary graphs with dimensions $N = p\,2^k$, where $p > 1$ is an odd integer, has a classical limit with a spectral gap $\Delta = \log 2$ independent of p. The decomposition (8) of the USEs is unique and the matrices $\tilde{U}$ are orthogonal, consisting of $N/2$ nested (2×2) matrices of the form

$$\tilde{u} = \frac{1}{\sqrt{2}} \begin{pmatrix} 1 & 1 \\ 1 & -1 \end{pmatrix}.$$

The spectral statistics of binary graphs in terms of periodic cycle correlations has been studied by Tanner (2000) and convergence towards RMT has been found considering transition matrices up to $N = 6$. The complexity of the combinatorial formulae describing the cycle length correlations made it difficult to advance to larger matrix sizes. The form factor can be obtained numerically by performing the ensemble average (11). Figure 1 shows the ensemble averaged form factor for matrix sizes $N = 6$ and 24, that is, two members of the $p = 3$ family. Deviations from the RMT result for the CUE clearly decreases when going from $N = 6$ to 24. The rate of convergence is measured in terms of the mean standard deviation σ averaged here over the τ interval shown, see the inset of figure 1. The numerical findings indicate a power-law behaviour $\sigma(N) \approx N^{-4/3}$ both for the $p = 1$ and the $p = 3$ family; that is, the rate of convergence does not depend on the size of the spectral gap.

4.1.2. Uniformly connected star-graphs. Fully connected graphs with constant transition probabilities, that is,

$$t_{ij} = \frac{1}{N} \qquad \text{for all} \quad i, j = 1, \ldots, N$$

display stochastic dynamics with an instant complete decay of correlations. Every initial probability distribution is mapped onto the equilibrium state $\tilde{p} = (1/N, \ldots, 1/N)$ in one step and all eigenvalues of the transition matrix are zero except for the leading eigenvalue $\Lambda_0 = 1$.

By interpreting the vertices i as the edges of a graph with a single central vertex, we may view the stochastic process as taking place on a star-shaped graph where all transitions between the edges through the central vertex are equally likely (including the 'backscattering' processes $i \to i$). Note that binary graphs of de Bruijn type with $N = 2^k$ are identical to a uniformly connected star-graph after exactly k steps. The topological entropy h_t measuring the exponential growth rate of periodic cycles diverges for star-graphs in the classical limit which is in contrast to binary graphs with[2] $h_t = \log 2$.

A possible choice for the matrix $\tilde{\boldsymbol{U}}$ in (8) defining USEs of uniformly connected transition matrices are symmetric Fourier matrices of the form

$$\tilde{u}_{nm} = \frac{1}{\sqrt{N}} \mathrm{e}^{\frac{2\pi \mathrm{i}}{N}(n-1)(m-1)}.$$

As a consequence of the symmetry of $\tilde{\boldsymbol{U}}$, we expect COE statistics which is indeed observed numerically, see figure 2. More surprising is the fact that convergence towards the RMT result is governed by the same power law as for binary graphs, see the insets of figures 1 and 2. One finds numerically $\sigma(N) \approx \frac{3}{4} N^{-4/3}$ for star-graphs; that is, the standard deviation falls off with the same exponent but a slightly smaller pre-factor. The rate of convergence is thus insensitive to the topology of the graph measured for example by the topological entropy or the spectrum of the transition matrix as long as a non-zero spectral gap is established.

4.2. Critical ensembles and deviations from RMT behaviour

Next we consider two types of systems, namely quantum star-graphs and diffusive networks, for which the spectral gap closes exactly or faster than the critical rate $\Delta \propto 1/N$. The deviations from RMT statistics have been well studied for both types of systems but have not, to our knowledge, been considered in terms of USEs and associated transition matrices.

4.2.1. Quantum star-graphs. Quantum star-graphs arise naturally when one quantizes a graph with a single central vertex attached to N undirected edges. Typical boundary conditions imposed on the wave equation at the central vertex result in restrictions on the possible transition rates and backscattering is greatly favoured. The vertex scattering matrix mentioned in (1), which is essentially equivalent to the matrix $\tilde{\boldsymbol{U}}$ in (8), is for Neumann boundary conditions of the form

$$\tilde{u}_{ij} = -\delta_{ij} + \frac{2}{N}. \tag{22}$$

The transition matrix corresponding to this orthogonal matrix describes a Markov process of weakly coupled one-dimensional systems with vanishing coupling strength in the limit

[2] A diverging topological entropy indicates a singularity in the classical dynamics and a star-graph may indeed serve as a model for a system with a point-like central scatterer (Berkolaiko *et al* 2001).

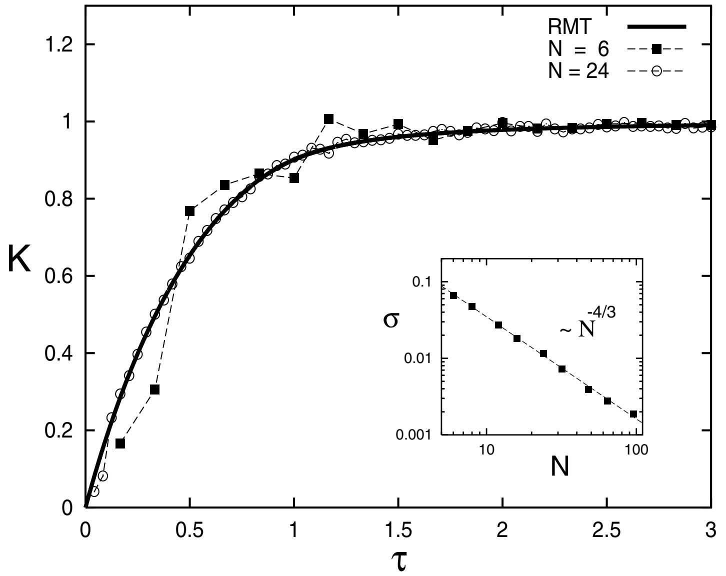

Figure 2. The form factor for uniformly connected star-graphs and the standard deviation σ.

$N \to \infty$; the system is thus extended in the sense that it consists of an increasing number of almost decoupled equivalent subsystems.

The Markov processes associated with quantum star-graphs are topologically equivalent to uniformly connected graphs discussed in section 4.1; that is, one can move from every vertex to every other vertex in one step. They do, however, differ greatly in their dynamical properties. The spectrum of the transition matrix associated with (22) is highly degenerate and can be given explicitly (Kottos and Smilansky 1999), i.e.

$$\lambda_0 = 0 \qquad \lambda_1, \ldots, \lambda_{N-1} = -\log\left(1 - \tfrac{4}{N}\right) \approx \tfrac{4}{N}.$$

Therefore, quantum star-graphs have a critical classical spectrum with a spectral gap vanishing proportional to $1/N$ and one finds spectral statistics intermediate between Poisson and COE/CUE statistics. Due to the strong enhancement of backscattering, multiple traversals of the period-1 orbits running along the N edges give the dominant contributions to the form factor for small $\tau = \frac{n}{N}$. Multiple repetitions of these orbits are invariant under cyclic permutations of the symbol code and the diagonal approximation takes on a form differing from equation (18) (Kottos and Smilansky 1999), i.e.

$$K(\tau) \approx \overline{P}(\tau) = \mathrm{e}^{-4\tau}$$

for fixed τ and $N \to \infty$. The form factor approaches one for large τ due to periodic orbit length correlations worked out in detail by Berkolaiko and Keating (1999) (see also Berkolaiko *et al* (2001)).

4.2.2. Diffusive networks. The quantum mechanics of classical diffusive systems has been studied mainly in the context of Anderson localization and insulator–metal (i.e. localization–delocalization) transitions. A variety of systems have been considered ranging from disordered conductors to dynamical localization in low-dimensional Hamiltonian systems as well as various discrete network models, see Dittrich (1996) and Janssen (1998) for recent reviews.

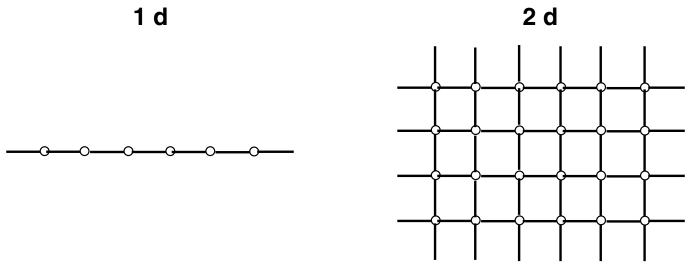

Figure 3. Diffusive network models in one and two dimensions where opposite sides are identified.

The network models considered here are similar to those studied by Shapiro (1982) consisting of regular lattices as shown in figure 3. Each vertex is connected to $2d$ neighbouring vertices via undirected edges and d is identified with the dimension of the system. We choose periodic boundary conditions and consider cubical networks having the same number of vertices, L, along each coordinate axis. The total number of vertices is thus L^d, and the number of edges equals $2\,d\,L^d$.

We consider a classical Markov process on these networks given by a transition matrix $\boldsymbol{T}_d$ with constant transition probabilities

$$t_{ij} = \frac{1}{2d} \qquad \text{if} \quad i \text{ and } j \text{ are connected}$$

and L is even. The stochastic dynamics on these networks is in the continuum limit $L \to \infty$ in appropriately rescaled units equivalent to d-dimensional diffusion governed by the diffusion equation

$$\left(\frac{\partial}{\partial t} - D\nabla^2\right)\rho(\boldsymbol{x}, t) = 0 \tag{23}$$

with diffusion constant $D = \frac{1}{2d}$. $\rho(x)$ is the continuum limit of the discrete probability distributions p. The low-lying eigenvalues λ of $\boldsymbol{T}_d$ can be recovered by solving (23) with periodic boundary conditions. The eigenvalue spectrum of (23) is given by

$$\lambda_{\boldsymbol{m}} = -\frac{4\pi^2 D}{L^2}\sum_{i=1}^{d} m_i^2 \tag{24}$$

where $\boldsymbol{m}$ is a d-dimensional integer lattice vector. The eigenvalues of $\boldsymbol{T}_d$ converge to the spectrum (24) in the large wavelength limit $m_i \ll L$ for all i. Writing the mean return probability (19) of the Markov process in terms of the spectrum (24), one obtains

$$\overline{P}(n) = \frac{1}{L^d}\,\mathrm{Tr}\,\boldsymbol{T}_d^n \approx \frac{1}{L^d}\sum_{\boldsymbol{m}}\exp\left(-\frac{4\pi^2 Dn}{L^2}\sum_{i=1}^{d} m_i^2\right) \tag{25}$$

$$= \frac{1}{(4\pi Dn)^{d/2}}\sum_{\boldsymbol{k}}\exp\left(-\frac{L^2}{4Dn}\sum_{i=1}^{d} k_i^2\right) \tag{26}$$

where the sums are over all lattice vectors $\boldsymbol{m}$, $\boldsymbol{k}$, respectively, and the last equation (26) is obtained by Poisson summation. The return probability approaches

$$\overline{P}(n) = (4\pi n D)^{-d/2} = \left(\frac{d}{2\pi n}\right)^{d/2}$$

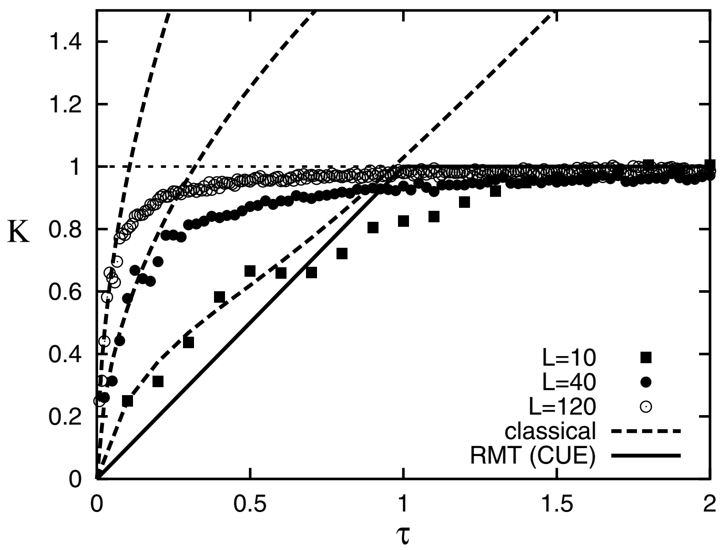

Figure 4. The form factor for one-dimensional diffusive quantum networks of different sizes. The data are compared with $n\overline{P}(n)/2d$ (dashed curve).

for large L and $n < L^2$ and converges to $\overline{P}(n) = 1/L^d$ in the limit $n \to \infty$ for fixed L. The system is thus extended having a well-defined classical limit which is of course nothing but the diffusion process (23) in an infinite domain.

The transition matrices $\boldsymbol{T}_d$ corresponding to a network of vertices on a regular lattice as shown in figure 3 are not unitary stochastic. USEs on the network can be constructed when considering the Markov process describing transitions between adjacent edges of the network instead. Edge–edge transition probabilities are again chosen to be $\tilde{t}_{ij} = 1/2d$ if i and j are incoming and outgoing edges, respectively, meeting at the same vertex. The transition matrix $\tilde{\boldsymbol{T}}_d$ of dimension $N = 2\,d\,L^d$ is unitary stochastic; furthermore it is easy to see that the non-zero eigenvalues of $\tilde{\boldsymbol{T}}_d$ coincide with the eigenvalues of $\boldsymbol{T}_d$, i.e.

$$\mathrm{Tr}\,\boldsymbol{T}_d^n = \mathrm{Tr}\,\tilde{\boldsymbol{T}}_d^n \qquad \text{for all} \quad n.$$

The matrix $\tilde{\boldsymbol{T}}_d$ consists of L coupled $2d \times 2d$-matrices. The corresponding USE can be written, for example, in terms of L coupled uniformly connected star-graphs with $2d$ edges, as described in section 4.1. Using the diagonal approximation, equation (18), together with the expression for the return probability (26), the form factor can for small τ be written as[3]

$$K(\tau) \approx \frac{n}{2dL^d}\,\mathrm{Tr}\,\tilde{\boldsymbol{T}}_d^n = n\frac{L^d}{2dL^d}\overline{P}(n) \approx \frac{1}{2d}\frac{1}{(4\pi D)^{d/2}}(N\tau)^{1-d/2} \qquad (27)$$

where we first made the diagonal approximation valid in the limit $n/L^d \to 0$ and $n \to \infty$ and the second approximation is applicable for $n < L^2$. One finds in particular for one-dimensional diffusion

$$K(\tau) \approx \frac{1}{2}\sqrt{\frac{N}{2\pi}\tau} \qquad \text{for small}\ \tau.$$

[3] There is yet another minor complication; the transition matrices introduced are not primitive. The network dynamics decomposes into two unconnected, identical networks when considering the graph for $\boldsymbol{T}_d^2$, i.e. the two-step dynamics between next-to-nearest-neighbour vertices and edges. Figures 4 and 5 therefore show $K(\tau) = \langle \frac{1}{2N}|\,\mathrm{Tr}\,\boldsymbol{U}^{2n}|^2\rangle_{U(N,\boldsymbol{T}_d)}$ with $\tau = 2n/N$.

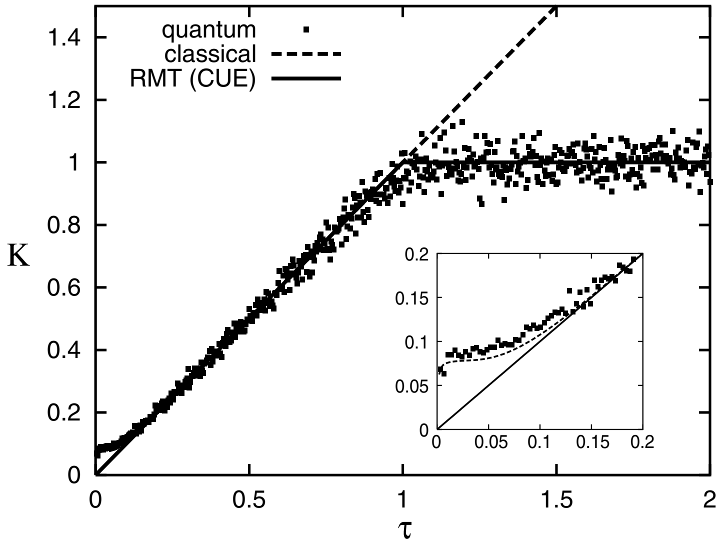

Figure 5. The quantum form factor for a two-dimensional network of side length $L = 12$ compared with classical data (dashed line). A plateau forms for small τ at $K = (4\pi)^{-1} = 0.0795\ldots$ (see also inset).

Quantum interference leads to deviations from the diagonal approximation at $\tau \approx \max(\frac{8\pi}{N}, 1)$ (Schanz and Smilansky 2000b) at which the form factor approaches one, see figure 4. The eigenstates of the USE are all localized in the classical limit, level repulsion between eigenvalues vanishes and the spectral statistics converges to the Poisson limit. The form factor forms a plateau for $d = 2$ and small τ values, that is,

$$K(\tau)_{U(N,\boldsymbol{T}_2)} \approx \frac{1}{4\pi} \qquad \text{for} \quad \tau < \frac{1}{4\pi}$$

which persists in the limit $N \to \infty$, see figure 5. We thus find a stationary distribution which converges neither to the CUE nor to the Poisson limit which is a clear indication for an ensemble being critical. Finally, considering $d > 2$, we expect convergence of the form factor to the CUE result for large N which is confirmed by numerical calculations (not shown here).

The influence of the dimension d on the small τ behaviour of $K(\tau)$ in diffusive systems has been described in detail by, for example, Dittrich (1996) and references therein. It is interesting to reconsider these results in terms of the spectral gap as described in section 3.2. The spectral gap between the leading and next-to-leading eigenvalues of $\boldsymbol{T}_d$ (and thus of $\tilde{\boldsymbol{T}}_d$) can be read off from equation (24); one obtains

$$\Delta_N = \frac{4\pi^2 D}{L^2} = \frac{4\pi^2 D (2d)^{2/d}}{N^{2/d}}$$

that is, the spectral gap falls off slower than $1/N$ for $d > 2$ only! The case $d = 2$ is critical and deviations from RMT indeed remain stationary in the classical limit. One-dimensional diffusion is in this sense supercritical leading to Poisson statistics. It is worthwhile noting that the KS entropy for the lattice dynamics considered here is positive for all d including $d = 1$ and 2, i.e. $K_{\text{KS}} = \log 2d > 0$. A positive KS entropy does therefore not necessarily imply RMT statistics.

5. Conclusion

We propose a new way to partition the unitary group into ensembles of unitary matrices specified in terms of unitary-stochastic transition matrices. This provides a framework to study systematically the connections between eigenvalue statistics of unitary matrices and the properties of an associated classical dynamics, here the stochastic dynamics on a graph. We define a classical limit of a family of stochastic networks with increasing network size. This makes it possible to give a strict criterion distinguishing between USEs whose spectral statistics converge towards the standard RMT results for $N \to \infty$ and those whose statistics do not. Arguing in the same spirit, Berkolaiko (2001) has recently shown that the spectral gap of unitary-stochastic matrices approaches infinity on average for large N when performing the average over the unitary group.

Many questions, however, remain unanswered. The most interesting one certainly is how to link the universal properties of spectra of unitary matrices found on all scales (and not only for small τ or for long-range correlations) to properties of a classical dynamics. Universality suggests a common principle; the attempts made so far to describe spectral properties of graphs beyond the diagonal approximation do, however, all rely heavily on the specific system under consideration (Kottos and Smilansky 1999, Berkolaiko and Keating 1999, Schanz and Smilansky 2000a, 2000b, Tanner 2000) and a general scheme is not yet in sight. One might furthermore expect that the spectral properties of almost all matrices within an ensemble (after applying local averaging within a given spectrum) coincide with the ensemble average. Finally, it would be interesting to study general quantum systems corresponding to a classically deterministic dynamics in terms of graphs. Connections between the semiclassical limit of a series of USEs and the semiclassical limit of a quantum map might be a way forward to understanding universality in quantum spectra in general.

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