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Spectral statistics for quantum graphs: periodic orbits and combinatorics

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ABSTRACT

We consider the Schrödinger operator on graphs and study the spectral statistics of a unitary operator which represents the quantum evolution, or a quantum map on the graph. This operator is the quantum analogue of the classical evolution operator of the corresponding classical dynamics on the same graph. We derive a trace formula, which expresses the spectral density of the quantum operator in terms of periodic orbits on the graph, and show that one can reduce the computation of the two-point spectral correlation function to a well defined combinatorial problem. We illustrate this approach by considering an ensemble of simple graphs. We prove by a direct computation that the two-point correlation function coincides with the circular unitary ensemble expression for 2×2 matrices. We derive the same result using the periodic orbit approach in its combinatorial guise. This involves the use of advanced combinatorial techniques which we explain.

§ 1. INTRODUCTION

We have recently shown (Kottos and Smilansky 1997, 1999) that the Schrödinger operator on graphs provides a useful paradigm for the study of spectral statistics and their relations to periodic orbit theory. In particular, the universal features that are observed in quantum systems whose classical counterpart is chaotic, appear also in the spectra of quantum graphs. This observation was substantiated by several numerical studies. The relevance to quantum chaology was established by identifying the underlying *mixing* classical evolution on the graphs, which provides the stability coefficients and actions of periodic orbits in whose terms an exact trace formula can be written (Kottos and Smilansky 1997, 1999, Roth 1983).

In spite of the large amount of effort invested in the past 15 years (Berry 1985, Bogomolny and Keating, 1996), we have only a limited understanding of the reasons for the universality of spectral statistics in systems whose classical dynamics are chaotic. The main stumbling block is the lack of understanding of the intricate and delicate interference between the contributions of (exponentially many) periodic

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orbits. This genuinely quantum quantity, (also known as the 'off-diagonal' contribution) is the subject of several research studies, which address it from various points of view (Argaman *et al.* 1993, Agam *et al.* 1995, Bogomolny and Keating 1966, Cohen *et al.* 1998, Miller 1998). The present contribution attempts to illuminate this issue from yet another angle, and we harness for this purpose quantum graphs and combinatorics.

Our material is presented in the following way. We shall start by defining the quantum dynamics on the graph in terms of a quantum map. This map will be represented by a unitary matrix, which is the quantum analogue of the classical Frobenius–Perron operator of the properly defined classical dynamics on the graph. The spectrum of the quantum operator is on the unit circle, and its statistics are the main object of the present work. After defining the two-point correlation function of interest, we shall write it down in terms of periodic orbits and discuss the combinatorial problem which should be addressed in order to obtain a complete expression which includes the 'off-diagonal' contribution. Since the random-matrix theory (RMT) is known to reproduce the two-point correlation function for generic graphs, we propose that the RMT expression could be obtained from a combinatorial theory, perhaps as the leading term in an asymptotic expansion. For one particular example we show that this is indeed the case in the last section. There we construct an ensemble of simple graphs with non-trivial spectral statistics, which can be solved in two independent ways. The direct way yields the statistics of RMT for the 2×2 circular unitary ensemble (CUE). The corresponding periodic orbit calculation is converted into a combinatorial problem, which is solved by proving a previously unknown combinatorial identity.

§ 2. The quantum scattering map and its classical analogue

2.1. *General definitions for quantum graphs*

We shall start with a few general definitions. Graphs consist of V *vertices* connected by B *bonds* (or *edges*). The *valency* v_i of a vertex i is the number of bonds meeting at that vertex. Associated with every graph is its *connectivity (adjacency) matrix* $C_{i,j}$. It is a square matrix of size V whose matrix elements $C_{i,j}$ are given in the following way

$$C_{i,j} = C_{j,i} = \left\{ \begin{matrix} 1 & \text{if } i, j \text{ are connected} \\ 0 & \text{otherwise} \end{matrix} \right\} \quad (i, j = 1, \ldots, V). \tag{1}$$

The valency of a vertex is given in terms of the connectivity matrix, by $v_i = \sum_{j=1}^{V} C_{i,j}$ and the total number of bonds is $B = \frac{1}{2}\sum_{i,j=1}^{V} C_{i,j}$.

When the vertices i and j are connected, we shall assume that the connection is achieved by a single bond, such that multiple bonds are excluded. We denote the connecting bond by $b = [i, j]$. Note that the notation $[i, j]$ will be used whenever we do not need to specify the *direction* on the bond. Hence $[i, j] = [j, i]$. *Directed bonds* will be denoted by (i, j), and we shall always use the convention that the bond is directed from the first index to the second one. To each bond $[i, j]$ we assign a length $L_{[i,j]} = L_{(i,j)} = L_{(j,i)}$. In most applications we would avoid non-generic degeneracies by assuming that the $L_{[i,j]}$ are *rationally independent.* The mean length is defined by $\langle L \rangle \equiv (1/B) \sum_{b=1}^{B} L_b$.

For the quantum description we assign to each bond $b = [i, j]$ a coordinate x_b which measures distances along the bond. We may use $x_{(i,j)}$ which is defined to take the value 0 at the vertex i and the value $L_{(i,j)} \equiv L_{(j,i)}$ at the vertex j. We can also use $x_{(j,i)}$ which vanishes at j and takes the value $L_{(i,j)}$ at i.

The wavefunction Ψ is a B-component vector and will be written as $(\Psi_{b_1}(x_{b_1}), \Psi_{b_2}(x_{b_2}), \ldots, \Psi_{b_B}(x_{b_B}))^{\mathrm{T}}$ where the set $\{b_i\}_{i=1}^{B}$ consists of all the B distinct bonds on the graph. We shall call $\Psi_b(x_b)$ the component of Ψ on the bond b. The bond coordinates x_b were defined above. When there is no danger of confusion, we shall use the shorthand notation $\Psi_b(x)$ for $\Psi_b(x_b)$ and it is understood that x is the coordinate on the bond b to which the component Ψ_b refers.

The Schrödinger equation is defined on the graph in the following way (Alexander 1985, Avron 1994) (see also Kottes and Smilansky (1999) for an extensive list of references on the subject): on each bond b, the component Ψ_b of the total wavefunction Ψ is a solution of the one-dimensional equation

$$\left(-\mathrm{i}\frac{\mathrm{d}}{\mathrm{d}x_{(i,j)}} - A_{(i,j)}\right)^2 \Psi_b(x_{(i,j)}) = k^2 \Psi_b(x_{(i,j)}) \qquad (b = [i,j]). \tag{2}$$

We included a 'magnetic vector potential' $A_{(i,j)}$, with $A_{(i,j)} = -A_{(j,i)}$ which breaks time-reversal symmetry.

On each of the bonds, the general solution of equation (2) is a superposition of two counter-propagating waves

$$\begin{aligned} \psi_{(i,j)}(x_{(i,j)}) &= \exp[\mathrm{i}(kx_{(i,j)} + A_{(i,j)}x_{(i,j)})], \\ \psi_{(j,i)}(x_{(j,i)}) &= \exp[\mathrm{i}(kx_{(j,i)} + A_{(j,i)}x_{(j,i)})]. \end{aligned} \tag{3}$$

Note that the above functions are normalized to have an amplitude 1 at the points from which they 'emerge', namely $\psi_{(i,j)} = 1$ at the vertex i and $\psi_{(j,i)} = 1$ at the vertex j. The Hilbert space of the solutions of equation (2) is spanned by the set of functions defined above, such that, for all $b = [i, j]$,

$$\Psi_b = a_{(i,j)}\psi_{(i,j)}(x_{(i,j)}) + a_{(j,i)}\psi_{(j,i)}(x_{(j,i)}). \tag{4}$$

Thus, the as yet undetermined coefficients $a_{(i,j)}$ form a $2B$-dimensional vector of complex numbers, which uniquely determines an element in the Hilbert space of solutions. This space corresponds to 'free-wave' solutions since we have not yet imposed any conditions which the solutions of equations (2) have to satisfy at the vertices.

2.2. *The quantum scattering map*

The *quantum scattering map* is a unitary transformation acting in the space of free waves, and it is defined as follows.

In a first step, we prescribe at each vertex $i = 1, \ldots, V$ a *vertex scattering matrix* which is a unitary matrix of dimension v_i. The vertex scattering matrices may be k dependent and they are denoted by $\sigma_{l,m}^{(i)}(k)$, where the indices l, m take the values of the vertices which are connected to i, that is $C_{i,l} = C_{i,m} = 1$. The vertex scattering matrix is a property which is attributed to the vertex under consideration. Either it can be derived from appropriate boundary conditions as in the work of Kottos and Smilamnsky (1997, 1999) or it can be constructed to model other physical situations. The important property of $\sigma_{l,m}^{(i)}(k)$ in the present context is that any wave which is *incoming* to the vertex i from the bonds (l, i), and which has an amplitude 1 at the vertex, is scattered and forms *outgoing* waves in the bonds (i, m) with amplitudes $\sigma^{(i)}_{l,m}(k)$.

Now, the quantum scattering map is represented by its effect on the $2B$-dimensional vector of coefficients $\mathbf{a} = \{a_{(i,j)}\}$, namely $\mathbf{a}$ is mapped to $\mathbf{a}'$ with components

$$a'_{b'} = \sum_{b=1}^{2B} a_b S_{B_{b,b'}}, \tag{5}$$

where b and b' run over all directed bonds and, if we define $b = (i, j)$ and $b' = (l, m)$,

$$S_{B_{(i,j),(l,m)}}(k) = \delta_{j,l} \exp[\mathrm{i}L_{(i,j)}(k + A_{(i,j)})]\sigma^{(j)}_{i,m}(k). \tag{6}$$

The effect of $\mathbf{S}_B$ on a wavefunction can be intuitively understood as follows. The coefficient $a_{(i,j)}$ is the (complex) amplitude of the wave which emerges from the vertex i and propagates to the vertex j. Once it reaches the vertex j, it has accumulated a phase $\exp[\mathrm{i}L_{(i,j)}(k + A_{(i,j)})]$ and it scatters into the bonds which emanate from j with an amplitude given by the appropriate vertex scattering matrix. The new amplitude $a'_{(l=j,m)}$ consists of the superposition of all the amplitudes contributed by waves which impinge on the vertex $l = j$ and then scatter. The name 'quantum scattering' map is justified by this intuitive picture.

The resulting matrix $\mathbf{S}_B$ is a $2B \times 2B$ unitary matrix. The unitarity follows simply from the unitarity of the vertex scattering matrices, and from the fact that $\mathbf{S}_B$ has non-vanishing entries only between connected directed bonds: the incoming bond aims at the vertex from which the outgoing bond emerges. The unitarity of $\mathbf{S}_B$ implies that its spectrum is restricted to the unit circle. In this paper we shall mainly be concerned with the spectral statistics of the eigenphases, and their relation to the underlying classical dynamics on the graph. The spectral statistics will be discussed in the next section. We shall use the remaining part of the present section to clarify two important issues. We shall first show how one can use the quantum scattering map to construct the space of solutions of the Schrödinger operator on the graph with boundary conditions. Then, we shall introduce the classical dynamics which correspond to the scattering map.

To define the space of 'bound states' on the graph, one has to restrict the space of wavefunctions by imposing appropriate boundary conditions on the vertices. The boundary conditions guarantee that the resulting Schrödinger operator is self-adjoint. We previously (Kottos and Smilansky 1997, 1999) described and used one particular set of boundary conditions, which ensure continuity (uniqueness) and current conservation. Here we shall use a slight generalization, which matches well the spirit of the present article. We shall impose the boundary conditions in terms of a consistency requirement that the coefficients $a_{(i,j)}$ have to obey. Namely, we require that the wavefunction (4) is *stationary* under the action of the quantum scattering map. In other words, the vector $\mathbf{a}$ must be an eigenvector of $\mathbf{S}_B(k)$ with a unit eigenvalue. (See also Klesse (1996) and Klesse and Metzler (1997).) This requirement can be fulfilled when

$$\det[\mathbf{I} - \mathbf{S}_B(k)] = 0. \tag{7}$$

We have actually derived (7) (Kottos and Smilansky 1997, 1999) for the particular case in which the vertex scattering matrices were computed from a particular set of vertex boundary conditions which impose continuity and current conservation on the vertices. The resulting vertex scattering matrices are

$$\sigma_{j,j'}^{(i)} = \left(-\delta'_{j,j} + \frac{1+\exp(-\mathrm{i}\omega_i)}{v_i} \right) C_{i,j} C_{i,j'}, \quad \omega_i = 2 \arctan \left(\frac{\lambda_i}{v_i k} \right). \tag{8}$$

Here, $0 \leqslant \lambda_i \leqslant \infty$ are arbitrary constants. The 'Dirichlet' ('Neumann') boundary conditions correspond to $\lambda_i = \infty(0)$. The Dirichlet case implies total reflection at the vertex, $\sigma_{j,j'}^{(i)} = -\delta_{j,j'}$. For the Neumann boundary condition we have $\sigma_{j,j'}^{(i)} = -\delta_{j,j'} + 2/v_i$, which is independent of k. For any intermediate boundary condition, the scattering matrix approaches the Neumann expression as $k \to \infty$. Note that, in all non-trivial cases ($v_i > 2$), back-scattering ($j = j'$) is singled out both in sign and in magnitude: $\sigma_{j,j}^{(i)}$ always has a negative real part, and the reflection probability $|\sigma_{j,j}^{(i)}|^2$ approaches unity as the valency v_i increases. One can easily check that $\boldsymbol{\sigma}^{(i)}$ is a symmetric unitary matrix, ensuring flux conservation and time-reversal symmetry at the vertex. For Neumann boundary conditions, $\boldsymbol{\sigma}^{(i)}$ is a real orthogonal matrix.

The spectral theory of the Schrödinger operators on graphs can be developed using equation (7) as the starting point. In particular, the corresponding trace formula (Roth 1983) can naturally be derived and is related to the underlying classical dynamics (Kottos and Smilansky 1997, 1999). Here, we shall study the quantum scattering map in its own right, without a particular reference to its role in the construction of the spectrum. We shall consider the ensemble of unitary $2B \times 2B$ matrices $\mathbf{S}_B(k)$, where k is allowed to vary in a certain interval to be specified later. Our main concern will be the statistical properties of the eigenvalues of $\mathbf{S}_B$. This will be explained in the next section.

2.3. *The classical scattering map*

The last point to be introduced and discussed in the present section is the classical dynamics on the graph and the corresponding scattering map.

We consider a classical particle which moves freely as long as it is on a bond. The vertices are singular points, and it is not possible to write down the analogue of Newton's equations at the vertices. Instead, one can employ a Liouvillian approach based on the study of the evolution of phase-space densities. This phase-space description will be constructed on a Poincaré section which is defined in the following way. Crossing of the section is registered as the particle encounters a vertex, thus the 'coordinate' on the section is the vertex label. The corresponding 'momentum' is the direction in which the particle moves when it emerges from the vertex. This is completely specified by the label of the next vertex to be encountered. In other words,

$$\left\{ \begin{matrix} \text{position} \\ \text{momentum} \end{matrix} \right\} \leftrightarrow \left\{ \begin{matrix} \text{vertex index} \\ \text{next index} \end{matrix} \right\}. \tag{9}$$

The set of all possible vertices and directions is equivalent to the set of $2B$ directed bonds. The evolution on this Poincaré section is well defined once we postulate the transition probabilities $P_{j \to j'}^{(i)}$ between the directed bonds $b = \{j, i\}$ and $b' = \{i, j'\}$. To make the connection with the quantum description, we adopt the quantum transition probabilities, expressed as the absolute squares of the $\mathbf{S}_B$ matrix elements

$$P_{j \to j'}^{(i)} = |\sigma_{j,j'}^{(i)}(k)|^2. \tag{10}$$

When the vertex scattering matrices are constructed from the standard matching conditions on the vertices (8), we obtain the explicit expression

$$P^{(i)}_{j\to j'} = \left| -\delta'_{j,j} + \frac{1+\exp(\mathrm{i}\omega_i)}{v_i} \right|^2. \tag{11}$$

For the two extreme cases corresponding to Neumann and Dirichlet boundary conditions, this results in

$$P^{(i)}_{j\to j'} = \begin{cases} \left(-\delta_{j,j'} + \dfrac{2}{v_i}\right)^2, & \text{Neumann case,} \\ \delta'_{j,j}, & \text{Dirichlet case.} \end{cases} \tag{12}$$

The transition probability $P^{(i)}_{j\to j'}$ for the Dirichlet case admits the following physical interpretation. The particle is confined to the bond where it started and thus the phase space is divided into non-overlapping ergodic components ('tori'). For all other boundary conditions the graph is dynamically connected.

The classical Frobenius–Perron evolution operator is a $2B \times 2B$ matrix whose elements $U_{b,b'}$ are the classical transition probabilities between the bonds b and b':

$$U_{ij,nm} = \delta_{j,n} P^{(j)}_{i\to m}. \tag{13}$$

$\mathbf{U}$ does not involve any metric information on the graph and, for Dirichlet or Neumann boundary conditions, $\mathbf{U}$ is independent of k. This operator is the classical analogue of the quantum scattering matrix $\mathbf{S}_B$. Usually, one 'quantizes' the classical operator to generate the quantum analogue. For graphs the process is reversed, and the classical evolution is derived from the more fundamental quantum dynamics.

Let $\rho_b(t)$, $b = 1, \ldots, 2B$ denote the distribution of probabilities to occupy the directed bonds at the (topological) time t. This distribution will evolve until the first return to the Poincaré section according to

$$\rho_b(t+1) = \sum_{b'} U_{b,b'} \rho_{b'}(t). \tag{14}$$

This is a Markovian master equation which governs the evolution of the classical probability distribution. The unitarity of the graph scattering matrix $\mathbf{S}_B$ guarantees $\sum_{b=1}^{2B} U_{b,b'} = 1$ and $0 \leqslant U_{b,b'} \leqslant 1$, such that the probability that the particle is on any of the bonds is conserved during the evolution. The spectrum of $\mathbf{U}$ is restricted to the unit circle and its interior, and $\nu_1 = 1$ is always an eigenvalue with the corresponding eigenvector $|1\rangle = (1/2B)(1, 1, \ldots, 1)^{\mathrm{T}}$. In most cases, the eigenvalue 1 is the only eigenvalue on the unit circle. Then, the evolution is ergodic since any initial density will evolve to the eigenvector $|1\rangle$ which corresponds to a uniform distribution (equilibrium).

$$\rho(t) \underset{t\to\infty}{\longrightarrow} |1\rangle. \tag{15}$$

The mixing rate $-\ln|\nu_2|$ at which equilibrium is approached is determined by the gap between the next largest eigenvalue ν_2 and 1. This is characteristic of a classically mixing system.

However, there are some non-generic cases such as bipartite graphs when -1 belongs to the spectrum. In this case the asymptotic distribution is not stationary. Nevertheless an equivalent description is possible for bipartite graphs when $\mathbf{U}$ is replaced by $\mathbf{U}^2$ which has then two uncoupled blocks of dimension B. The example that we are going to discuss in the last section will be of this type.

Periodic orbits (POs) on the graph will play an important role in the following and we define them in the following way. An *orbit* on the graph is an itinerary (finite or infinite) of successively connected *directed* bonds $(i_1, i_2), (i_2, i_3), \ldots$. For graphs without loops or multiple bonds this is uniquely defined by the sequence of vertices $i_1, i_2, \ldots$ with $i_m \in [1, V]$ and $C_{i_m, i_{m+1}} = 1$ for all m. An *orbit* is *periodic* with period n if, for all k, $(i_{n+k}, i_{n+k+1}) = (i_k, i_{k+1})$. The *code* of a PO of period n is the sequence of n vertices $i_1, \ldots, i_n$ and the orbit consists of the bonds (i_m, i_{m+1}) (with the identification $i_{m+n} \equiv i_m$). In this way, any cyclic permutation of the code defines the same PO.

The POs can be classified in the following way:

(*a*) *Irreducible POs.* These are POs which do not intersect themselves such that any vertex label in the code can appear at most once. Since the graphs are finite, the maximum period of irreducible POs is V. To each irreducible PO corresponds its time-reversed partner whose code is read in the reverse order. The only POs that are both irreducible and conjugate to itself under time reversal are the POs of period 2.

(*b*) *Reducible POs.* These are POs whose code is constructed by inserting the code of any number of irreducible POs at any position which is consistent with the connectivity matrix. All the POs of period $n > V$ are reducible.

(*c*) *Primitive POs.* These are POs whose code cannot be written down as a repetition of a shorter code.

We introduced above the concept of orbits on the graph as strings of vertex labels whose ordering obeys the required connectivity. This is a finite coding which is governed by a Markovian grammar provided by the connectivity matrix. In this sense, the symbolic dynamics on the graph are Bernoulli. This property adds another piece of evidence to the assertion that the dynamics on the graph are chaotic. In particular, one can obtain the topological entropy Γ from the symbolic code. Using the relation

$$\Gamma = \lim_{n \to \infty} \left(\frac{1}{n} \log \left[\operatorname{Tr} (C^n) \right] \right), \tag{16}$$

one obtains $\Gamma = \log \bar{v}$, where $\bar{v}$ is the largest eigenvalue of C.

Of prime importance in the discussion of the relation between the classical and the quantum dynamics are the traces $u_n = \operatorname{Tr} (\mathbf{U}^n)$ which are interpreted as the mean classical probability to perform n-periodic motion. Using the definition (13) one can write the expression for u_n as a sum over contributions of n-POs:

$$u_n = \sum_{p \in \mathcal{P}_n} n_p \exp(-r \gamma_p n_p), \tag{17}$$

where the sum is over the set $\mathcal{P}_n$ of primitive POs whose period n_p is a divisor of n, with $r = n/n_p$. To each primitive orbit one can assign a *stability factor* $\exp(-\gamma_p n_p)$ which is accumulated as a product of the transition probabilities as the trajectory traverses its successive vertices:

$$\exp(-\gamma_p n_p) \equiv \prod_{j=1}^{n_p} P^{(i_j)}_{i_{j-1} \to i_{j+1}}. \tag{18}$$

The stability exponents γ_p correspond to the Lyapunov exponents in periodic orbit theory.

When only one eigenvalue of the classical evolution operator $\mathbf{U}$ is on the unit circle, one has $u_n \underset{n\to\infty}{\longrightarrow} 1$. This leads to a classical sum rule

$$u_n = \sum_{p \in P_n} n_p \exp(-r\gamma_p n_p) \underset{n\to\infty}{\longrightarrow} 1. \tag{19}$$

This last relation shows again that the number of periodic orbits must increase exponentially with increasing n to balance the exponentially decreasing stability factors of the individual POs. The topological entropy can be related to the mean stability exponent through this relation.

Using equation (17) for u_n, one can easily write down the complete thermodynamic formalism for the graph. Here, we shall only quote the PO expression for the Ruelle ζ function:

$$\begin{aligned}\zeta_{\mathrm{R}}(z) &\equiv [\det(I - z\mathbf{U})]^{-1}\\ &= \exp\{-\mathrm{Tr}[\ln(\mathbf{I} - z\mathbf{U})]\}\\ &= \exp\left(\sum_n \frac{z^n}{n} u_n\right)\\ &= \prod_p \frac{1}{1 - z^{n_p}\exp(-n_p\gamma_p)},\end{aligned} \tag{20}$$

where the product extends over all primitive periodic orbits.

The above discussion of the classical dynamics on the graph shows that it bears a striking similarity to the dynamics induced by area-preserving hyperbolic maps. The reason underlying this similarity is that even though the graph is a genuinely one-dimensional system, it is not simply connected, and the complex connectivity is the origin and reason for the classically chaotic dynamics.

§ 3. The spectral statistics of the quantum scattering map

We consider the matrices $\mathbf{S}_B$ defined in equation (6). Their spectrum consists of $2B$ points confined to the unit circle (eigenphases). Unitary matrices of this type are frequently studied since they are the quantum analogues of classical area-preserving maps. Their spectral fluctuations depend on the nature of the underlying classical dynamics (Smilansky 1989). The quantum analogues of classically integrable maps display Poissonian statistics while, in the opposite case of classically chaotic maps, the statistics of eigenphases conform quite accurately with the results of Dyson's RMT for the *circular* ensembles. The ensemble of unitary matrices which will be used for the statistical study will be the set of matrices $\mathbf{S}_B(k)$ with k in the range $|k - k_0| \leqslant \Delta_k/2$. The interval size Δ_k must be sufficiently small that the vertex matrices do not vary appreciably when k scans this range of values. Then the k averaging can be performed with the vertex scattering matrices replaced by their value at k_0. When the vertex scattering matrices are derived from Neumann or Dirichlet boundary conditions, the averaging interval is unrestricted because the dimension of $\mathbf{S}_B$ is independent of k. In any case, Δ_k must be much larger than the correlation length between the matrices $\mathbf{S}_B(k)$, which was estimated by Kottos and Smilansky (1999) to be inversely proportional to the width of the distribution of the bond lengths. The ensemble average with respect to k will be denoted by

$$\langle\cdot\rangle_k \equiv \frac{1}{\Delta_k}\int_{k_0-\Delta_k/2}^{k_0+\Delta_k/2} \cdot\, \mathrm{d}k. \tag{21}$$

Another way to generate an ensemble of matrices $\mathbf{S}_B$ is to randomize the length matrix $\mathbf{L}$ or the magnetic vector potentials $A_{(i,j)}$, while the connectivity (topology of the graph) is kept constant. In most cases, the ensembles generated in this way will be equivalent. In the last section we shall also consider an *additional* average over the vertex scattering matrices.

In § 3.1 we compare statistical properties of the eigenphases $\{\theta_l(k)\}$ of $\mathbf{S}_B$ with the predictions of RMT (Brody *et al.* 1981, Mehta 1990) and with the results of PO theory for the spectral fluctuations of quantized maps (Blümel and Smilansky 1988, 1990). The statistical measure that we shall investigate is the spectral form factor. Explicit expressions for this quantity are given by RMT (Haake *et al.* 1996), and a semiclassical discussion can be found in the papers by Bogomolny and Keating (1996) and Smilansky (1997a,b).

3.1. *The form factor*

The matrix $\mathbf{S}_B$ for a fixed value of k is a unitary matrix with eigenvalues $\exp[\mathrm{i}\theta_l(k)]$. The spectral density of the eigenphases is

$$\begin{aligned} d(\theta;k) &\equiv \sum_{l=1}^{2B} \delta[\theta-\theta_l(k)] \\ &= \frac{2B}{2\pi} + \frac{1}{2\pi}\sum_{n=1}^{\infty} \exp(-\mathrm{i}\theta n)\,\mathrm{Tr}\,[\mathbf{S}_B^n(k)] + \mathrm{cc}, \end{aligned} \tag{22}$$

where the first term on the right-hand side is the smooth density $\bar{d} = 2B/2\pi$. The oscillatory part is a Fourier series with the coefficients Tr $[\mathbf{S}_B^n(k)]$. This set of coefficients will play an important role in the following. Using the definitions (6) one can expand $\mathrm{Tr}\,[\mathbf{S}_B^n(k)]$ directly as a sum over $n-$POs on the graph:

$$\mathrm{Tr}\,[\mathbf{S}_B^n(k)] = \sum_{p\in\mathcal{P}_n} n_p \mathcal{A}_p^r \exp[\mathrm{i}(kl_p + \Phi_p)r] \exp(\mathrm{i}\mu_p r), \tag{23}$$

where the sum is over the set $\mathcal{P}_n$ of primitive POs whose period n_p is a divisor of n, with $r = n/n_p$. $l_p = \sum_{b\in p} L_b$ is the length of the PO. $\Phi_p = \sum_{b\in p} L_b A_b$ is the 'magnetic flux' through the orbit. If all the parameters A_b have the same absolute size A, we can write $\Phi_p = Ab_p$, where b_p is the directed length of the orbit. μ_p is the phase accumulated from the vertex matrix elements along the orbit, and it is the analogue of the Maslov index. For the standard vertex matrices (8) μ_p/π gives the number of *back scatterings* along p. The amplitudes $\mathcal{A}_p$ are given by

$$\mathcal{A}_p = \prod_{j=1}^{n_p} |\sigma_{i_{j-1},i_{j+1}}^{(i_j)}| \equiv \exp\left(-\frac{\gamma_p}{2}\,n_p\right), \tag{24}$$

where i_j runs over the vertex indices of the PO, and j is understood mod n_p. The Lyapunov exponent γ_p was defined in equation (18). It should be mentioned that equation (23) is the building block of the PO expression for the spectral density of the graph, which can be obtained starting from the secular equation (7). In the quantization of classical area-preserving maps, similar expressions appear as the leading semiclassical approximations. In the present context, equation (23) is an identity.

The two-point correlations are expressed in terms of the excess probability density $R_2(r)$ of finding two phases at a distance r, where r is measured in units of the mean spacing $2\pi/2B$:

$$R_2(r;k_0) = \frac{2}{2\pi}\sum_{n=1}^{\infty}\cos\left(\frac{2\pi rn}{2B}\right)\frac{1}{2B}\langle|\mathrm{Tr}\,\mathbf{S}_B^n|^2\rangle_k. \tag{25}$$

The form factor

$$K\left(\frac{n}{2B}\right) = \frac{1}{2B}\langle|\mathrm{Tr}\,\mathbf{S}_B^n|^2\rangle_k \tag{26}$$

is the Fourier transform of $R_2(r,k_0)$. For a Poisson spectrum, $K(n/2B) = 1$ for all n. RMT predicts that $K(n/2B)$ depends on the scaled time $n/2B$ only (Smilansky 1989), and explicit expressions for the orthogonal and the unitary circular ensembles are known (Haake *et al.* 1996).

As was indicated above, if the vertex scattering matrices are chosen by imposing Dirichlet boundary conditions on the vertices, the classical dynamics are 'integrable'. One expects therefore the spectral statistics to be Poissonian:

$$K\left(\frac{n}{2B}\right) = 1 \qquad \text{for all } n \geqslant 1. \tag{27}$$

For Dirichlet boundary conditions the vertex scattering matrices (8) couple only time-reversed bonds. $\mathbf{S}_B$ is reduced to a block diagonal form where each bond and its time reversed partner are coupled by a 2×2 matrix of the form

$$\mathbf{S}^{(b)}(k,A) = \begin{pmatrix} 0 & \exp[\mathrm{i}(k+A)L_b] \\ \exp[\mathrm{i}(k-A)L_b] & 0 \end{pmatrix}. \tag{28}$$

The spectrum of each block is the pair $\pm\exp(\mathrm{i}kL_b)$, with the corresponding symmetric and antisymmetric eigenvectors $(1/2^{1/2})\,(1,\pm 1)$. As a result, we obtain

$$K\left(\frac{n}{2B}\right) = 1 + (-1)^n \quad \text{for all } n \geqslant 1. \tag{29}$$

This deviation from the expected Poissonian result arises because the extra symmetry reduces the matrix $\mathbf{S}_B$ further into the symmetric and antisymmetric subspaces. The spectrum in each of them is Poissonian but, when combined together, the fact that the eigenvalues in the two spectra differ only by a sign leads to the anomaly (29).

Having successfully disposed of the integrable case, we address now the more general situation. In figure 1 we show typical examples of form factors, computed numerically for a fully connected graph with $V = 20$. The data for Neumann boundary conditions and $A = 0$ (figure 1 (*a*)) or $A \neq 0$ (figure 1 (*b*)) are reproduced quite well by the predictions of RMT, which are shown by the smooth lines. For this purpose, one has to scale the topological time n by the corresponding 'Heisenberg time', which is the dimension of the matrix, that is $2B$. The deviations from the smooth curves are not statistical and cannot be ironed out by further averaging. Rather, they arise because the graph is a dynamical system which cannot be

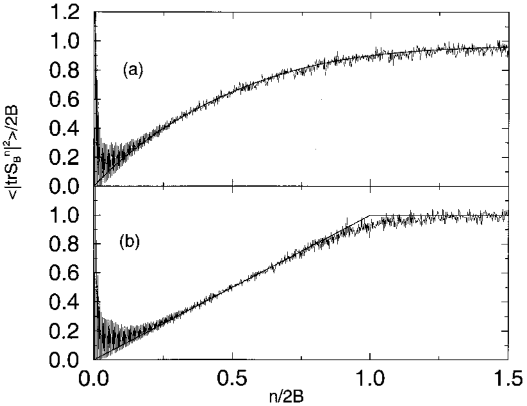

Figure 1. Form factor for a fully connected graph (*a*) with $V = 20$ with and (*b*) without time-reversal symmetry. The smooth curves show the predictions of the corresponding random matrix ensembles COE and CUE respectively.

described by RMT in all details. To study this point in depth we shall express the form factor in terms of the PO expression (23).

$$K\left(\frac{n}{2B}\right) = \frac{1}{2B}\left\langle\left|\sum_{p\in\mathcal{P}_n} n_p \mathcal{A}_p^r \exp[\mathrm{i}(kl_p + Ab_p + \pi\mu_p)r]\right|^2\right\rangle_k$$

$$= \frac{1}{2B}\sum_{p,p'\in\mathcal{P}_n} n_p n_{p'} \mathcal{A}_p^r \mathcal{A}_{p'}^{r'} \exp\left[\mathrm{i}A(rb_p - r'b_{p'}) + \mathrm{i}\pi(r\mu_p - r'\mu_{p'})\right]\Big|_{rl_p = r'l_{p'}}. \quad (30)$$

The k averaging is carried out over such a large interval that the double sum above is restricted to pairs of POs that have exactly the same length. The fact that we choose the lengths of the bonds to be rationally independent will enter the considerations which follow in a crucial way.

The largest deviations between the numerical data and the predictions of RMT occur for $n = 1, 2$. For $n = 1$, one obtains zero instead of the circular orthogonal ensemble (COE) (CUE) values $1/B$ $(1/2B)$, simply because the graph has no POs of period 1. This could be modified by allowing loops, which were excluded here from the outset. The 2-POs are self-retracing (i.e. invariant under time reversal), and each has a distinct length. Their contribution is enhanced because back scattering is favoured when the valency is large. Self-retracing implies also that their contribution is insensitive to the value of A. The form factor for $n = 2$ calculated for a fully connected graph with $v = V - 1$ is

$$K\left(\frac{n}{2B}\right) = 2\left(1 - \frac{2}{v}\right)^4, \quad (31)$$

independent of the value of A. This is different from the value expected from RMT. The repetitions of the 2-POs are also the reason for the odd–even staggering which is seen for low values of $\tau \equiv n/2B$. They contribute a term which is approximately $2\exp(-2V\tau)$ and thus decays faster with the scaled time τ when the graph increases.

The deviations between the predictions of RMT and PO theory for low values of τ are typical and express the fact that for deterministic systems in general, the short-time dynamics are not fully chaotic. The short-time domain becomes less prominent as B becomes larger because the time n has to be scaled by $2B$. This limit is the analogue of the limit $\hbar \to 0$ in a general quantum system.

Consider now the domain $2 < n \ll 2B$. The POs are mostly of the irreducible type, and the length restriction limits the sum to pairs of orbits that are conjugate under time reversal. Neglecting the contributions from repetitions and from self-retracing orbits we obtain

$$K\left(\frac{n}{2B}\right) \approx \frac{1}{2B} \sum_{p \in \mathcal{P}_n} n^2 \mathcal{A}_p^2 \, 4 \cos^2(Ab_p)$$
$$= \frac{2n}{2B} u_n \langle \cos^2(Ab_p) \rangle_n. \tag{32}$$

The classical return probability u_n approaches unity as n increases (see equation (19)). Neglecting the short-time deviations, we can replace u_n by one, and we see that the remaining expression is the classical expectation of $\cos^2(Ab_p)$ over POs of length n. For $A = 0$ this factor is identically unity and one obtains the leading term of the COE expression for $n \ll 2B$. If A is sufficiently large $\langle \cos^2(Ab_p) \rangle_n \approx \frac{1}{2}$, one obtains the short-time limit of the CUE result. The transition between the two extreme situations is well described by

$$\langle \cos^2(Ab_p) \rangle_n \approx \tfrac{1}{2} \left[\exp\left(- A^2 \langle L_b^2 \rangle \frac{n}{2} \right) + 1 \right]. \tag{33}$$

This formula is derived by assuming that the total directed length b_p of a PO is a sum of elementary lengths with random signs.

The basic approximation so far was to neglect the interference between contributions of POs with different codes (up to time reversal). This can be justified as long as POs with different codes have different lengths. This is the case for low values of n. As n approaches B, the degeneracy of the length spectrum increases, and for $n > 2B$ all the orbits are degenerate. In other words, the restriction $rl_p = r'l_{p'}$ in equation (30) does not pick up a unique orbit and its time reversed partner, but rather a group of *isometric* but distinct orbits. Therefore, the interference of the contributions from these orbits must be calculated. The relative sign of the terms is determined by the 'Maslov' index. The computation of the interfering contributions from different POs with neighbouring actions is an endemic problem in the semiclassical theory of spectral statistics. These contributions are referred to as the *non-diagonal* terms, and they are treated by invoking the concept of PO correlations (Argaman *et al.* 1993, Cohen *et al.* 1998). The dynamic origin of these correlations is not known. In the case of graphs, they appear as correlations of the 'Maslov' signs within a class of isometric n-POs.

To compute $K(n/2B)$ from equation (30), one has to sum the contributions of all the n-POs after grouping together those that have exactly the same lengths. We shall discuss the case $A = 0$; so a further restriction on the orbits to have the same directed length is not required here. Since the lengths of the individual bonds are assumed to be rationally independent, a group of isometric n-POs is identified by the non-negative integers q_i, $i = 1, \ldots, B$, such that

$$l_{\mathbf{q}} \equiv \sum_{i=1}^{B} q_i l_i \qquad \text{with} \qquad \sum_{i=1}^{B} q_i = n, \tag{34}$$

that is, each bond i is traversed q_i times. The orbits in the group differ only in the *order* by which the bonds are traversed. We shall denote the number of isometric POs by $D_n(\mathbf{q})$. Note that not all the integer vectors $\mathbf{q}$ which satisfy equation (34) correspond to POs. Rather, the connectivity required by the concept of an orbit imposes restrictions, which render the problem of computing $D_n(\mathbf{q})$ a very hard combinatorial problem (U. Gavish 1998, private communication). Writing equation (30) explicitly for the case of a fully connected graph with Neumann vertex scattering matrices, we obtain

$$K\left(\frac{n}{2B}\right) = \frac{1}{2B}\left(\frac{2}{v}\right)^{2n} \sum_{\mathbf{q}} \left| \sum_{\alpha=1}^{D_n(\mathbf{q})} \frac{n}{r_\alpha} (-\xi)^{\mu_\alpha} \right|^2, \quad \text{with } \xi \equiv \left(\frac{v-2}{2}\right), \tag{35}$$

and the α summation extends over the n-POs in the class $\mathbf{q}$. μ_α is the number of back scatterings along the orbit, and r_α is different from unity if the orbit is a repetition of a shorter primitive orbit of period n/r_α.

Equation (35) is the starting point of the new approach to spectral statistics, which we would like to develop in the present paper. The actual computation of equation (35) can be considered as a *combinatorial* problem, since it involves the counting of loops on a graph, and adding them with appropriate (signed) weights. For Neumann boundary conditions, the weights are entirely determined by the connectivity of the graph. Our numerical data convincingly show that in the limit of large B the form factors for sufficiently connected graphs reproduce the results of RMT. The question is whether this relation can be derived using asymptotic combinatorial theory. The answer is not yet known, but we would like to show in the next section that, for a very simple graph, one can use combinatorics to evaluate the PO sums and recover in this way the exact values of the form factor.

§4. The 2-star model

In this section we shall investigate classical and quantum dynamics in a very simple graph using two different methods. We shall use PO theory to reduce the computation of the trace of the classical evolution operator u_n and the spectral form factor $K(n/2B)$ to combinatorial problems, namely sums over products of binomial coefficients. The result will be compared with a straightforward computation starting from the eigenvalues of the classical and quantum scattering maps.

An n-star graph consists of a 'central' vertex (with vertex index o) out of which emerge n bonds, all terminating at vertices (with indices $j = 1, \ldots, n$) with valencies $v_j = 1$. The bond lengths are $L_{oj} \equiv L_j$. This simple model (sometimes called a *hydra*) was studied at some length in Kottos and Smilansky (1999) and Berkolaiko and Keating (1999). The star with $n = 2$ is not completely trivial if the central vertex scattering matrix is chosen as

$$\boldsymbol{\sigma}^{(o)}(\eta) = \begin{pmatrix} \cos\eta & \mathrm{i}\sin\eta \\ \mathrm{i}\sin\eta & \cos\eta \end{pmatrix} \tag{36}$$

where the value $0 \leqslant \eta \leqslant \pi/2$ is still to be fixed. The scattering matrices at the two other vertices are taken to be unity and correspond to Neumann boundary conditions. The dimensions of $\mathbf{U}$ and $\mathbf{S}_B$ are 4, but can be immediately reduced to 2; owing to the trivial scattering at the reflecting tips, $a_{jo} = a_{oj} \equiv a_j$ for $j = 1, 2$. In this representation the space is labelled by the indices of the two loops (of lengths $2L_1$ and $2L_2$ respectively) which start and end at the central vertex. After this simplification the matrix $\mathbf{S}_B$ is

$$\mathbf{S}_B(k;\eta) = \begin{pmatrix} \exp(2\mathrm{i}kL_1) & 0 \\ 0 & \exp(2\mathrm{i}kL_2) \end{pmatrix} \begin{pmatrix} \cos\eta & \mathrm{i}\sin\eta \\ \mathrm{i}\sin\eta & \cos\eta \end{pmatrix}. \tag{37}$$

We shall compute the form factor for two ensembles. The first is defined by a fixed value of $\eta = \pi/4$, and the average is over an infinitely large k range. The second ensemble includes an additional averaging over the parameter η. We shall show that the measure for the integration over η can be chosen such that the model yields the CUE form factor. This is surprising at first sight, since the model defined above is clearly time-reversal invariant. However, if we replace kL_1 and kL_2 in equation (37) by $L(k \pm A)$, equation (37) will allow for an interpretation as the quantum scattering map of a graph with a single loop of length L and a vector potential A, that is of a system with broken time-reversal invariance (see figure 2 below). In particular, the form factors of the two systems will coincide exactly, when an ensemble average over L is performed. Clearly, this is a very special feature of the model considered, and we shall not discuss it here in more detail.

4.1. *Periodic orbit representation of u_n*

The classical evolution operator corresponding to equation (37) is

$$\mathbf{U}(\eta) = \begin{pmatrix} \cos^2\eta & \sin^2\eta \\ \sin^2\eta & \cos^2\eta \end{pmatrix}. \tag{38}$$

The spectrum of $\mathbf{U}$ consists of $\{1, \cos(2\eta)\}$, such that

$$u_n(\eta) = 1 + \cos^n(2\eta). \tag{39}$$

We shall now show how this result can be obtained from a sum over the POs of the system, grouped into classes of isometric orbits. This grouping is not really necessary for a classical calculation, but we would like to stress the analogy to the quantum case considered below.

The POs are uniquely encoded by the loop indices, such that each n-tuple of two symbols 1 and 2 corresponds (up to a cyclic permutation) to a single PO. When n is prime, the number of different POs is $N_2(n) = 2 + (2^n - 2)/n$ otherwise there are small corrections due to the repetitions of shorter orbits. These corrections are the reason why it is more convenient to represent a sum over POs of length n as a sum over all possible code words, although some of these code words are related by a cyclic permutation and consequently denote the same orbit. If we do so and moreover replace the stability factor of each orbit by equation (18), the PO expansion of the classical return probability becomes

$$u_n = \sum_{i_1=1,2} \cdots \sum_{i_n=1,2} \prod_{j=1}^{n} P_{i_j \to i_{j+1}}, \tag{40}$$

where j is a cyclic variable such that $i_{n+1} \equiv i_1$. In fact, equation (40) can be obtained without any reference to POs if one expands the intermediate matrix products contained in $u_n = \mathrm{Tr}\,\mathbf{U}^n$ and uses $P_{i_j \to i_{j+1}} = U_{i_j, i_{j+1}}(\eta)$.

We shall now order the terms in the multiple sum above according to the classes of isometric orbits. In the present case a class is completely specified by the integer $q \equiv q_1$ which counts the traversals of the loop 1, that is the number of symbols 1 in the code word. Each of the q symbols 1 in the code is followed by an uninterrupted sequence of $t_j \geqslant 0$ symbols 2 with the restriction that the total number of symbols 2 is given by

$$\sum_{j=1}^{q} t_j = n - q. \tag{41}$$

We conclude that each code word in a class $0 < q < n$ which starts with a symbol $i_1 = 1$ corresponds to an ordered partition of the number $n - q$ into q non-negative integers, while the words starting with $i_1 = 2$ can be viewed as partition of q into $n - q$ summands.

To make this step very clear, consider the following example: all code words of length $n = 5$ in the class $q = 2$ are 11222, 12122, 12212, 12221 and 22211, 22121, 21221, 22112, 21212, 21122. The first four words correspond to the partitions $0 + 3 = 1 + 2 = 2 + 1 = 3 + 0$ of $n - q = 3$ into $q = 2$ terms, while the remaining five words correspond to $2 = 0 + 0 + 2 = 0 + 1 + 1 = 1 + 0 + 1 = 0 + 2 + 0 = 1 + 1 + 0 = 2 + 0 + 0$.

In the multiple products in equation (40), a forward scattering along the orbit is expressed by two different consecutive symbols $i_j \neq i_{j+1}$ in the code and leads to a factor $\sin^2 \eta$, while a back scattering contributes a factor $\cos^2 \eta$. Since the sum is over POs, the number of forward scatterings is always even and we denote it by 2ν. It is then easy to see that ν corresponds to the number of positive terms in the partitions introduced above, since each such term corresponds to an uninterrupted sequence of symbols 2 enclosed between two symbols 1 or vice versa and thus contributes two forward scatterings. For the codes starting with a symbol 1 there are $\binom{q}{\nu}$ ways to choose the ν positive terms in the sum of q terms, and there are $\binom{n-q-1}{\nu-1}$ ways to decompose $n - q$ into ν *positive* summands. After similar reasoning for the codes starting with the symbol 2 we find for the PO expansion of the classical return probability

$$\begin{aligned} u_n(\eta) &= 2\cos^{2n}\eta + \sum_{q=1}^{n-1}\sum_{\nu}\left[\binom{q}{\nu}\binom{n-q-1}{\nu-1} + \binom{n-q}{\nu}\binom{q-1}{\nu-1}\right]\sin^{4\nu}\eta\cos^{2n-4\nu}\eta \\ &= 2\cos^{2n}\eta + \sum_{q=1}^{n-1}\sum_{\nu}\frac{n}{\nu}\binom{q-1}{\nu-1}\binom{n-q-1}{\nu-1}\sin^{4\nu}\eta\cos^{2n-4\nu}\eta \\ &= 2\sum_{\nu}\binom{n}{2\nu}\sin^{4\nu}\eta\cos^{2n-4\nu}\eta \\ &= (\cos^2\eta + \sin^2\eta)^n + (\cos^2\eta - \sin^2\eta)^n, \end{aligned} \tag{42}$$

which is obviously equivalent to equation (39). The summation limits for the variable ν are implicit since all terms outside vanish owing to the properties of the binomial coefficients. In order to reach the third line we have used the identity

$$\sum_{q=1}^{n-1}\binom{q-1}{\nu-1}\binom{n-q-1}{\nu-1} = \binom{n-1}{2\nu-1} = \frac{2\nu}{n}\binom{n}{2\nu}. \tag{43}$$

It can be derived by some straightforward variable substitutions from

$$\sum_{k=l}^{n-m}\binom{k}{l}\binom{n-k}{m} = \binom{n+1}{l+m+1}. \tag{44}$$

which, in turn, is found in the literature (Prudnikov *et al.* 1986).

4.2. *Quantum mechanics: spacing distribution and form factor*

Starting from equation (37), and writing the eigenvalues as $\exp[\mathrm{i}k(L_1+L_2)]$ $\exp(\pm\mathrm{i}\lambda/2)$, we obtain for λ, the difference between the eigenphases:

$$\lambda = 2\arccos\{\cos\eta\,\cos[k(L_1-L_2)]\}. \tag{45}$$

For fixed η, the k-averaged spacing distribution (which is essentially equivalent to $R_2(r)$ for the considered model) is given by

$$\begin{aligned} P(\theta;\eta) &= \frac{1}{\Delta_k}\int_{k_0-\Delta_k/2}^{k_0+\Delta_k/2} \mathrm{d}k\,\delta k\,(\theta - 2\arccos\{\cos\eta\cos[k(L_1-L_2)]\}) \\ &= \begin{cases} 0, & \cos\left(\dfrac{\theta}{2}\right) > |\cos\eta|, \\ \dfrac{\sin(\theta/2)}{[\cos^2\eta - \cos^2(\theta/2)]^{1/2}}, & \cos\left(\dfrac{\theta}{2}\right) < |\cos\eta|. \end{cases} \end{aligned} \tag{46}$$

We have assumed that θ is the smaller of the intervals between the two eigenphases, that is $0 \leqslant \theta \leqslant \pi$.

The spacings are excluded from a domain centred about 0 (π), that is they show very strong level repulsion. The distribution is square-root singular at the limits of the allowed domain.

$P(\theta;\eta)$ can be written as

$$P(\theta;\eta) = \frac{1}{2\pi} + \frac{1}{\pi}\sum_{n=1}^{\infty}\cos(n\theta)\{\tfrac{1}{2}\langle|\mathrm{Tr}\,[\mathbf{S}_B(\eta)^n]|^2\rangle_k - 1\}, \tag{47}$$

and, by a Fourier transformation, we can compute the form factor

$$K_2(n;\eta) = \tfrac{1}{2}\langle|\mathrm{Tr}\,[\mathbf{S}_B(\eta)^n]|^2\rangle. \tag{48}$$

In particular, for $\eta = \pi/4$, one finds that

$$K_2\left(n;\frac{\pi}{4}\right) = 1 + \frac{(-1)^{m+n}}{2^{2m+1}}\binom{2m}{m} \tag{49}$$

$$\approx 1 + \frac{(-1)^{m+n}}{2(\pi n)^{1/2}}. \tag{50}$$

Where $m = [n/2]$ and $[\cdot]$ stands for the integer part. The slow convergence of $K_2(n;\pi/4)$ to the asymptotic value of one is a consequence of the singularity of $P(\theta;\pi/4)$.

We now consider the ensemble for which the parameter η is distributed with the measure $\mathrm{d}\mu(\eta) = |\cos\eta\sin\eta|\,\mathrm{d}\eta$. The *only* reason for the choice of this measure is that, upon integrating equation (47), one obtains

$$P(\theta) = 2\sin^2\left(\frac{\theta}{2}\right), \tag{51}$$

which coincides with the CUE result for 2×2 matrices. A Fourier transformation results in

$$K_2(n) = \begin{cases} \frac{1}{2} & \text{for } n = 1, \\ 1 & \text{for } n \geqslant 2. \end{cases} \tag{52}$$

The form factors (49), (50) and (52) are displayed in figure 2 below.

4.3. *Periodic orbit expansion of the form factor*

As pointed out at the end of § 3.1, the k-averaged form factor can be expressed as a sum over classes of isometric periodic orbits. The analogue of equation (35) for the 2-star is

$$K_2(n;\eta) = \tfrac{1}{2}\sum_{q=0}^{n}\left|\sum_{\alpha=1}^{D_n(q)}\frac{n}{r_\alpha}\,\mathrm{i}^{2\nu_\alpha}\sin^{2\nu_\alpha}\eta\cos^{n-2\nu_\alpha}\eta\right|^2, \tag{53}$$

where the number of forward and backward scatterings along the orbits are $2\nu_\alpha$ and $\mu_\alpha = n - 2\nu_\alpha$, respectively. Again, it is very inconvenient to work with the repetition number r_α, and consequently we replace (as in the derivation of equation (42)) the sum over orbits by a sum over all code words and use the analogy with the compositions of integer numbers to obtain

$$K_2(n;\eta) = \cos^{2n}\eta + \frac{n^2}{2}\sum_{q=1}^{n-1}\left[\sum_{\nu}\frac{(-1)^\nu}{\nu}\binom{q-1}{\nu-1}\binom{n-q-1}{\nu-1}\sin^{2\nu}\eta\,\cos^{n-2\nu}\eta\right]^2. \tag{54}$$

The inner sum over ν can be written in terms of Krawtchouk polynomials as

$$K_2(n;\eta) = \cos^{2n}\eta + \tfrac{1}{2}\sum_{q=1}^{n-1}\binom{n-1}{n-q}\cos^{2q}\eta\sin^{2(n-q)}\eta\left[\frac{n}{q}P_{n-1,n-q}^{(\cos^2\eta,\sin^2\eta)}(q)\right]^2, \tag{55}$$

and the Krawtchouk polynomials are defined as (Szegö 1959, Nikiforov *et al.* 1991)

$$P_{N,k}^{(u,v)}(x) = \left[\binom{N}{k}(uv)^k\right]^{-1/2}\sum_{\nu=0}^{k}(-1)^{k-\nu}\binom{x}{\nu}\binom{N-x}{k-\nu}u^{k-\nu}v^{\nu},$$
$$0 \leqslant k \leqslant N,\ u+v=1. \tag{56}$$

These functions form a complete system of orthogonal polynomials of integer x with $0 \leqslant x \leqslant N$. They have quite diverse applications ranging from the theory of covering codes (Cohen *et al.* 1997) to the statistical mechanics of polymers (Schulten *et al.* 1980) and have been studied extensively in the mathematical literature (Szegö 1959, Nikiforov *et al.* 1991). The same functions appear also as a building block in our PO theory of Anderson localization on graphs (Schanz and Smilansky 2000). Unfortunately, we were not able to reduce the above expression any further by using the known sum rules and asymptotic representations for Krawtchouk polynomials. The main obstacle stems from the fact that in our case the three numbers N, k and x in the definition (56) are constrained by $N = k + x - 1$.

We shall now consider the special case $\eta = \pi/4$ for which we obtained in § 4.2 the solution (49). The result can be expressed in terms of Krawtchouk polynomials with $u = v = \frac{1}{2}$, which is also the most important case for the applications mentioned above. We adopt the common practice of omitting the superscript (u, v) in this special case and find that

$$K_2\left(n;\frac{\pi}{4}\right) = \frac{1}{2^n} + \frac{1}{2^{n+1}}\sum_{q=1}^{n-1}\binom{n-1}{n-q}\left[\frac{n}{q}P_{n-1,n-q}(q)\right]^2. \tag{57}$$

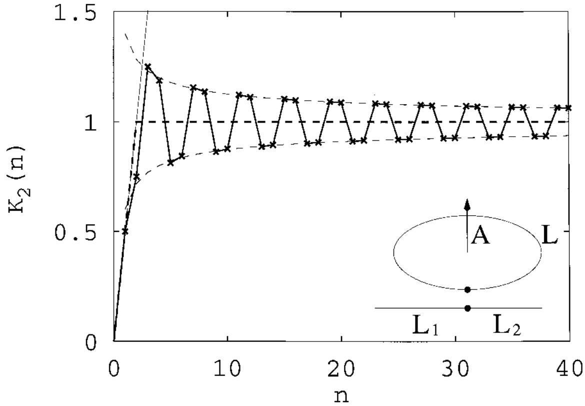

Figure 2. Form factor for the 2-star quantum graph. The crosses and the connecting heavy full line show the two equivalent exact results (49) and (57) for $\eta = \pi/4$. The broken lines represent the approximation (50), and the thin straight line corresponds to the diagonal approximation, when repetitions of primitive PO are neglected. The heavy broken line exhibits the form factor of a CUE ensemble of 2×2 random matrices (52), which can be obtained from the 2-star by an appropriate averaging over η. Finally, the inset shows a sketch of the two possible realizations of the system: a time-reversal invariant 2-star with bond lengths L_1 and L_2 or a graph with a single loop of length L and a magnetic flux A breaking time-reversal symmetry.

It is convenient to introduce

$$\begin{aligned}\mathcal{N}(s,t) &= (-1)^{s+t}\binom{s+t-1}{s}^{1/2} P_{s+t-1,s}(t)\\ &= \sum_{\nu}(-1)^{t-\nu}\binom{t}{\nu}\binom{s-1}{\nu-1}\end{aligned} \tag{58}$$

and to rewrite equation (57) with the help of some standard transformations of binomial coefficients:

$$\begin{aligned}K_2\left(n;\frac{\pi}{4}\right) &= \frac{1}{2^n}+\frac{1}{2^{n+1}}\sum_{q=1}^{n-1}\left(\frac{n}{q}\mathcal{N}(q,n-q-1)\right)^2\\ &= \frac{1}{2^n}+\frac{1}{2^{n+1}}\sum_{q=1}^{n-1}[\mathcal{N}(q,n-q)+(-1)^n\mathcal{N}(n-q,q)]^2.\end{aligned} \tag{59}$$

This expression is displayed in figure 2 together with equation (49) in order to illustrate the equivalence of the two results. An independent proof for this equivalence can be given by comparing the generating functions of $K_2(n;\pi/4)$ in the two representations.† We defer this to appendix A.

It should be noted, that in this way we have found a proof for two identities involving the Krawtchouk polynomials

† This idea was suggested by G. Berkolaiko.

$$\sum_{q=1}^{2m-1} \binom{2m-1}{2m-q} \left(\frac{2m}{q} P_{2m-1,2m-q}(q) \right)^2 = 2^{2m+1} + (-1)^m \binom{2m}{m} - 2 \tag{60}$$

and

$$\sum_{q=1}^{2m} \binom{2m}{2m+1-q} \left(\frac{2m+1}{q} P_{2m,2m+1-q}(q) \right)^2 = 2^{2m+2} - 2(-1)^m \binom{2m}{m} - 2, \tag{61}$$

which were obtained by separating even and odd powers of n in equations (49) and (57). To the best of our knowledge, equations (60) and (61) were derived here for the first time.

Finally we shall derive the CUE result (52) for the ensemble of graphs defined in the § 4 starting from the PO expansion (54). We find that

$$K_2(n) = \int_0^{\pi/2} \mathrm{d}\mu(\eta)\, K_2(n;\eta). \tag{62}$$

Inserting equation (54), expanding into a double sum and using

$$\int_0^{\pi/2} \mathrm{d}\eta \sin^{2(\nu+\nu')+1} \eta \cos^{2(n-\nu-\nu')+1} \eta = \frac{1}{2(n+1)} \binom{n}{\nu+\nu'}^{-1}, \tag{63}$$

we obtain

$$\begin{aligned} K_2(n) = {} & \frac{1}{n+1} \\ & + \frac{n^2}{4(n+1)} \sum_{q=1}^{n-1} \sum_{\nu,\nu'} \frac{(-1)^{\nu+\nu'}}{\nu\nu'} \binom{n}{\nu+\nu'}^{-1} \binom{q-1}{\nu-1} \binom{n-q-1}{\nu-1} \\ & \times \binom{q-1}{\nu'-1} \binom{n-q-1}{\nu'-1}. \end{aligned} \tag{64}$$

Comparing this with the equivalent result (52), we were again led to a previously unknown identity involving a multiple sum over binomial coefficients. It can be expressed as

$$S(n,q) = \sum_{\nu,\nu'} F_{\nu,\nu'}(n,q) = 1 \qquad (1 \leqslant q < n), \tag{65}$$

with

$$\begin{aligned} F_{\nu,\nu'}(n,q) = {} & \frac{(n-1)n}{2} \frac{(-1)^{\nu+\nu'}}{\nu\nu'} \binom{n}{\nu+\nu'}^{-1} \binom{q-1}{\nu-1} \binom{q-1}{\nu'-1} \\ & \times \binom{n-q-1}{\nu-1} \binom{n-q-1}{\nu'-1}. \end{aligned} \tag{66}$$

In this case, an independent computer-generated proof was found (A. Tefera 1999, private communication), which is based on the recursion relation

$$q^2 F_{\nu,\nu'}(n,q) - (n-q-1)^2 F_{\nu,\nu'}(n,q+1) + (n-1)(n-2q-1) F_{\nu,\nu'}(n+1,q+1) = 0. \tag{67}$$

This recursion relation was obtained with the help of a Mathematica routine (Wegschaider 1997), but it can be checked manually in a straightforward calculation.

By summing equation (67) over the indices ν, ν', the same recursion relation is shown to be valid for $S(n, q)$ (Petkovšek *et al.* 1996, Wegschaider 1997) and the proof is completed by demonstrating the validity of equation (65) for a few initial values. Having proven equation (65), we can use it to perform the summation over ν, ν' in equation (64) and find

$$K_2(n) = \frac{1}{n+1} + \sum_{q=1}^{n-1} \frac{n}{n^2 - 1}$$
$$= \frac{1}{n+1} + \frac{n}{n+1}(1 - \delta_{n,1}), \tag{68}$$

which is now obviously equivalent to the random matrix form factor (52). To the best of our knowledge, this is the first instance in which a combinatorial approach to RMT is employed.

§ 5. Conclusions

We have shown how within PO theory the problem of finding the form factor (the spectral two-point correlation function) for a quantum graph can be exactly reduced to a well defined combinatorial problem. For this purpose it was necessary to go beyond the diagonal approximation and to take into account the correlations between the POs.

In our model, these correlations are restricted to groups of isometric POs. This fits very well the results of Cohen *et al.* (1998), where for a completely different system (the Sinai billiard), the classical correlations between POs were analysed and found to be restricted to relatively small groups of orbits. The code words of the orbits belonging to one group were conjectured to be related by a permutation and a symmetry operation, which is in complete analogy to the isometric orbits on graphs.

Even for the very small and simple graph model that we considered in the last section the combinatorial problems involved were highly non-trivial. In fact we encountered previously unknown identities which we could not have obtained if it were not for the second independent method of computing the form factor. However, since the pioneering work documented by Petkovšek *et al.* (1996), investigation of sums of the type that we encountered in this paper is a rapidly developing subject, and it can be expected that finding identities such as equations (60), (61) and (65) will shortly be a matter of computer power.

The universality of the correlations between POs in all chaotic systems poses the problem of identifying the common dynamic reasons for their occurrence and of finding a common mathematical structure which is capable of describing them. A very interesting question in this respect is whether the correlations between POs in a general chaotic system can be related to combinatorial problems.

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APPENDIX A

PROOF OF EQUIVALENCE OF EQUATIONS (49) AND (59)

In this appendix we give an independent proof of the equivalence between the two results (49) and (50) obtained in §§4.2 and 4.3 respectively, for the form factor of the 2-star with $\eta = \pi/4$. We define the generating function

$$G(x) = \sum_{x=1}^{\infty} K_2\left(n; \frac{\pi}{4}\right)(2x)^n \qquad (|x| < \tfrac{1}{2}) \tag{A 1}$$

and find from equation (49) that

$$\begin{aligned} G(x) &= \frac{2x}{1-2x} - \frac{1}{2} + \sum_{m=0}^{\infty} \frac{(-1)^m}{2} \binom{2m}{m} x^{2m}(1-2x) \\ &= \frac{1}{2}\frac{1-2x}{(1+4x^2)^{1/2}} - \frac{1}{2}\frac{1-6x}{1-2x}. \end{aligned} \tag{A 2}$$

On the other hand we have from equation (59)

$$G(x) = \frac{x}{1-x} + G_1(x) + G_2(-x) \tag{A 3}$$

with

$$G_1(x) = \sum_{s,t=1}^{\infty} \mathcal{N}^2(s,t)\, x^{s+t} \tag{A 4}$$

and

$$G_2(x) = \sum_{s,t=1}^{\infty} \mathcal{N}(s,t)\mathcal{N}(t,s) x^{s+t}. \tag{A 5}$$

A convenient starting point for obtaining G_1 and G_2 is the integral representation

$$\mathcal{N}(s,t) = -\frac{(-1)^t}{2\pi \mathrm{i}} \oint \mathrm{d}z\, (1+z^{-1})^t (1-z)^{s-1}, \tag{A 6}$$

where the contour encircles the origin. With the help of equation (A 6) we find that

$$\begin{aligned} g(x,y) &= \sum_{s,t=1}^{\infty} \mathcal{N}(s,t)\, x^s\, y^t \\ &= -\frac{1}{2\pi \mathrm{i}} \sum_{s,t=1}^{\infty} \oint \mathrm{d}z \sum_{s,t=1}^{\infty} (1+z^{-1})^t (1-z)^{s-1}\, x^s\, (-y)^t \\ &= \frac{xy}{2\pi \mathrm{i}} \sum_{s,t=0}^{\infty} \oint \mathrm{d}z\, \frac{1}{1-x(1-z)}\, \frac{1+z}{z+y(1+z)} \\ &= \frac{xy}{(1+y)(1-x+y-2xy)} \qquad \left(|x|, |y| < \frac{1}{2^{1/2}}\right). \end{aligned} \tag{A 7}$$

The contour $|1+z^{-1}| = |1-z| = 2^{1/2}$ has been chosen such that both geometric series converge everywhere on it. Now we have

$$
\begin{aligned}
G_1(x^2) &= \frac{1}{(2\pi i)^2} \oint \frac{dz\, dz'}{zz'} \sum_{s,t=1}^{\infty} \sum_{s',t'=1}^{\infty} \mathcal{N}(s,t)\mathcal{N}(s',t')(xz)^s \left(\frac{x}{z}\right)^{s'} (xz')^t \left(\frac{x}{z'}\right)^{t'} \\
&= \frac{x^4}{(2\pi i)^2} \oint dz\, dz' \, \frac{1}{(1+xz')[1+x(z'-z)-2x^2zz']} \\
&\quad \times \frac{z'}{(z'+x)[zz'+x(z-z')-2x^2]},
\end{aligned}
\tag{A 8}
$$

where $|x| < 1/2^{1/2}$ and the contour for z, z' is the unit circle. We perform the double integral using the residua inside the contour and obtain

$$
G_1(x) = \frac{x}{2x-1}\left(\frac{1}{(4x^2+1)^{1/2}} - \frac{1}{1-x}\right). \tag{A 9}
$$

In complete analogy we find that

$$
G_2(x) = \frac{1}{2}\,\frac{4x^2+2x+1}{(2x+1)(4x^2+1)^{1/2}} - \frac{1}{2} \tag{A 10}
$$

such that

$$
G(x) = \frac{x}{1-x} + \frac{x}{2x-1}\left(\frac{1}{(4x^2+1)^{1/2}} - \frac{1}{1-x}\right) + \frac{1}{2}\,\frac{4x^2-2x+1}{(1-2x)(4x^2+1)^{1/2}} - \frac{1}{2}. \tag{A 11}
$$

The proof is completed by a straightforward verification of the equivalence between the functions (A 2) and (A 11).

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† Note that in this edition the relation contains a misprint; the correct form which we provided in the text can easily be proven using the method of Petkovšek *et al.* (1996).