

## Two constructions of quantum graphs and two types of spectral statistics

G. Berkolaiko

ABSTRACT. The purpose of this article is to address two questions on fundamentals of quantum graphs.

Quantum graphs are usually introduced either through the differential operator acting on the functions defined on the edges of a graph or through directly specifying the scattering matrices at the vertices of the graphs. The first question addressed in this article is the connection between these constructions, mostly from the point of view of spectral statistics. Our answer to this question is, in most part, a review of the already available results.

The second question we address is the equivalence of two types of spectral statistics of a graph. When spectral statistics of quantum graphs are discussed, the spectrum can refer to one of two things: the eigenvalue spectrum of the differential operator or the eigenphases of the scattering matrix associated to the graph. In the second part of the article we announce and discuss new results explaining in which limit the two types of statistics will agree (complete proofs of the results will appear in [1]).

In addition, we discuss the effect on the spectral statistics of the possible energy-dependence of the  $\mathbf{S}$ -matrix of the graph.

### 1. Introduction

Quantum graphs have attracted much attention in recent years due both to their applicability as physical models, and their interesting mathematical properties. We refer the reader to [2] and to the present volume for a selection of recent results as well as to the reviews [3, 4].

In this article we mostly focus on the aspects of quantum graphs pertaining to their use as models to probe the universality of the spectral characteristics of quantum systems. One of the most intriguing phenomena of quantum mechanics is the observation that many quantum systems are remarkably similar when one makes statistical observations in the semi-classical regime. This manifests itself both in the energy levels, and associated energy eigenfunctions. Quantum graphs are completely typical in this regard, and represent the most likely system for which a full mathematically rigorous proof of this universal behavior will be found.

---

2000 *Mathematics Subject Classification.* 34B45,81Q50.

The author was supported by NSF through the research grant DMS-0604859 and special meeting grant DMS-0648786.

Quantum graphs are usually introduced through one of the two constructions. The first construction identifies edges of the graph with intervals of the real line, hence introducing spaces of functions suitable for defining Laplace differential operator on the graph. The functions are required to satisfy certain conditions on the vertices of the graph, where several edges meet. This setup has a long history of being used in physical models [5, 6, 7]. It was studied by mathematicians since at least the 1980s [8, 9, 10, 11, 12, 13, 14]. The study of spectral statistics of quantum graphs was initiated in [15, 16].

The second construction considers the wave propagation in the graph by specifying the scattering matrices of the vertices and declaring the propagation along the edges to be free. The first known to us use of this construction was by Chalker and co-authors [17, 18]. Spectral statistics of such models were first studied in [19, 20].

Both constructions result in a simple *secular equation* for the eigenvalues  $\{\lambda_n^2\}$  of a quantum graph,

$$(1.1) \quad \det(\mathbf{I} - \mathbf{D}(\lambda)\mathbf{S}(\lambda)) = 0,$$

where  $\mathbf{S}(\lambda)$  is the *bond scattering matrix* in terminology of [16] (also called *global scattering matrix* in [21]). The matrix  $\mathbf{D}(\lambda)$  is an explicitly specified diagonal matrix. We describe the above constructions in more detail in Section 2.

A simple but important question is whether the two constructions are fully analogous. A straightforward observation is that most authors, when using the scattering approach, consider only  $\lambda$ -independent (*energy-independent*) matrices  $\mathbf{S}$ . However, a self-adjoint Laplace operator leads to the  $\mathbf{S}$ -matrix which, in general, depends on  $\lambda$  in a special way. Thus, a study of the spectral statistics of the graphs defined via scattering matrices would appear to be losing some generality. In Section 3.3 we will argue that this is not so.

On the other hand, in the case when the Laplace operator produces an energy-independent  $\mathbf{S}$ -matrix, the matrix  $\mathbf{S}$  has some very special properties (see Lemma 2.1 and preceding discussion). For example, this condition excludes such a popular choice of a scattering matrix, as the Fourier matrix [20, 22]. In Section 2.3 we will discuss two differential operators on quantum graphs, one due to Carlson [23] and the other due to Bolte and Harrison [24], with spectrum actually described by equation (1.1) with arbitrary energy-independent matrix  $\mathbf{S}$ . We will also explain how to obtain solutions of (1.1) with arbitrary  $\mathbf{S}$  as one half of the spectrum of a self-adjoint Laplacian.

Finally we will discuss the connection between the  $\lambda$ -spectrum and the eigenphases of the matrix  $\mathbf{D}(\lambda)\mathbf{S}(\lambda)$ . It is the latter that is usually studied in the works on spectral statistics on graphs with the underlying belief that the statistics of the Laplace operator are the same. In Sections 3.1 and 3.2 we announce and discuss the theorems proved in a forthcoming article [1] which provide a rigorous basis for the said beliefs. The results are obtained for both the statistics of the eigenvalue spectrum and the statistics of the eigenfunctions.

## 2. Two descriptions of quantum graphs

For both constructions of a quantum graph we begin with a graph  $G = (\mathcal{V}, \mathcal{B})$  where  $\mathcal{V}$  is a finite set of vertices (sometimes referred to as nodes), and  $\mathcal{B}$  is the set of edges. Each edge  $e$  has a positive finite length, denoted  $L_e$ . The total number of

edges is  $B$ . We denote by  $d_v$  the degree of the vertex  $v \in \mathcal{V}$ , which is the number of edges emanating from it.

**2.1. The Laplace operator approach.** The first way to define a quantum graph is to identify each edge  $e$  with the interval  $[0, L_e]$  of the real line and thus define the  $L^2$ -space of functions on the graph. Implicitly, we have introduced the *principal direction* on the edge  $e$ : from the vertex corresponding to 0 to the vertex corresponding to  $L_e$ . The choice of this direction is unimportant.

One can now consider the eigenproblem

$$(2.1) \quad -\frac{d^2}{dx^2}u_e(x) = \lambda^2 u_e(x).$$

A solution to the eigenvalue equation (2.1) on the edge  $e$  can be written as a linear combination of plane waves,

$$(2.2) \quad u_e(x_e) = c_e e^{-i\lambda x_e} + \hat{c}_e e^{-i\lambda(L_e - x_e)},$$

where the factor  $e^{-i\lambda L_e}$  is introduced for symmetry with respect to the choice of the principal direction on  $e$ : choosing the other direction would merely result in  $c_e$  and  $\hat{c}_e$  exchanging places.

A solution on the whole graph can be uniquely defined by specifying the corresponding vector of coefficients  $\mathbf{c} = (c_1, \dots, c_B, \hat{c}_1, \dots, \hat{c}_B)^T$ . The elements of the vector  $\mathbf{c}$  are naturally associated with *directed* edges of the graph  $G$ , henceforth referred to as *bonds* and denoted by Greek letters. The start- and end-vertices of a bond  $\alpha$  will be denoted by  $\text{start}(\alpha)$  and  $\text{end}(\alpha)$ . In the absence of multi-edges,  $\text{start}(\alpha)$  and  $\text{end}(\alpha)$  fully specify the bond  $\alpha$ . Each edge of the graph corresponds to two bonds, related by the reversal operation. The reversal of a bond  $\alpha$  is denoted by  $\bar{\alpha}$ . For future reference we rewrite (2.2) in the bond notation,

$$(2.3) \quad u_\alpha(x_\alpha) = c_\alpha e^{-i\lambda x_\alpha} + c_{\bar{\alpha}} e^{-i\lambda(L_\alpha - x_\alpha)}.$$

To make the operator in (2.1) self-adjoint one needs to impose matching conditions on the behavior of  $u$  at the vertices of the graph. The most natural are the Kirchhoff (or ‘‘Neumann’’) conditions: we require that  $u$  is continuous at the vertices, and that the probability current is conserved, i.e.

$$(2.4) \quad \sum_{\alpha: v \rightarrow \alpha} \frac{d}{dx} u_\alpha(v) = 0 \quad \text{for all } v \in \mathcal{V},$$

where the sum is over all bonds  $\alpha$  that originate ( $\rightarrow$ ) from the vertex  $v$  and the derivatives are taken at the vertex  $v$  in the outward direction. All matching conditions giving rise to a self-adjoint operator were classified in, among other sources, [25, 26, 27, 21].

We will describe the general conditions following [25] and [21]. Let  $d_v$  be the degree of the vertex  $v$  (the number of emanating edges). Denote by  $\mathbf{F}(v)$  the vector of values of the function  $f$  at the vertex  $v$  and by  $\mathbf{F}'(v)$  the vector of outgoing derivatives. Both vectors have dimension  $d_v$ . The general self-adjoint conditions can be written in the form

$$(2.5) \quad A_v \mathbf{F}(v) + B_v \mathbf{F}'(v) = 0,$$

where the matrices  $A_v$  and  $B_v$  are such that the  $d_v \times 2d_v$  matrix  $(A_v, B_v)$  has full rank and  $A_v B_v^*$  is Hermitian [25]. An alternative parameterization [21] involves

splitting the conditions into “Neumann”, “Dirichlet” and “Robin” parts:

$$(2.6) \quad P_v F(v) = 0, \quad Q_v F'(v) = 0, \quad R_v F'(v) = C_v R_v F(v),$$

where  $P_v, Q_v$  and  $R_v$  are orthogonal (and mutually orthogonal) projectors operating on  $\mathbb{C}^{d_v}$  and satisfying  $P_v + Q_v + R_v = \mathbf{I}$  and  $C_v$  is a self-adjoint matrix operating on  $\text{Range } R_v$ . Setting  $A_v = P_v - C_v R_v$  and  $B_v = Q_v + R_v$  one can change from parameterization (2.6) to parameterization (2.5).

The scattering matrix  $\sigma^{(v)}$  at the vertex  $v$  describes the evolution of the plain wave  $e^{-i\lambda x}$  coming towards the vertex along one of the incoming bonds. More precisely, we consider the set (indexed by the outgoing bonds  $\alpha$ ) of scattering problems

$$(2.7) \quad \begin{cases} -\frac{d^2 f}{dx^2} = \lambda^2 f(x) \text{ on each edge } e \in E_v, \\ f^{(\alpha)}(x_\alpha) = e^{-i\lambda x} + \sigma_{\alpha\alpha}^{(v)} e^{i\lambda x} \text{ on } \alpha, \\ f^{(\alpha)}(x_\beta) = \sigma_{\beta\alpha}^{(v)} e^{i\lambda x} \text{ on } \beta \neq \alpha, \\ \text{vertex conditions are satisfied at } v, \end{cases}$$

where  $x$  are measured from the vertex  $v$ .

Solving for  $\sigma^{(v)}$  we obtain the following formula [25],

$$(2.8) \quad \sigma^{(v)} = -(A_v + i\lambda B_v)^{-1}(A_v - i\lambda B_v),$$

or, in terms of projectors [21],

$$\sigma^{(v)} = -P_v + Q_v - (C_v - i\lambda)^{-1}(C_v + i\lambda)R_v.$$

For small  $\lambda$  we can write it as

$$\sigma^{(v)} = -P_v + Q_v - R_v - 2i\lambda(C_v - i\lambda)^{-1}R_v = -P_v + Q_v - R_v + O(\lambda),$$

while for large  $\lambda$

$$(2.9) \quad \sigma^{(v)} = -P_v + Q_v + R_v - 2(C_v - i\lambda)^{-1}C_v R_v = -P_v + Q_v + R_v + O(1/\lambda).$$

We note that, although  $\sigma^{(v)}$  is a square matrix, it acts from a space indexed by incoming bonds to the space indexed by the outgoing bonds at the vertex  $v$ .

It is intuitively clear (and can be verified by direct computation) that an eigenfunction of (2.1) with given boundary conditions can be represented locally around  $v$  as a sum of functions  $f^{(\alpha)}(x)$ . Comparing this representation with (2.3) we conclude that *outgoing amplitudes* are related to *incoming amplitudes* through

$$(2.10) \quad (e^{-i\lambda L_1} c_{\bar{e}_1}, \dots, e^{-i\lambda L_d} c_{\bar{e}_d})^T = \sigma^{(v)} (c_{e_1}, \dots, c_{e_d})^T.$$

Noting that outgoing amplitudes  $c_{\bar{e}}$  are incoming for another vertex, we combine all vertex conditions into a  $2B \times 2B$  system

$$(2.11) \quad \mathbf{c} = \mathbf{U}(\lambda)\mathbf{c}, \quad \mathbf{U}(\lambda) = e^{i\lambda \mathbf{L}} \mathbf{S}(\lambda),$$

where the elements of the  $2B \times 2B$  matrix  $\mathbf{S}$  are given by

$$(2.12) \quad (\mathbf{S})_{\beta\alpha} = \delta_{\text{end}(\alpha), \text{start}(\beta)} \sigma_{\beta\alpha}^{(v)}, \quad v = \text{end}(\alpha).$$



amplitude  $a_\beta$ , where  $\beta$  is a bond, being multiplied by the phase factor  $e^{i\lambda L_\beta}$ . Scattering at vertices is described by a unitary<sup>1</sup> matrix  $\mathbf{T}$ , having the property that

$$T_{(v_1, v_2)(v_3, v_4)} = 0 \quad \text{if } v_4 \neq v_1.$$

Altogether we arrive to the *quantum evolution operator*  $\mathbf{U}(\lambda) = e^{i\lambda \mathbf{L}} \mathbf{T}$  and the same secular equation for the eigenvalues,

$$(2.15) \quad \det(\mathbf{I} - e^{i\lambda \mathbf{L}} \mathbf{T}) = 0.$$

In effect, the second construction is simply prescribing the scattering matrices  $\sigma^{(v)}$ . Since one can prescribe arbitrary (in particular,  $\lambda$ -dependent) matrices, the scattering approach is in principle more general than the operator approach. In practice, only  $\lambda$ -independent matrices are considered. One of the most popular choices is the so-called Fourier matrix,

$$(2.16) \quad \sigma_{\beta_k \alpha_j} = \frac{\exp(2\pi i j k / d)}{\sqrt{d}},$$

where  $j = 1 \dots d$  indexes the incoming bonds and  $k = 1 \dots d$  indexes outgoing ones. This matrix is popular because it is “democratic” in assigning equal classical probability  $|\sigma_{\beta_k \alpha_j}|^2$  to each transition. Another interesting choice is *equitransmitting matrices* [34] which prohibit back-scattering and are intimately connected with combinatorial Ihara-Selberg zeta functions.

In general, the above choices of  $\sigma$  do not satisfy the condition of Lemma 2.1 and therefore cannot be obtained from self-adjoint Laplace operator on graphs. There is a real difference in the spectra  $\{\lambda_n\}$  as well: the spectrum of equation (2.1) is obviously symmetric with respect to 0 by construction. This property can be derived from the condition of Lemma 2.1 too.

However, the solutions of (2.15) do not have to be symmetric with respect to the negation. A simple example is with  $L_1 = 1$  and

$$\mathbf{T} = \begin{pmatrix} 1 & 0 \\ 0 & -i \end{pmatrix},$$

for which the solutions of (2.15) are  $\lambda = 0, \pi/2 + 2\pi j$ ,  $j \in \mathbb{Z}$  and are obviously not symmetric.

Interestingly, the symmetry of the spectrum does not imply compliance with Lemma 2.1. An example to this effect is

$$\mathbf{T} = \sigma = \begin{pmatrix} \sin(\phi) & i \cos(\phi) \\ i \cos(\phi) & \sin(\phi) \end{pmatrix},$$

which, for general values of  $\phi$ , does not satisfy  $\sigma^2 = \mathbf{I}$ .

Having highlighted the principal difference between the results of two approaches, in the next section we discuss some differential operators with spectrum that is determined as a solution of (2.15) with arbitrary  $\sigma$ .

---

<sup>1</sup>The unitarity of this matrix implies that at each vertex of the graph the number of outgoing bonds must be equal to the number of incoming bonds.

**2.3. The operator  $iD$  and its relatives.** The first construction we borrow from a work of Carlson [23]. There, the operator  $iD = i\frac{d}{dx}$  is considered on a *directed* graph. At each vertex the number of incoming bonds is equal to the number of outgoing bonds and is denoted by  $\delta_v$ . Given a function  $f$ , the vectors of its incoming and outgoing values at the vertex  $v$  are defined by

$$F_i(v) = \begin{pmatrix} f_{\alpha_1}(L_{\alpha_1}) \\ \vdots \\ f_{\alpha_\delta}(L_{\alpha_\delta}) \end{pmatrix}, \quad F_o(v) = \begin{pmatrix} f_{\beta_1}(0) \\ \vdots \\ f_{\beta_\delta}(0) \end{pmatrix},$$

where  $\alpha_j$  denote the incoming bonds and  $\beta_j$  denote the outgoing ones. The matching condition takes the form

$$F_i(v) = \sigma^{(v)} F_o(v),$$

where  $\sigma^{(v)}$  is a  $\delta \times \delta$ -dimensional matrix. A quick calculation shows that the operator  $-iD$  is self-adjoint if and only if the matrices  $\sigma^{(v)}$  are unitary for every  $v$ .

Solving the eigenvalue problem

$$iDf = \lambda f$$

explicitly, one finds that  $\lambda$  is an eigenvalue if and only if condition

$$\det(\mathbf{I} - e^{i\lambda\mathbf{L}}\mathbf{T}) = 0,$$

is satisfied where the matrix  $\mathbf{T}$  is made up of smaller matrices  $\sigma^{(v)}$  in the familiar manner, see (2.12). The only difference to (2.15) is that the diagonal matrix of lengths  $\mathbf{L}$  is not required to have any structure (all lengths can be different, unlike (2.13)). Thus we can establish the following correspondence: let  $G$  be an (undirected) graph with bond lengths  $\ell = (L_1, \dots, L_B)$  and the bond scattering matrix  $T$ . Denote by  $G_d$  the *directed* graph obtained by splitting each edge of  $G$  into two directed bonds, each of the same length as the original edge. Then equation (2.15) describes the spectrum of the operator  $iD$  on the graph  $G_d$ . It is obvious from the construction that at each vertex of the graph  $G_d$  the number of incoming bonds equals the number of outgoing ones, as required.

Another, rather similar construction, is to consider the Dirac operator of graphs. Most of the discussion below originates from [24] and we refer the reader to it for more details. The Dirac operator is

$$(2.17) \quad \mathcal{D} = -i\hbar c \alpha \frac{d}{dx} + mc^2 \beta,$$

where  $\alpha$  and  $\beta$  are 4-dimensional matrices satisfying  $\alpha^2 = \beta^2 = \mathbf{I}$  and  $\alpha\beta + \beta\alpha = 0$ . Several simplifications can be done. One can take the matrices  $\alpha$  and  $\beta$  to be 2-dimensional (although some physical interpretations will be lost as a result), for example

$$\alpha = \begin{pmatrix} 0 & -i \\ i & 0 \end{pmatrix} \quad \beta = \begin{pmatrix} 1 & 0 \\ 0 & -1 \end{pmatrix}.$$

We will also set the mass  $m$  to zero (this does not affect the high energy statistics). Finally, we will rescale  $\hbar c = 1$ . With these simplifications, the (two-component) eigenvalue equation  $\mathcal{D}\psi = \lambda\psi$  becomes

$$(2.18) \quad \begin{pmatrix} \psi' \\ \phi' \end{pmatrix} = \begin{pmatrix} \lambda\phi \\ -\lambda\psi \end{pmatrix}.$$

We denote by  $\Psi(v)$  the vector of first components of the wavefunction at the vertex  $v$ . Since the operator  $\mathcal{D}$  is first-order, the *principal* direction of an edge becomes important. This manifests itself in the definition of  $\Phi(v)$ ,

$$\Phi(v) = (-\phi_{e_1}(0), \dots, -\phi_{e_j}(0), \phi_{e_{j+1}}(L_{e_{j+1}}), \dots, \phi_{e_\delta}(L_{e_\delta}),$$

where the edges  $e_1$  to  $e_j$  are going out of the vertex  $v$  (according to their principal direction) and the rest are coming in. Comparing with (2.18) we can interpret  $\Phi$  simply as  $\frac{1}{\lambda}\Psi'(v)$ , where  $\Psi'(v)$  is the vector of the derivatives of the functions  $\psi$  taken in the *outward direction*. From this point of view, the factor  $1/\lambda$  is the only difference from the setup for the Laplace operator.

All matching conditions making the Dirac operator self-adjoint can be written as

$$A_v\Psi(v) + B_v\Phi(v) = 0, \quad (A_v, B_v) \text{ has maximal rank and } A_v B_v^* = B_v A_v^*,$$

in analogy to (2.5). Solving the scattering problem shows [24] that the spectrum is again precisely determined by equation (2.15) with the matrix  $\mathbf{T}$  made up of unitary matrices

$$(2.19) \quad \sigma^{(v)} = -(A_v + i\gamma(\lambda)B_v)^{-1}(A_v - i\gamma(\lambda)B_v),$$

where  $\gamma(\lambda) = 1$  when  $m = 0$  and  $\gamma(\lambda) \rightarrow 1$  as  $\lambda \rightarrow \infty$  in the general case. Thus we see that, for a massless Dirac equation, we can obtain an arbitrary  $\lambda$ -independent unitary scattering matrix on every vertex. Indeed, for an arbitrary  $U_v$ , we can set

$$A_v = \frac{1}{2}(U_v + \mathbf{I}) \quad B_v = \frac{i}{2}(U_v - \mathbf{I})$$

and obtain

$$\sigma^{(v)} = -(A_v + iB_v)^{-1}(A_v - iB_v) = U_v.$$

The final construction, reported here for the first time, allows to realize the set  $\Lambda$  of solutions of (2.15) as a subset of density  $1/2$  of a spectrum of a self-adjoint Laplace operator. To do so, we replace each edge with 2 edges of equal length connecting the same points. Equation (2.10) then becomes

$$\begin{aligned} & \left( e^{-i\lambda L_1} c_{\beta_1}, \dots, e^{-i\lambda L_d} c_{\beta_d}, e^{-i\lambda L_1} c_{\beta'_1}, \dots, e^{-i\lambda L_d} c_{\beta'_d} \right)^T \\ & = \tilde{\sigma}^{(v)} \left( c_{\alpha_1}, \dots, c_{\alpha_d}, c_{\alpha'_1}, \dots, c_{\alpha'_d} \right)^T, \end{aligned}$$

where  $\alpha_j$  and  $\alpha'_j$  are incoming bonds and  $\beta_j$  and  $\beta'_j$  are the outgoing ones. If we set

$$\tilde{\sigma} = \begin{pmatrix} 0 & \sigma \\ \sigma^* & 0 \end{pmatrix}$$

at each vertex, the condition of Lemma 2.1 is clearly satisfied. An easy calculation shows that the secular equation factorizes

$$(2.20) \quad \det(\mathbf{I} - e^{i\lambda\mathbf{L}}\mathbf{S}) \det(\mathbf{I} - e^{-i\lambda\mathbf{L}}\mathbf{S}) = 0,$$

which shows that the spectrum of the doubled graph is the set  $\Lambda \cup (-\Lambda)$ . While we do not know of any *a priori* connections between the spectral statistics of  $\Lambda$  and  $\Lambda \cup (-\Lambda)$ , this construction brings us back to the fundamental difference between the solutions of (2.15) and the eigenvalues of (2.1): the latter are symmetric with respect to 0 and the former, in general, are not.



### 3. Two meanings of “spectrum” of quantum graphs and their statistics

Unless explicitly noted to the contrary, we will now assume that the scattering matrix  $\mathbf{S}$  is  $\lambda$ -independent, whether it is obtained from a Laplace operator (see section 2.1) or directly specified (see section 2.2). In section 3.3 we will discuss what happens to the spectral statistics when this condition is dropped.

In various sources the notion of the “spectrum  $\sigma(G)$  of the graph  $G$ ” can refer to:-

- (1) the eigenproblem (2.1) and thus the solutions  $\{\lambda_n\}$  of (2.14),
- (2) the eigenphases of the matrix  $\mathbf{U}(\lambda) = e^{i\lambda\mathbf{L}}\mathbf{S}(\lambda)$  for an arbitrary  $\lambda$ , i.e. to the set of  $2B$  numbers  $\{\theta_j\}$  such that  $e^{i\theta_j}$  is the  $j$ -th eigenvalue of  $\mathbf{U}(\lambda)$ .

We will refer to the first definition of the spectrum as the  $\lambda$ -spectrum, and the second as the  $\theta$ -spectrum.

In a similar way, the “eigenvector” of  $G$  can refer to one of three objects:-

- (1) the function  $u(x)$  that solves (2.1), subject to boundary conditions, for some  $\lambda_n$  in the  $\lambda$ -spectrum,
- (2) the eigenvector of  $\mathbf{U}(\lambda_n) = \mathbf{1}$  corresponding to the eigenvalue 1, i.e. to the solution  $\mathbf{c}$  of  $\mathbf{U}(\lambda_n)\mathbf{c} = \mathbf{c}$ . These eigenvectors will be denoted by  $\phi_n$ ,
- (3) any of the  $2B$  eigenvectors of  $\mathbf{U}(\lambda)$  for arbitrary  $\lambda$ , denoted by  $\psi_j(\lambda)$ ,  $j = 1, \dots, 2B$ .

The correspondence between the first two types of eigenvectors is given by formula (2.3). A heuristic formula which connects properties of the second and the third types of eigenvectors was suggested in [35, Eq. (5)]. In this article we explain the results of [1] which prove this and some other useful relationships between statistics of different types of eigenvectors and eigenvalues.

**3.1. Eigenvalue statistics.** Starting with the seminal work by Kottos and Smilansky [15, 16], the quantum graphs became a popular model of quantum chaos. One of the more pertinent questions of quantum chaos is the universality of the eigenvalue correlations among systems of a certain type. On graphs, [15] showed some preliminary numerical evidence that eigenvalue spectrum of graphs follow the general prediction [36, 37] which says that the spectrum of classically chaotic system should have correlations typical associated to eigenvalues of large random matrices. Persistent deviations from the predicted behavior were found in star graphs [16, 38] and Tanner [20] proposed a precise condition on the graphs to follow the random matrix theory prediction. This question was then attacked analytically by various methods, with results reported, in particular, in [39, 40, 41]. For more information we refer the reader to a recent review [4].

While the original interest was in level statistics, i.e. the statistical functions of the spectrum  $\{\lambda_n\}$ , most of the analytical studies were in fact concentrating on the eigenphase statistics of the  $\theta$ -spectrum. There are heuristic reasons why the corresponding statistics should coincide, but the formal link between the two has hitherto not been explored.

The most work in spectral statistics on graphs has been done on nearest-neighbor spacing distribution (mostly numeric, starting from [15]; but see also [28]), form factor ([15, 16, 38, 20, 39, 22, 41] and others) and the two-point correlation function (see [29, 42, 40]). Most articles proceed to study properties of the statistical functions without considering whether the sought functions exist and in what sense. However, for quantum graphs this question can and should be

considered (flat tori is an example of another system where the existence question is well understood, see for example [43]).

In this article we discuss a theorem (proved in [1]) showing that, in the correct limit, the two statistics exist and are equivalent. We take the example of nearest-neighbor spacing distribution, i.e. the distribution of gaps  $\{\lambda_n - \lambda_{n-1}\}$  on one hand and of the values of the functions  $\{\theta_j(\lambda) - \theta_{j-1}(\lambda)\}$  on the other. Formally, the level spacing distribution is given by

$$P(s) = \lim_{N \rightarrow \infty} \frac{1}{N} \sum_{n=1}^N \delta(s - (\lambda_n - \lambda_{n-1})),$$

where  $\delta$  is the Dirac delta-function. Mathematically, the distributions are defined via a family of test functions.

**THEOREM 3.1 ([1]).** *Let  $h$  be a continuous function. If  $\mathbf{L}$  is linearly independent over  $\mathbb{Q}$ , the limits*

$$(3.1) \quad P_\lambda[h] := \lim_{N \rightarrow \infty} \frac{1}{N} \sum_{n=1}^N h(\lambda_n - \lambda_{n-1})$$

and

$$(3.2) \quad P_\theta[h] = \lim_{\Lambda \rightarrow \infty} \frac{1}{\Lambda} \int_0^\Lambda \frac{1}{2B} \sum_{j=1}^{2B} h(\theta_j(\lambda) - \theta_{j-1}(\lambda)) d\lambda$$

exist and define bounded linear functionals of  $h$ . If we take the limit

$$\mathbf{L} \rightarrow (\ell_0, \ell_0, \dots, \ell_0)$$

for some  $\ell_0 > 0$ , while keeping  $\mathbf{L}$  linearly independent over  $\mathbb{Q}$ , the two functionals coincide. Namely,

$$(3.3) \quad \lim_{\Delta L \rightarrow 0} P_\lambda[h] = \lim_{\Delta L \rightarrow 0} P_\theta[h],$$

where  $\Delta L := L_{\max} - L_{\min}$  is the spread of the distribution of the bond lengths.

The proof of this theorem is similar but slightly more complicated than the proof of Theorem 3.2. We will present the main ideas behind both proofs in the next section, following the statement of Theorem 3.2.

If  $\mathbf{L}$  is *not* linearly independent over  $\mathbb{Q}$ , the limits (3.1) and (3.2) still exist but are highly sensitive to the changes in individual bond length. Thus the limits in equation (3.3) are, in general, singular. In particular, when all bond lengths are equal ( $\Delta L = 0$ ), the  $\lambda$ -spectrum is periodic and spacings in  $\theta$ -spectrum are independent of  $\lambda$ . The nearest-neighbor distribution in this case is highly degenerate.

It is straightforward to extend the result to  $r$ -th nearest neighbor spacing distributions, i.e. the distributions of  $\lambda_n - \lambda_{n-r}$  and  $\theta_j(\lambda) - \theta_{j-r}(\lambda)$ . Moreover, when all  $r$ -th nearest spacing distributions coincide, so do other statistical functions such as the  $n$ -point correlation functions.

**3.2. Eigenvector statistics.** The equivalence between the statistics of the  $\lambda$ -spectrum and the  $\theta$ -spectrum can be extended to eigenfunction statistics.

To proceed, we need to introduce more notation. By  $\psi_j(\lambda)$  we will denote the  $j$ -th eigenvector of  $\mathbf{S}(\lambda)$ . The matrix  $\mathbf{L}$ , as before, is the diagonal matrix of the bond lengths. The total length of the graph is  $\mathcal{L} = \sum_{b=1}^B L_b$  and the average bond length,  $\mathcal{L}/B$ , is denoted by  $\bar{L}$ .

Let  $A$  be a  $2B \times 2B$  matrix (“observable”). We denote  $A_n = \langle \phi_n | A | \phi_n \rangle$  and  $A_j(\lambda) = \langle \psi_j(\lambda) | A | \psi_j(\lambda) \rangle$ , which corresponds to the “expected value of the observable  $A$ ”. Without loss of generality [35] we can assume that  $A$  has zero mean or, equivalently,  $\text{Tr } A = 0$ . Similarly we define  $L(\lambda_n) = \langle \phi_n | \mathbf{L} | \phi_n \rangle$ .

Further, let  $\mathbf{D}$  denote a diagonal unitary matrix of the form

$$\mathbf{D} = \text{diag}(e^{ix_1}, \dots, e^{ix_B}, e^{ix_1}, \dots, e^{ix_B})$$

and

$$A_j(\mathbf{D}) = \langle \psi_j(\mathbf{D}) | A | \psi_j(\mathbf{D}) \rangle$$

be the expectation of  $A$  with respect to the  $j$ -th eigenvector  $\psi_j(\mathbf{D})$  of the matrix  $\mathbf{D}\mathbf{S}$ . By  $\mathbb{E}^D(\cdot)$  we denote the average with respect to the natural uniform probability measure on matrices  $\mathbf{D}$ : each of the  $B$  distinct diagonal elements of  $\mathbf{D}$  is an independent random variable uniformly distributed on the unit circle.

One of the central results in the study of statistical properties of eigenvectors is “quantum ergodicity”. Quantum ergodicity is the property of almost all eigenvectors to equidistribute [44, 45, 46]. In our context, this corresponds to vanishing of the variance of either  $A_n$  or  $A_j(\lambda)$  in some limit. We shall not discuss here the important question of which limit is appropriate; we refer the interested reader to [35]. Instead we present a result that the moments of  $A_n$  and  $A_j(\lambda)$  are equivalent. This result first appeared in a note by Keating and Smilansky, where a heuristic argument using periodic orbit theory was proposed (it later got published in [35]). In [1] it is proved rigorously using ergodicity considerations.

**THEOREM 3.2 ([1]).** *Let  $\mathbf{L}$  be linearly independent over  $\mathbb{Q}$ . Then, for all  $m \geq 0$ ,*

$$(3.4) \quad \lim_{N \rightarrow \infty} \frac{1}{N} \sum_{n=1}^N \frac{A_n^m}{L(\lambda_n)/\bar{L}} = \lim_{\Lambda \rightarrow \infty} \frac{1}{\Lambda} \int_0^\Lambda \frac{1}{2B} \sum_{k=1}^{2B} A_j(\lambda)^m d\lambda = \mathbb{E}^D \left( \frac{1}{2B} \sum_{k=1}^{2B} A_j(\mathbf{D})^m \right).$$

The weights  $L(\lambda_n)/\bar{L}$  on the left-hand side of (3.4) shows that the exact equivalence of the moments should only be expected in the additional limit  $\Delta \rightarrow 0$ . This limit was necessary in Theorem 3.1 and was also used previously in [38, 47]. Still, provided the distribution of lengths is bounded away from zero and infinity, the two types of moments would go to the zero limit simultaneously or not at all. Moreover, the second part of equation (3.4) relates the moments of the eigenvectors of a fixed graph to the averaged properties of an *ensemble* of random matrices. This is extremely important as it allows one to use such disorder-average methods as super-symmetry (see [42, 40]).

The main idea of the proof of Theorem 3.2 is to introduce a family of spectra,  $\{\lambda_{\alpha,n}\}_{n=1}^\infty$ , indexed by  $\alpha \in [0, 2\pi]$ . The value  $\lambda_{\alpha,n}$  is  $n$ -th solution to a modified version of equation (2.14),

$$\det(\mathbf{I} - e^{i\alpha} e^{i\lambda \mathbf{L}} \mathbf{S}(\lambda)) = 0.$$

The original spectrum  $\{\lambda_n\}$  coincides with  $\{\lambda_{0,n}\}$ . One can then show that the statistics (in this case, eigenvector statistics) of all such spectra coincide. This is done using an idea of Barra and Gaspard [28] that visualizes the levels  $\lambda_n$  as piercings of the manifold  $\det(\mathbf{I} - e^{ix} \mathbf{S}) = 0$  by an ergodic flow on  $B$ -dimensional torus.

Since statistics for all  $\alpha$  coincide, one can substitute  $A_{\alpha,n}$  for  $A_n$  in the left-hand side of (3.4) and add an averaging with respect to  $\alpha$ . It then turns out that

the average with respect to  $\alpha$  coincides precisely with the right-hand side of (3.4). The proof of Theorem 3.2 follows the same basic outline.

Finally, we would like to mention that in [35], quantum ergodicity was proved for a special family of graphs of increasing size, originally due to [48]. The variance was shown to vanish *without* any spectral or disorder averaging, i.e. it was shown that

$$\lim_{B \rightarrow \infty} \frac{1}{2B} \sum_{k=1}^{2B} A_j(\lambda, B)^m = 0.$$

This is a rather strong result which used absence of loops of a certain type on the said graphs. In general, we cannot expect such “individual” quantum ergodicity on graphs, forcing one to use an averaging as in (3.4).

**3.3. Statistics of  $\lambda$ -dependent matrices.** Now suppose that  $\mathbf{S}(\lambda)$  has a dependence on  $\lambda$  of the type (2.8). Equation (2.9) shows that  $\mathbf{S}(\lambda) \rightarrow \mathbf{S}_\infty$  as  $\lambda \rightarrow \infty$ , where  $\mathbf{S}_\infty = \mathbf{I} - 2P_v$ . Then, if  $\{\lambda_j\}_{j=1}^\infty$  is the solutions of  $\det(\mathbf{I} - e^{i\lambda\mathbf{L}}\mathbf{S}_\infty) = 0$ , then the solutions of the equation  $\det(\mathbf{I} - e^{i\lambda\mathbf{L}}\mathbf{S}(\lambda)) = 0$  are  $\tilde{\lambda}_j = \lambda_j + \kappa_j$ , where  $\kappa_j \rightarrow 0$  as  $j \rightarrow \infty$ . In this situation, the spectral statistics of  $\{\lambda_j\}_{j=1}^\infty$  and  $\{\tilde{\lambda}_j\}_{j=1}^\infty$  are the same. We illustrate this on the level spacing distribution.

**THEOREM 3.3.** *Let  $h$  be a bounded equicontinuous function (e.g. a continuous function with a compact support). If  $\tilde{\lambda}_j = \lambda_j + \kappa_j$  with  $\kappa_j \rightarrow 0$  as  $j \rightarrow \infty$ , then*

$$(3.5) \quad P_\lambda[h] = P_{\tilde{\lambda}}[h],$$

where  $P_\lambda[h]$  is defined by

$$P_\lambda[h] := \lim_{N \rightarrow \infty} \frac{1}{N} \sum_{n=1}^N h(\lambda_n - \lambda_{n-1}).$$

**REMARK 3.4.** Theorem 3.1 guarantees that  $P_\lambda[h]$  exists, therefore (3.5) will imply that  $P_{\tilde{\lambda}}[h]$  exists too.

**PROOF.** The proof is a simple exercise in classical analysis. Given  $\epsilon > 0$  choose  $\delta > 0$  such that  $|h(x) - h(y)| < \epsilon$  whenever  $|x - y| \leq \delta$  (equicontinuity). Choose  $J$  such that  $\kappa_j < \delta/2$  whenever  $j \geq J$ . Then, denoting  $\lambda_n - \lambda_{n-1} = s_n$  and  $\tilde{\lambda}_n - \tilde{\lambda}_{n-1} = \tilde{s}_n$ ,

$$\begin{aligned} & \left| \frac{1}{N} \sum_{n=1}^N h(s_n) - \frac{1}{N} \sum_{n=1}^N h(\tilde{s}_n) \right| \\ & \leq \frac{1}{N} \sum_{n=1}^{J-1} |h(s_n) - h(\tilde{s}_n)| + \frac{1}{N} \sum_{n=J}^N |h(s) - h(\tilde{s}_n)| \\ & \leq \frac{2(J-1)M}{N} + \frac{(N-J)\epsilon}{N}, \end{aligned}$$

where  $M$  is an upper bound of  $|h(x)|$ . Taking first the limit  $N \rightarrow \infty$  and then the limit  $\epsilon \rightarrow 0$  (the left-hand side does not depend on  $\epsilon$ ), we conclude that

$$\lim_{N \rightarrow \infty} \left| \frac{1}{N} \sum_{n=1}^N h(\lambda_n - \lambda_{n-1}) - \frac{1}{N} \sum_{n=1}^N h(\tilde{\lambda}_n - \tilde{\lambda}_{n-1}) \right| = 0.$$

□

### Acknowledgement

The author would like to thank B. Gutkin and T. Kottos for asking questions I could not (then) answer, B. Winn for allowing to use material from our joint paper [1], Isaac Newton Institute for Mathematical Sciences, Cambridge, UK for hosting such an interesting programme (where the questions resurfaced again) and to NSF for support through the research grant DMS-0604859 and special meeting grant DMS-0648786.

### References

- [1] G. Berkolaiko and B. Winn, “Relationship between scattering matrix and spectrum of quantum graphs.” preprint arXiv:0801.4104 [math-ph], 2008.
- [2] G. Berkolaiko, R. Carlson, S. Fulling, and P. Kuchment, eds., *Proceedings of Joint Summer Research Conference on Quantum Graphs and Their Applications, 2005*. Contemporary Mathematics, AMS, 2006.
- [3] P. Kuchment, “Graph models for waves in thin structures,” *Waves Random Media*, vol. 12, no. 4, pp. R1–R24, 2002.
- [4] S. Gnutzmann and U. Smilansky, “Quantum graphs: Applications to quantum chaos and universal spectral statistics,” *Advances in Physics*, vol. 55, no. 5, pp. 527–625, 2006.
- [5] L. Pauling, “The dimagnetic entropy of aromatic molecules,” *J. Chem. Phys.*, vol. 4, pp. 673–677, 1936.
- [6] J. Griffith, “A free-electron theory of conjugated molecules. i. polycyclic hydrocarbons,” *Trans. Faraday Soc.*, vol. 49, pp. 345–351, 1953.
- [7] K. Ruedenberg and C. W. Scherr, “Free-electron network model for conjugated systems. I. Theory,” *J. Chem. Physics*, vol. 21, no. 9, pp. 1565–1581, 1953.
- [8] G. Lumer, “Espaces ramifiés, et diffusions sur les réseaux topologiques,” *C. R. Acad. Sci. Paris Sér. A-B*, vol. 291, no. 12, pp. A627–A630, 1980.
- [9] J.-P. Roth, “Le spectre du laplacien sur un graphe,” in *Théorie du potentiel (Orsay, 1983)*, vol. 1096 of *Lecture Notes in Math.*, pp. 521–539, Berlin: Springer, 1984.
- [10] J. von Below, “A characteristic equation associated to an eigenvalue problem on  $c^2$ -networks,” *Linear Algebra Appl.*, vol. 71, pp. 309–325, 1985.
- [11] S. Nicaise, “Spectre des réseaux topologiques finis,” *Bull. Sci. Math. (2)*, vol. 111, no. 4, pp. 401–413, 1987.
- [12] O. M. Penkin and Y. V. Pokornyy, “On a boundary value problem on a graph (in Russian),” *Differentsial'nye Uravneniya*, vol. 24, no. 4, pp. 701–703, 734–735, 1988.
- [13] N. I. Gerasimenko and B. S. Pavlov, “A scattering problem on noncompact graphs,” *Teoret. Mat. Fiz.*, vol. 74, no. 3, pp. 345–359, 1988.
- [14] P. Exner and P. Šeba, “Free quantum motion on a branching graph,” *Rep. Math. Phys.*, vol. 28, no. 1, pp. 7–26, 1989.
- [15] T. Kottos and U. Smilansky, “Quantum chaos on graphs,” *Phys. Rev. Lett.*, vol. 79, pp. 4794–4797, 1997.
- [16] T. Kottos and U. Smilansky, “Periodic orbit theory and spectral statistics for quantum graphs,” *Ann. Phys.*, vol. 274, pp. 76–124, 1999.
- [17] J. Chalker and P. Coddington, “Percolation, quantum tunnelling and the integer hall effect,” *Journal of Physics C: Solid State Physics*, vol. 21, no. 14, pp. 2665–2679, 1988.
- [18] J. T. Chalker and S. Siak, “Anderson localisation on a cayley tree: a new model with a simple solution,” *Journal of Physics: Condensed Matter*, vol. 2, no. 11, pp. 2671–2686, 1990.
- [19] H. Schanz and U. Smilansky, “Spectral statistics for quantum graphs: periodic orbits and combinatorics,” *Phil. Mag. B*, vol. 80, no. 12, pp. 1999–2021, 2000.
- [20] G. Tanner, “Unitary-stochastic matrix ensembles and spectral statistics,” *J. Phys. A*, vol. 34, no. 41, pp. 8485–8500, 2001.
- [21] S. A. Fulling, P. Kuchment, and J. H. Wilson, “Index theorems for quantum graphs,” *J. Math. Phys. A*, vol. 40, pp. 14165–14180, 2007.
- [22] G. Berkolaiko, H. Schanz, and R. S. Whitney, “Form factor for a family of quantum graphs: an expansion to third order,” *J. Phys. A*, vol. 36, no. 31, pp. 8373–8392, 2003.

- [23] R. Carlson, “Inverse eigenvalue problems on directed graphs,” *Trans. Amer. Math. Soc.*, vol. 351, no. 10, pp. 4069–4088, 1999.
- [24] J. Bolte and J. Harrison, “Spectral statistics for the dirac operator on graphs,” *J. Phys. A*, vol. 36, no. 11, pp. 2747–2769, 2003.
- [25] V. Kostrykin and R. Schrader, “Kirchhoff’s rule for quantum wires,” *J. Phys. A*, vol. 32, no. 4, pp. 595–630, 1999.
- [26] M. Harmer, “Hermitian symplectic geometry and extension theory,” *J. Phys. A*, vol. 33, no. 50, pp. 9193–9203, 2000.
- [27] P. Kuchment, “Quantum graphs. I. Some basic structures,” *Waves Random Media*, vol. 14, no. 1, pp. S107–S128, 2004. Special section on quantum graphs.
- [28] F. Barra and P. Gaspard, “On the level spacing distribution in quantum graphs,” *J. Stat. Phys.*, vol. 101, no. 1-2, pp. 283–319, 2000.
- [29] G. Berkolaiko, E. B. Bogomolny, and J. P. Keating, “Star graphs and Šeba billiards,” *J. Phys. A*, vol. 34, no. 3, pp. 335–350, 2001.
- [30] J. P. Keating, J. Marklof, and B. Winn, “Value distribution of the eigenfunctions and spectral determinants of quantum star graphs,” *Comm. Math. Phys.*, vol. 241, no. 2-3, pp. 421–452, 2003.
- [31] G. Berkolaiko, J. P. Keating, and B. Winn, “Intermediate wave-function statistics,” *Phys. Rev. Lett.*, vol. 91, 2003.
- [32] V. Kostrykin, J. Potthoff, and R. Schrader, “Heat kernels on metric graphs and a trace formula.” math-ph/0701009, Jan. 2007.
- [33] T. Kottos and U. Smilansky, “Chaotic scattering on graphs,” *Phys. Rev. Lett.*, vol. 85, no. 5, pp. 968–971, 2000.
- [34] J. M. Harrison, U. Smilansky, and B. Winn, “Quantum graphs where back-scattering is prohibited,” *Journal of Physics A: Mathematical and Theoretical*, vol. 40, no. 47, pp. 14181–14193, 2007.
- [35] G. Berkolaiko, J. P. Keating, and U. Smilansky, “Quantum ergodicity for graphs related to interval maps,” *Comm. Math. Phys.*, vol. 273, no. 1, pp. 137–159, 2007.
- [36] O. Bohigas, M.-J. Giannoni, and C. Schmit, “Characterization of chaotic quantum spectra and universality of level fluctuation laws,” *Phys. Rev. Lett.*, vol. 52, no. 1, pp. 1–4, 1984.
- [37] G. Casati, F. Valz-Griz, and I. Guarneri, “On the connection between the quantization of nonintegrable systems and statistical theory of spectra,” *Lett. Nuovo Cimento*, vol. 28, pp. 279–282, 1980.
- [38] G. Berkolaiko and J. P. Keating, “Two-point spectral correlations for star graphs,” *J. Phys. A*, vol. 32, no. 45, pp. 7827–7841, 1999.
- [39] G. Berkolaiko, H. Schanz, and R. S. Whitney, “Leading off-diagonal correction to the form factor of large graphs,” *Phys. Rev. Lett.*, vol. 88, no. 10, p. 104101, 2002.
- [40] S. Gnuzmann and A. Altland, “Spectral correlations of individual quantum graphs,” *Phys. Rev. E*, vol. 72, no. 5, p. 056215, 2005.
- [41] G. Berkolaiko, “Correlations within the spectrum of a large quantum graph: a diagrammatic approach,” in *Proceedings of Joint Summer Research Conference on Quantum Graphs and Their Applications, 2005* (G. Berkolaiko, R. Carlson, S. Fulling, and P. Kuchment, eds.), AMS, 2006.
- [42] S. Gnuzmann and A. Altland, “Universal spectral statistics in quantum graphs,” *Phys. Rev. Lett.*, vol. 93, no. 19, p. 194101, 2004.
- [43] J. Marklof, “Pair correlation densities of inhomogeneous quadratic forms,” *Ann. of Math. (2)*, vol. 158, no. 2, pp. 419–471, 2003.
- [44] A. I. Šnirel’man, “Ergodic properties of eigenfunctions,” *Uspehi Mat. Nauk*, vol. 29, no. 6(180), pp. 181–182, 1974.
- [45] S. Zelditch, “Uniform distribution of eigenfunctions on compact hyperbolic surfaces,” *Duke Math. J.*, vol. 55, no. 4, pp. 919–941, 1987.
- [46] Y. Colin de Verdière, “Ergodicité et fonctions propres du laplacien,” *Comm. Math. Phys.*, vol. 102, no. 3, pp. 497–502, 1985.
- [47] G. Berkolaiko, J. P. Keating, and B. Winn, “No quantum ergodicity for star graphs,” *Comm. Math. Phys.*, vol. 250, no. 2, pp. 259–285, 2004.
- [48] P. Pakoński, K. Życzkowski, and M. Kuś, “Classical 1D maps, quantum graphs and ensembles of unitary matrices,” *J. Phys. A*, vol. 34, no. 43, pp. 9303–9317, 2001.

DEPARTMENT OF MATHEMATICS, TEXAS A&M UNIVERSITY, COLLEGE STATION, TX 77843,  
USA