

Relationship between scattering matrix and spectrum of quantum graphs

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Abstract

We investigate the equivalence between spectral characteristics of the Laplace operator on a metric graph, and the associated unitary scattering operator. We prove that the statistics of level spacings, and moments of observations in the eigenbases coincide in the limit that all bond lengths approach a positive constant value.

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 [1] and the forthcoming volume [2] for a *pot-pourri* of new results. Recent reviews, dedicated to quantum graphs, include [3, 4].

In this article we focus on one feature of interest which is the use of graph models to probe the the universality of quantum systems. One of the unsolved paradoxes of quantum mechanics is the observation that a great many quantum systems are remarkably similar when one makes statistical observations in the semi-classical régime. This manifests itself both in the energy levels, and associated energy eigenfunctions. Despite a great deal of effort, this universality is poorly understood mathematically. Generic quantum graphs exhibit this universal behavior, and represent the most likely system for which a full mathematically rigorous proof of this universality will first be found. Important steps in this direction have been taken in [5].

A *quantum graph* can be defined in two different, but related, ways (a complete description appears in the following section). One may consider a self-adjoint realisation of the Laplace operator, or a scattering matrix approach. Mathematically, the scattering approach appears to be more tractable, and has formed the basis of most investigations [6, 7, 8, 9, 10]. Moreover, the spectra arising from these quantizations are subtly different. This is not as confusing as it might seem, since the statistical properties of both versions of the spectrum are believed to coincide when averaged over a large interval. It is the purpose of this article to put a concrete mathematical foundation behind this belief.

The plan of the article is as follows: In the next section we give precise definitions of the two ways to describe quantum graphs, and in section 3 describe our main results. In section 4 we describe the tools used and then present in section 5 the proofs of our results.

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 bonds (or edges). Each bond b has a positive length, denoted L_b . The total number of bonds is B . We denote by d_v the degree of the vertex $v \in \mathcal{V}$, which is the number of bonds emanating from it.

2.1 The Laplace operator approach

The first way to define a quantum graph is to identify each bond b with the interval $[0, L_b]$ of the real line and thus define the L^2 -space of functions on the graph. Then one can consider the eigenproblem

$$-\frac{d^2}{dx^2}u_b(x) = \lambda^2 u_b(x). \quad (1)$$

This setup has a long history of being used in physical models [11, 12, 13]. It was studied by mathematicians since at least the 1980s [14, 15, 16, 17, 18, 19, 20]. The study of spectral statistics of quantum graphs was initiated in [21, 22].

To make the operator in (1) self-adjoint one needs to impose matching conditions on the behavior of u at the vertices of the graph. One possibility is to impose Kirchhoff conditions:¹ we require that u is continuous at the vertices, and that the probability current is conserved, i.e.

$$\sum_{v \in b} \frac{d}{dx} u_b(v) = 0 \quad \text{for all } v \in \mathcal{V}, \quad (2)$$

where the sum is over all bonds that originate from the vertex v and the derivatives are taken at the vertex v in the outward direction. The admissible matching conditions were classified in, among other sources, [23, 24, 25].

A solution to the eigenvalue equation (2) on the bond b , can be written as a linear combination of plane waves,

$$\psi_b(x_b) = c_b e^{ikx_b} + \hat{c}_b e^{-ikx_b}. \quad (3)$$

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* bonds of the graph G .

Imposing the matching conditions, we find that λ^2 is an eigenvalue if and only if $S(\lambda)\mathbf{c} = \mathbf{c}$ for some explicitly given matrix $S(\lambda)$. For instance, in the case of Kirchhoff conditions given above,

$$S(\lambda) = e^{i\lambda \mathbf{L}} S_0, \quad (4)$$

where the elements of the $2B \times 2B$ matrix S_0 are given by

$$(S_0)_{(v_1, v_2)(v_3, v_4)} = \delta_{v_2, v_3} \left(\frac{2}{d_{v_2}} - \delta_{v_1, v_4} \right),$$

¹sometimes called ‘‘Neumann’’ conditions

for (v_1, v_2) and (v_3, v_4) directed bonds of the graph. By \mathbf{L} we denoted the vector of bond lengths $\mathbf{L} = (L_1, \dots, L_B)$ and defined, in a slight abuse of notation, a $2B \times 2B$ diagonal matrix

$$e^{i\mathbf{x}} := \begin{pmatrix} e^{ix_1} & & & & & \\ & \ddots & & & & \\ & & e^{ix_B} & & & \\ & & & e^{ix_1} & & \\ & & & & \ddots & \\ & & & & & e^{ix_B} \end{pmatrix}, \quad (5)$$

where $\mathbf{x} \in \mathbb{R}^{2B}$. Note the doubling of dimension which signifies the move from undirected to directed bonds.

The general conditions for factorization (4) are given in [26, 27]. Even when these conditions are not satisfied and S depends on λ in a non-trivial fashion, the above factorization is valid in the limit $\lambda \rightarrow \infty$. Thus, for the purpose of studying the spectral statistics it is not a strong restriction to assume that (4) applies, as we will do below.

2.2 The scattering approach

The second construction considers wave propagation on the graph where each vertex is treated as a scatterer and propagation along the bonds is free. This construction was first considered in the context of studying spectral statistics in [22] and generalized in [28] to directed graphs. On each bond the waves travel in both directions. Therefore, at any given moment, the system is fully specified by a $2B$ -dimensional vector of wave amplitudes \mathbf{a} , indexed again by the directed bonds. Scattering at vertices is described by a unitary matrix T , having the property that

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

The free propagation results in the amplitude a_b (here b is a directed bond) being multiplied by the phase factor $e^{i\lambda L_b}$. Altogether we arrive to the *quantum evolution operator* $U(\lambda) = e^{i\lambda \mathbf{L}} T$.

Thus, in both constructions one ends up with a unitary matrix $S(\lambda) = e^{i\lambda \mathbf{L}} S_0$. This matrix specifies the eigenvalues $\{\lambda_n\}$ *via* the equation

$$\det[I - e^{i\lambda \mathbf{L}} S_0] = 0. \quad (6)$$

Actually, it was noted in [29] (see also [4, 27]) that the multiplicity of $\lambda = 0$ as a root of (6) can be different to its multiplicity as an eigenvalue of the Laplace operator, but that for all positive eigenvalues, the multiplicities coincide. To avoid this ambiguity we will omit the zero eigenvalues from the spectra that we consider. i.e. in our counting, λ_1 will be the first strictly positive eigenvalue. Since the multiplicity of the zero eigenvalue is necessarily finite (see corollary 4.2 below) this omission will not affect any spectral statistics.

2.3 Spectral quantities for quantum graphs

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

1. the eigenproblem (1) and thus solutions $\{\lambda_n\}$ of (6),
2. the eigenphases of the matrix $S(\lambda)$ for an arbitrary λ , i.e. to the set of $2B$ numbers $\{\theta_j\}$ such that $e^{i\theta_j}$ is the j -th eigenvalue of $S(\lambda)$.

To distinguish the two notions of the spectrum we will refer to the first definition above as the λ -spectrum, and to the second as the θ -spectrum.

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

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

There correspondence between first two types of eigenvectors is given by formula (3). A heuristic formula which connects properties of the second and the third types of eigenvectors was suggested in [10, Eq. (5)]. In this article we give a rigorous derivation of the formula.

3 Main results

Our results concern equivalences between statistical properties of two types of eigenvalues and eigenvectors of quantum graphs. These results are derived as an application of Proposition 4.4 introduced in Section 4.

3.1 Eigenvalue statistics

Starting with the seminal work of Kottos and Smilansky [21, 22], 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 certain type. On graphs, [21] showed some preliminary numerical evidence that eigenvalue spectrum of graphs follow the general prediction [30, 31] 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 [22, 32] and Tanner [7] 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 [8, 5, 9]. 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 θ -spectrum. There are heuristic reasons why the corresponding statistics should coincide, but the formal link between the two has hitherto not been explored.

In this article we prove that, in the correct limit, the two statistics 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 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 δ is the Dirac delta-function. Mathematically, the distributions are defined *via* a family of test functions.

Theorem 3.1. *Let \mathbf{L} be linearly independent over \mathbb{Q} and $\bar{L} = (L_1 + \dots + L_B)/B$ denote the mean bond length. If h be a continuous function, then the limits*

$$P_\lambda[h] := \lim_{N \rightarrow \infty} \frac{1}{N} \sum_{n=1}^N h(\bar{L}(\lambda_n - \lambda_{n-1})), \quad (7)$$

and

$$P_\theta[h] = \lim_{\Lambda \rightarrow \infty} \frac{1}{\Lambda} \int_0^\Lambda \frac{1}{2B} \sum_{j=1}^{2B} h(\theta_j(\lambda) - \theta_{j-1}(\lambda)) d\lambda \quad (8)$$

exist and define bounded linear functionals of h . If we take the limit $\mathbf{L} \rightarrow \ell_0(1, 1, \dots, 1)$ for some $\ell_0 > 0$, while keeping \mathbf{L} linearly independent over \mathbb{Q} , the two functionals coincide. Namely,

$$\lim_{\Delta L \rightarrow 0} P_\lambda[h] = \lim_{\Delta L \rightarrow 0} P_\theta[h], \quad (9)$$

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

Remark 3.2. If \mathbf{L} is *not* linearly independent over \mathbb{Q} , the limits (7) and (8) still exist but are highly sensitive to the changes in individual bond length. Thus the limits in equation (9) are, in general, singular. In particular when all bond lengths are equal ($\Delta L = 0$), the λ -spectrum is periodic and spacings in θ -spectrum are independent of λ . The nearest-neighbor distribution in this case is highly degenerate.

Remark 3.3. 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 neighbor spacing distributions coincide, so do other statistical functions such as the n -point correlation functions. (See, for example, equation (6.1.39) of [33].)

3.2 Eigenvector statistics

The equivalence between the statistics of the λ -spectrum and the θ -spectrum can be extended to eigenvector statistics.

To proceed, we need to introduce some notation in addition to that introduced previously in section 2.3. By $\psi_j(\lambda)$ we will denote the j -th eigenvector of $S(\lambda)$. As before, \mathbf{L} denotes the vector 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 ”. We define the bond-length observable by $L := \text{diag}(\mathbf{L}, \mathbf{L})$ and set $L(\lambda_n) = \langle \phi_n | L | \phi_n \rangle$.

Further, let D denote the $2B \times 2B$ random unitary matrix

$$D := e^{i\mathbf{X}},$$

where \mathbf{X} is a random vector distributed uniformly on $\mathbb{T}^B := [0, 2\pi)^B$, and $A_j(D) = \langle \psi_j(D) | A | \psi_j(D) \rangle$ be the expectation of A with respect to the j -th eigenvalue of the matrix DS_0 . By $\mathbb{E}^D(\cdot)$ we denote averages with respect to the distribution of D .

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 [34, 35, 36]. 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 [10]. Instead we prove that the variances (as indeed all other moments) of A_n and $A_j(\lambda)$ are equivalent.

Theorem 3.4. *Let \mathbf{L} be linearly independent over \mathbb{Q} . Then, for all $m \geq 0$,*

$$\lim_{N \rightarrow \infty} \frac{1}{N} \sum_{n=1}^N \frac{A_n^m}{L(\lambda_n)/\bar{L}} = \lim_{\Lambda \rightarrow \infty} \frac{1}{\Lambda} \int_0^\Lambda \frac{1}{2B} \sum_{k=1}^{2B} A_j(\lambda)^m d\lambda = \mathbb{E}^D \left(\frac{1}{2B} \sum_{k=1}^{2B} A_j(D)^m \right). \quad (10)$$

The weighting on the left-hand side of (10) shows that there is an exact equivalence of moments only in the (additional) limit $\Delta L \rightarrow 0$, as was taken in [32, 37]. However, provided ΔL is bounded away from zero and infinity, the centered moments would approach the zero limit either simultaneously or not at all. Another important feature of equation (10) is that its second part relates the moments of the eigenvectors of a fixed graph to the averaged properties of an *ensemble* of random matrices. While such averaging was not necessary in the proof of quantum ergodicity of models considered in [10], it is expected to be helpful in more general circumstances.

4 Main tools

4.1 Graph spectra and torus flow

Our methods are based on an idea going back to Barra and Gaspard [38], who suggested to view the eigenvalues λ_n as the Poincaré return times of a flow to a hypersurface defined by an extension of equation (6).

Let \mathbb{T}^B be the torus of side 2π in B dimensions. Define the surface $\Sigma \subseteq \mathbb{T}^B$ by

$$\Sigma := \{ \mathbf{x} : \det[e^{i\mathbf{x}} S_0 - I] = 0 \}, \quad (11)$$

where we use notation (5) for exponential of a vector.

Further, define a flow $\phi_t(\mathbf{x}_0)$ on \mathbb{T}^B by

$$\phi_t(\mathbf{x}_0) = \mathbf{x}_0 + t\mathbf{L} \pmod{2\pi}. \quad (12)$$

If the components of \mathbf{L} are linearly independent over \mathbb{Q} then the flow is equidistributing on the torus.

Since $\phi_\lambda(\mathbf{0}) = \lambda\mathbf{L} \pmod{2\pi}$, equation (6) can be rewritten as

$$\det[e^{i\phi_\lambda(\mathbf{0})} S_0 - I] = 0,$$

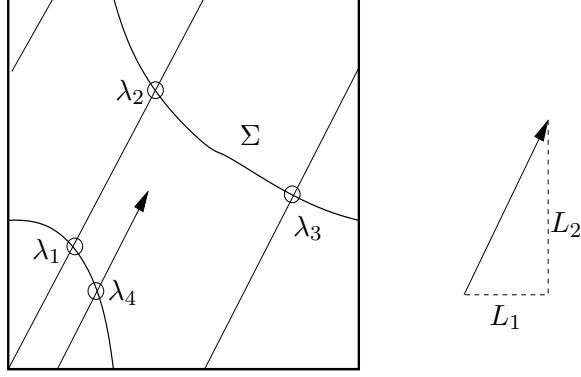


Figure 1: A cartoon of the flow piercing the surface Σ . The direction of increasing k is indicated by an arrow, and eigenvalues are indicated by little circles.

or simply as $\phi_\lambda(\mathbf{0}) \in \Sigma$. Thus the times $t = \lambda_n$, $n \in \mathbb{Z}$ of intersections of the flow $\phi_t(\mathbf{0})$ with the surface Σ give the set of points in the quantum spectrum of a graph (see figure 1).

The idea of Barra and Gaspard [38] was to use the ergodicity of the flow (12) to compute averages like (7) as an integral over the surface Σ . In this paper we put their idea on a mathematical footing (in particular, tackling the problem of using the ergodic theorem to integrate over Σ which is measure zero subset of \mathbb{T}^B) and extend it to apply to the problems described in Section 3.

4.2 More about intersections with Σ

The following result goes back to at least [22, Eq. (70)]. For completeness, we provide it with a proof.

Lemma 4.1. *Let U be a $2B \times 2B$ unitary matrix, and let $D(t) := e^{i\phi_t(\mathbf{x}_0)}$ for fixed \mathbf{x}_0 . Let $e^{i\theta(t)}$ be an eigenvalue of the unitary matrix $D(t)U$ and $\mathbf{u}(t)$ be the corresponding normalised eigenvector. Then,*

$$\frac{d\theta}{dt} = \langle \mathbf{u}(t) | L | \mathbf{u}(t) \rangle, \quad (13)$$

where $L = \text{diag}(\mathbf{L}, \mathbf{L})$. In particular,

$$L_{\min} \leq \frac{d\theta}{dt} \leq L_{\max}. \quad (14)$$

Proof. Since $D(t)U$ is unitary and analytic, the function $\theta(t)$ can be chosen real analytic, and so there are no problems differentiating the eigenvalue equation,

$$D(t)U\mathbf{u}(t) = e^{i\theta(t)}\mathbf{u}(t), \quad (15)$$

with respect to t to obtain

$$iLD(t)U\mathbf{u}(t) + D(t)U\mathbf{u}'(t) = i\theta'(t)e^{i\theta(t)}\mathbf{u}(t) + e^{i\theta(t)}\mathbf{u}'(t). \quad (16)$$

Multiplying by $\mathbf{u}(t)^\dagger$ (the conjugate transpose of $\mathbf{u}(t)$),

$$ie^{i\theta(t)}\mathbf{u}(t)^\dagger L\mathbf{u}(t) + \mathbf{u}(t)^\dagger D(t)U\mathbf{u}'(t) = i\theta'(t)e^{i\theta(t)}, \quad (17)$$

where we used that $\mathbf{u}(t)^\dagger\mathbf{u}(t) = 1$ and $\mathbf{u}(t)^\dagger\mathbf{u}'(t) = 0$. To handle the second term on the left-hand side we notice that

$$\mathbf{u}(t)^\dagger D(t)U = \left((D(t)U)^\dagger \mathbf{u}(t) \right)^\dagger = \left(e^{-i\theta(t)} \mathbf{u}(t) \right)^\dagger = e^{i\theta(t)} \mathbf{u}(t)^\dagger \quad (18)$$

and so

$$\mathbf{u}(t)^\dagger D(t)U\mathbf{u}'(t) = e^{i\theta(t)}\mathbf{u}(t)^\dagger\mathbf{u}'(t) = 0.$$

Thus,

$$\frac{d\theta}{dt} = \mathbf{u}(t)^\dagger L\mathbf{u}(t) = \sum_{j=1}^B L_j (|u(t)_j|^2 + |u(t)_{j+B}|^2), \quad (19)$$

leading to the desired bounds. \square

We can fix bounds on the rate of crossing of the flow with Σ based on the fact that

$$\det[e^{i\phi_t(\mathbf{x}_0)}S_0 - I] = 0$$

if and only if one of the eigenphases $\theta(t)$ is equal to a multiple of 2π . Since all $\theta(t)$ are increasing functions and Lemma 4.1 gives us an estimate of the increase, we get the following corollary.

Corollary 4.2. *If t varies in an interval of length $\frac{2\pi}{L_{\min}}$ then the flow $\phi_t(\mathbf{x}_0)$ intersects the surface Σ at least $2B$ times.*

If t varies in an interval of length $\frac{2\pi}{L_{\max}}$ then the flow $\phi_t(\mathbf{x}_0)$ intersects the surface Σ at most $2B$ times.

On average, the flow $\phi_t(\mathbf{x}_0)$ intersects the surface $2B$ times in an interval of length $\frac{2\pi}{\bar{L}}$, where \bar{L} is the *average* bond length. This is a consequence of the asymptotic density of the λ -spectrum, the Weyl's law for graphs. This classical result has been known on graphs for some time. A particularly elegant proof has appeared recently in [39, Theorem 1].

Proposition 4.3. *Let $N(\Lambda) := \#\{0 < \lambda_n \leq \Lambda\}$ where spectral points are counted with multiplicity. Then*

$$N(\Lambda) \sim \frac{\mathcal{L}}{\pi}\Lambda \quad \text{as } \Lambda \rightarrow \infty, \quad (20)$$

where $\mathcal{L} := L_1 + \dots + L_B$.

We remark that, in fact, the stronger asymptotic

$$N(\Lambda) = \frac{\mathcal{L}}{\pi}\Lambda + \mathcal{O}(1).$$

is proved in [39], however we shall only make use of (20).

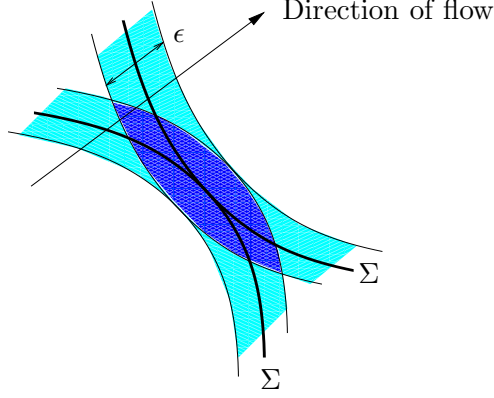


Figure 2: The region in which the “thickened” function Φ_ϵ is supported. If two branches of Σ come close together, the function takes the sums of the values on the different branches. In the figure this region is shaded in a darker tone.

4.3 The main proposition

Let Φ be a bounded function, defined on Σ . We extend it to the whole of \mathbb{T}^B , by the following “thickening”. Let $\epsilon > 0$ and define

$$\Phi_\epsilon(\mathbf{x}) := \sum_{\xi \in \Sigma} \Phi(\xi) \mathbb{I}_{\{\xi = \mathbf{x} + t\mathbf{L} : |t| \leq \epsilon/2\}}. \quad (21)$$

Thus Φ_ϵ takes the value $\Phi(\xi)$ at all points within a distance at most $\epsilon/2$ from $\xi \in \Sigma$ in the direction of the flow. Should two or more different branches of the surface Σ come close together, or intersect, the function Φ_ϵ takes the sum of the values of $\Phi(\xi)$ on the branches (see figure 2). The sum in (21) is finite as a consequence of corollary 4.2.

We permit the function Φ to be undefined on a set $\mathcal{U} \subseteq \Sigma$, provided that \mathcal{U} is small in the following sense. The projection of the set \mathcal{U} onto the $B - 1$ dimensional hyperplane $P := \{\mathbf{x} \in \mathbb{T}^B : x_1 = 0\}$ is required to have measure zero:

$$\text{meas}\{\mathbf{y} \in P : \exists t, 0 < t \leq 2\pi/L_1, \phi_t(\mathbf{y}) \in \mathcal{U}\} = 0. \quad (22)$$

This ensures that the discontinuities of Φ_ϵ have measure zero with respect to Σ .

Our main tool is the following proposition.

Proposition 4.4. *Let \mathbf{L} be linearly independent over \mathbb{Q} and let Φ be defined on all of Σ except possibly for a set \mathcal{U} satisfying (22), and be positive and bounded. Denote by $t_n = t_n(\mathbf{x}_0)$ the consecutive intersection times of the flow $\phi_t(\mathbf{x}_0)$ with the surface Σ . Then for any $\mathbf{x}_0 \in \mathbb{T}^B$ and $\epsilon > 0$*

$$\lim_{N \rightarrow \infty} \frac{1}{N} \sum_{n=1}^N \Phi(\phi_{t_n}(\mathbf{x}_0)) = \frac{1}{\bar{d}(2\pi)^B \epsilon} \int_{\mathbb{T}^B} \Phi_\epsilon(\mathbf{x}) \, d\mathbf{x}, \quad (23)$$

where $\bar{d} := \lim_{n \rightarrow \infty} n/t_n = \mathcal{L}/\pi$ is the mean density of the intersections t_n .

Remark 4.5. Since we want the result for *every* point $\mathbf{x}_0 \in \mathbb{T}^B$, simple ergodicity of the flow ϕ_t would not be enough. Instead we shall use the Weyl’s equidistribution which applies to intervals (and Riemann integrable functions) rather than Lebesgue measurable sets (and integrable function). Namely we use the following lemma, which follows directly from the results of Weyl [40].

Lemma 4.6. *Let $G: \mathbb{T}^B \rightarrow \mathbb{R}$ be a Riemann integrable function. Then, for every $\mathbf{x}_0 \in \mathbb{T}^B$,*

$$\lim_{T \rightarrow \infty} \frac{1}{T} \int_0^T G(\phi_t(\mathbf{x}_0)) dt = \frac{1}{|\mathbb{T}^B|} \int_{\mathbb{T}^B} G(\mathbf{x}) d\mathbf{x}. \quad (24)$$

If the integral on the left-hand side does not exist, equation (24) should be understood in terms of upper and lower Darboux integrals (limits of Darboux sums),

$$\lim_{T \rightarrow \infty} \frac{1}{T} \text{L.D.} \int_0^T G(\phi_t(\mathbf{x}_0)) dt = \lim_{T \rightarrow \infty} \frac{1}{T} \text{U.D.} \int_0^T G(\phi_t(\mathbf{x}_0)) dt = \frac{1}{|\mathbb{T}^B|} \int_{\mathbb{T}^B} G(\mathbf{x}) d\mathbf{x}. \quad (25)$$

Proof. The proof follows the standard procedure, see for example [41, Theorem 1.1]. Let

$$\mathbb{T}^B = \bigcup_j R_j \quad (26)$$

be a finite partition of \mathbb{T}^B into well-behaved sets, such as rectangles. Then

$$G(\mathbf{x}) \leq \hat{G}(\mathbf{x}) := \sum_j \mathbb{I}_{R_j}(\mathbf{x}) \sup_{\mathbf{y} \in R_j} G(\mathbf{y}),$$

where \mathbb{I}_A is the indicator function of set A . By [40, Satz 5],

$$\lim_{T \rightarrow \infty} \frac{1}{T} \int_0^T \mathbb{I}_{R_j}(\phi_t(\mathbf{x}_0)) dt = \frac{|R_j|}{|\mathbb{T}^B|},$$

the volume of the set R_j . Therefore,

$$\limsup_{T \rightarrow \infty} \frac{1}{T} \text{U.D.} \int_0^T G(\phi_t(\mathbf{x}_0)) dt \leq \lim_{T \rightarrow \infty} \frac{1}{T} \int_0^T \hat{G}(\phi_t(\mathbf{x}_0)) dt = \frac{1}{|\mathbb{T}^B|} \sum_j |R_j| \max_{\mathbf{y} \in R_j} G(\mathbf{y}),$$

which is the upper Darboux sum for the integral $|\mathbb{T}^B|^{-B} \int_{\mathbb{T}^B} G(\mathbf{x}) d\mathbf{x}$. Since G is Riemann integrable, the Darboux sums converge to the value of the integral in the limit as the partition (26) becomes finer. Analogous lower estimates lead to (25). \square

Proof of Proposition 4.4. Since the function Φ_ϵ is bounded and the discontinuity set has measure zero, Φ_ϵ is Riemann integrable and we can apply Lemma 4.6. According to the way that Φ_ϵ is a thickening of width ϵ of Φ on Σ , we have that

$$\frac{1}{N} \sum_{n=1}^N \Phi(\phi_{t_n}(\mathbf{x}_0)) = \frac{1}{N\epsilon} \int_0^{t_N + \epsilon/2} \Phi_\epsilon(\phi_t(\mathbf{x}_0)) dt + O\left(\frac{1}{N}\right), \quad (27)$$

as $N \rightarrow \infty$. The error term comes from a possible overlap of the integration range with crossings other than t_n , $1 \leq n \leq N$. Corollary 4.2 guarantees that the number of such crossings is uniformly bounded.

Now we let $N \rightarrow \infty$ which entails $T := t_N + \epsilon/2 \rightarrow \infty$ and apply Lemma 4.6,

$$\begin{aligned} \lim_{N \rightarrow \infty} \frac{1}{N} \sum_{n=1}^N \Phi(\phi_{\lambda_n}(\mathbf{x}_0)) &= \lim_{N \rightarrow \infty} \frac{t_N}{N\epsilon} \lim_{T \rightarrow \infty} \frac{1}{T} \int_0^T \Phi_\epsilon(\phi_t(\mathbf{x}_0)) dt \\ &= \frac{1}{d(2\pi)^B \epsilon} \int_{\mathbb{T}^B} \Phi_\epsilon(\mathbf{x}) d\mathbf{x}. \end{aligned} \quad (28)$$

Curiously, equation (28) provides a proof that the limit of n/t_n exists and is independent of \mathbf{x}_0 . Indeed, set $\Phi(\mathbf{x}) \equiv 1$ and observe that two other limits in equation (28) obviously exist. Thus, the limit of the sequence (n/t_n) is the same as for the case $\mathbf{x}_0 = 0$, which is covered by proposition 4.3 giving the limit \mathcal{L}/π . \square

5 Applications

With the tools developed in Section 4 we can prove Theorems 3.1 and 3.4. While the proofs follow the same set of basic ideas, the eigenvector statistics proof is slightly simpler and thus we present it first.

5.1 Eigenvector statistics

In this section we will prove Theorem 3.4. We will do it by introducing a family of spectra, $\{\lambda_{\alpha,n}\}$ indexed by $\alpha \in [0, 2\pi)$. We remind the reader that λ_n were defined as solutions of the equation $\det[e^{i\lambda\mathbf{L}}S_0 - I] = 0$. We extend this definition and denote by $\lambda_{\alpha,n}$ the solutions of the equation

$$\det[e^{-i\alpha}e^{i\lambda\mathbf{L}}S_0 - I] = 0. \quad (29)$$

Thus, $\lambda_{\alpha,n}\mathbf{L} - \boldsymbol{\alpha} \in \Sigma$, where $\boldsymbol{\alpha} = \alpha(1, \dots, 1)$ and Σ is the surface defined by (11). In other words, $\lambda_{\alpha,n}$ are the intersection times of the flow $\phi_t(-\boldsymbol{\alpha})$ with Σ .

Similarly to ϕ_n we can now define $\phi_{\alpha,n}$ to be the eigenvector of eigenvalue 1 of the matrix $e^{i\alpha}e^{i\lambda_{\alpha,n}\mathbf{L}}S_0$. Obviously, $\lambda_n = \lambda_{0,n}$ and $\phi_n = \phi_{0,n}$. We let $A_{\alpha,n} := \langle \phi_{\alpha,n} | A | \phi_{\alpha,n} \rangle$.

Lemma 5.1. *Let G be a bounded continuous and possibly nonlinear functional on \mathbb{C}^{2B} . For $\mathbf{x} \in \Sigma$ define $\Phi(\mathbf{x}) := G(\phi_{\mathbf{x}})$, where $\phi_{\mathbf{x}}$ satisfies*

$$e^{i\mathbf{x}}S_0\phi_{\mathbf{x}} = \phi_{\mathbf{x}}.$$

Then

$$\lim_{N \rightarrow \infty} \frac{1}{N} \sum_{n=1}^N G(\phi_{\alpha,n}) = \frac{1}{(2\pi)^B \epsilon} \int_{\mathbb{T}^B} \Phi_{\epsilon}(\mathbf{x}) d\mathbf{x}. \quad (30)$$

Proof. First we remark that $\Phi(\mathbf{x})$ is well-defined and continuous on Σ , except possibly at degenerate points of Σ .

By definition, $\phi_{\alpha,n} = \phi_{\mathbf{x}}$ with $\mathbf{x} = \lambda_{\alpha,n}\mathbf{L} - \boldsymbol{\alpha}$. Therefore,

$$G(\phi_{\alpha,n}) = \Phi(\lambda_{\alpha,n}\mathbf{L} - \boldsymbol{\alpha}) = \Phi(\phi_{\lambda_{\alpha,n}}(-\boldsymbol{\alpha})).$$

Now we can apply Proposition 4.4 to conclude the proof. \square

The important consequence of Lemma 5.1 is that the moments of $A_{\alpha,n}$ are independent of α .

Proof of Theorem 3.4. Let $\{e^{i\theta_j(\lambda)}\}_{j=1}^{2B}$ be the eigenvalues of the matrix $e^{i\lambda\mathbf{L}}S_0$, with $\theta_j(\lambda)$ chosen to be real analytic. As a consequence of lemma 4.1, θ_j has a smooth inverse.

Using a 2π -periodized Dirac delta function, $\delta_{2\pi}$ we can trivially write

$$A_j(\lambda)^m = \int_0^{2\pi} \delta_{2\pi}(\alpha - \theta_j(\lambda)) A_j(\lambda)^m d\alpha.$$

Then

$$\begin{aligned}
\int_0^\Lambda \sum_{j=1}^{2B} A_j(\lambda)^m d\lambda &= \int_0^{2\pi} \sum_{j=1}^{2B} \int_0^\Lambda \delta_{2\pi}(\alpha - \theta_j(\lambda)) A_j(\lambda)^m d\lambda d\alpha \\
&= \int_0^{2\pi} \sum_{j=1}^{2B} \int_{\theta_j(0)}^{\theta_j(\Lambda)} \delta_{2\pi}(\alpha - \xi) \frac{A_j(\theta_j^{-1}(\xi))^m}{\theta_j'(\theta_j^{-1}(\xi))} d\xi d\alpha. \\
&= \int_0^{2\pi} \sum_{0 < \lambda_{\alpha,n} \leq \Lambda} \frac{A_{j_{\alpha,n}}(\lambda_{\alpha,n})^m}{\theta_{j_{\alpha,n}}'(\lambda_{\alpha,n})} d\alpha, \tag{31}
\end{aligned}$$

We have chosen $j_{\alpha,n}$ so that $\theta_{j_{\alpha,n}}(\lambda_{\alpha,n}) = \alpha \pmod{2\pi}$. Therefore $\psi_{j_{\alpha,n}}(\lambda_{\alpha,n})$ is what we denoted by $\phi_{\alpha,n}$. Further, by Lemma 4.1, $\theta_j'(\lambda_{\alpha,n}) = \langle \phi_{\alpha,n} | L | \phi_{\alpha,n} \rangle$. We set

$$G(\phi) = \frac{\langle \phi | A | \phi \rangle^m}{\langle \phi | L | \phi \rangle}, \quad \text{so that} \quad \frac{A_{j_{\alpha,n}}(\lambda_{\alpha,n})^m}{\theta_{j_{\alpha,n}}'(\lambda_{\alpha,n})} = G(\phi_{\alpha,n}),$$

and obtain

$$\begin{aligned}
\int_0^\Lambda \sum_{j=1}^{2B} A_j(\lambda)^m d\lambda &= \int_0^{2\pi} \sum_{\lambda_{\alpha,n} \leq \Lambda} G(\phi_{\alpha,n}) d\alpha \\
&= N(\Lambda) \int_0^{2\pi} \frac{1}{N(\Lambda)} \sum_{\lambda_{\alpha,n} \leq \Lambda} G(\phi_{\alpha,n}) d\alpha. \tag{32}
\end{aligned}$$

Now we divide by $2B\Lambda$ and take the limit $\Lambda \rightarrow \infty$. By proposition 4.3, $N(\Lambda)/\Lambda \rightarrow \mathcal{L}/\pi$ in this limit. By the dominated convergence theorem we can take the limit inside the α -integral to get

$$\begin{aligned}
\lim_{\Lambda \rightarrow \infty} \frac{1}{\Lambda} \int_0^\Lambda \frac{1}{2B} \sum_{j=1}^{2B} A_j(\lambda)^m d\lambda &= \frac{\mathcal{L}}{2B\pi} \int_0^{2\pi} \lim_{\Lambda \rightarrow \infty} \frac{1}{N(\Lambda)} \sum_{\lambda_{\alpha,n} \leq \Lambda} G(\phi_{\alpha,n}) d\alpha \\
&= \frac{\mathcal{L}}{B} \lim_{\Lambda \rightarrow \infty} \frac{1}{N(\Lambda)} \sum_{n=1}^{N(\Lambda)} G(\phi_{0,n}) \\
&= \lim_{N \rightarrow \infty} \frac{1}{N} \sum_{n=1}^N \frac{A_n^m}{L(\lambda_n)/\bar{L}}, \tag{33}
\end{aligned}$$

where we used the fact that, by Lemma 5.1, the limit inside the integral is independent of α .

To prove the second equality in (10) we apply Weyl's equidistribution theorem to the limit on the left in (33). This is justified since eigenvector components of $e^{i\mathbf{x}}S_0$ vary continuously in \mathbf{x} except possibly at the points where the eigenvalues of $e^{i\mathbf{x}}S_0$ are non-simple. The set of such points is a C -analytic set and will have either measure 0 or full measure (see the discussion in Section 5.3). The latter situation is incompatible with condition (22). \square

5.2 Spectral statistics

We will use the previous results to prove that the spectral statistics of the matrix $e^{i\mathbf{x}}S_0$ averaged over \mathbb{T}^B converge to the empirical spectral statistics as the interval from which bond lengths are drawn shrinks in size.

5.2.1 A few more definitions

Let $d : \mathbb{T}^B \rightarrow \mathbb{R}_+$ be the “time” of the next crossing of the surface Σ ,

$$d(\mathbf{x}) := \inf\{t > 0 : \phi_t(\mathbf{x}) \in \Sigma\}. \quad (34)$$

For $\mathbf{x} \in \mathbb{T}^B$ let the eigenvalues of $e^{i\mathbf{x}}S_0$ be $e^{i\hat{\theta}_1(\mathbf{x})}, \dots, e^{i\hat{\theta}_{2B}(\mathbf{x})}$, ordered so that

$$0 < \hat{\theta}_{2B}(\mathbf{x}) \leq \hat{\theta}_{2B-1}(\mathbf{x}) \leq \dots \leq \hat{\theta}_2(\mathbf{x}) \leq \hat{\theta}_1(\mathbf{x}) \leq 2\pi. \quad (35)$$

This ordering ensures that if $\mathbf{x} \in \Sigma$ then $\hat{\theta}_1(\mathbf{x}) = 2\pi$. We use the hat in notation $\hat{\theta}_j$ to distinguish it from the eigenphases $\theta_j(\lambda)$ of the matrix $e^{i\lambda\mathbf{L}}S_0$ which can be chosen real analytic with respect to λ . Of course, the sets $\{\theta_j(\lambda)\}$ and $\{\hat{\theta}_j(\phi_\lambda(\mathbf{0}))\}$ coincide modulo 2π .

Define the eigenphase spacing functions by

$$\begin{aligned} \sigma_1(\mathbf{x}) &:= \hat{\theta}_1(\mathbf{x}) - \hat{\theta}_2(\mathbf{x}) \\ &\vdots \\ \sigma_{2B-1}(\mathbf{x}) &:= \hat{\theta}_{2B-1}(\mathbf{x}) - \hat{\theta}_{2B}(\mathbf{x}) \\ \sigma_{2B}(\mathbf{x}) &:= \hat{\theta}_{2B}(\mathbf{x}) + 2\pi - \hat{\theta}_1(\mathbf{x}). \end{aligned}$$

These definitions are illustrated in figure 3.

We will use shorthand $\sigma_j(\lambda)$ for $\sigma_j(\phi_\lambda(\mathbf{0}))$ and $d(\lambda)$ for $d(\phi_\lambda(\mathbf{0}))$.

5.2.2 Equivalence of spacing distributions

Proof of Theorem 3.1. Let h be a continuous test function. We want to compare

$$\lim_{\Lambda \rightarrow \infty} \frac{1}{\Lambda} \int_0^\Lambda \frac{1}{2B} \sum_{j=1}^{2B} h(\sigma_j(\lambda)) \, d\lambda \quad \text{and} \quad \lim_{N \rightarrow \infty} \frac{1}{N} \sum_{n=1}^N h(\bar{L}d(\lambda_n)).$$

Repeating the arguments of equations (31) and (32) we obtain

$$\begin{aligned} \int_0^\Lambda \sum_{j=1}^{2B} h(\sigma_j(\lambda)) \, d\lambda &= \int_0^\Lambda \int_0^{2\pi} \sum_{r=1}^{2B} \delta_{2\pi}(\alpha - \theta_r(\lambda)) h(\sigma_{j_r}(\lambda)) \, d\alpha d\lambda \\ &= \int_0^{2\pi} \int_0^\Lambda \delta(\lambda - \lambda_{\alpha,n}) \frac{h(\sigma_{j_{\alpha,n}}(\lambda))}{\theta'_{j_{\alpha,n}}(\lambda)} \, d\lambda d\alpha, \\ &= \int_0^{2\pi} \sum_{\lambda_{\alpha,n} \leq \Lambda} \Phi^\sigma(\phi_{\lambda_{\alpha,n}}(-\alpha)) \, d\alpha, \end{aligned}$$

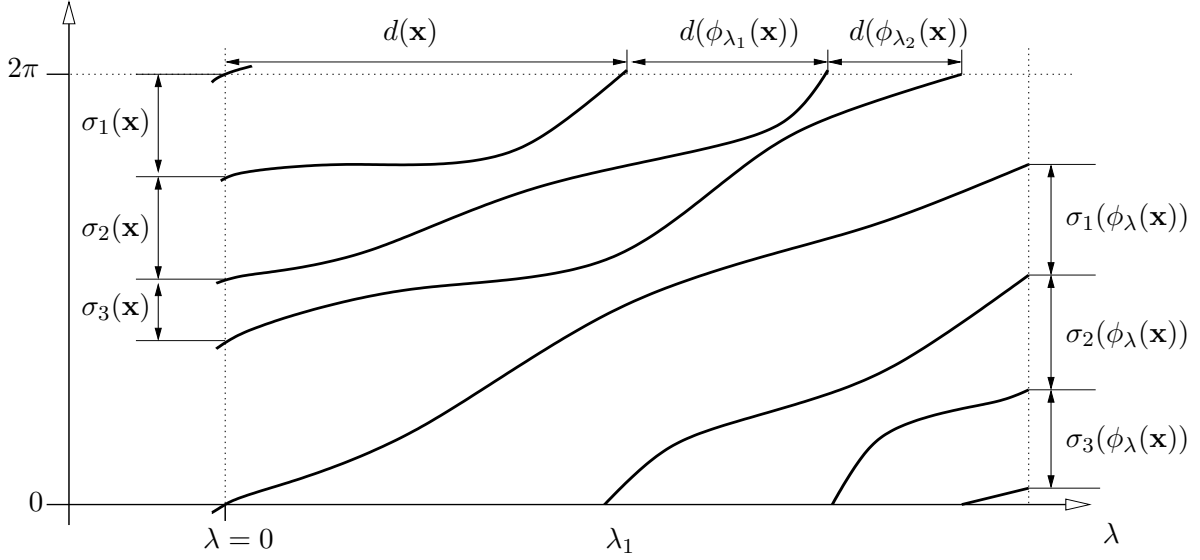


Figure 3: The eigenangles of $e^{i\phi_\lambda(\mathbf{x})} S_0$ and notation of Section 5.2.1

where, for $\mathbf{x} \in \Sigma$, we have defined

$$\Phi^\sigma(\mathbf{x}) = \frac{h(\sigma_1(\mathbf{x}))}{\left. \frac{d}{dt} \hat{\theta}_1(\phi_t(\mathbf{x})) \right|_{t=0}}, \quad (36)$$

where the derivative is taken from the left, since $\hat{\theta}_1$ is discontinuous on Σ . The function $\Phi^\sigma(\mathbf{x})$ is well defined if at \mathbf{x} we have $\hat{\theta}_2 < \hat{\theta}_1 = 2\pi$, i.e. the eigenvalue 1 of $e^{i\mathbf{x}} S_0$ is simple. Now we divide by $2B\Lambda$, take the limit $\Lambda \rightarrow \infty$ and use Proposition 4.4 to get, analogously to (33),

$$\begin{aligned} \lim_{\Lambda \rightarrow \infty} \frac{1}{\Lambda} \int_0^\Lambda \frac{1}{2B} \sum_{j=1}^{2B} h(\sigma_j(\lambda)) \, d\lambda &= \frac{\mathcal{L}}{2B\pi} \int_0^{2\pi} \lim_{\Lambda \rightarrow \infty} \frac{1}{N(\Lambda)} \sum_{\lambda_{\alpha,n} \leq \Lambda} \Phi^\sigma(\phi_{\lambda_{\alpha,n}}(\boldsymbol{\alpha})) \, d\boldsymbol{\alpha} \\ &= \frac{\bar{L}}{(2\pi)^B \epsilon} \int_{\mathbb{T}^B} \Phi_\epsilon^\sigma(\mathbf{x}) \, d\mathbf{x}. \end{aligned}$$

On the other hand, again by Proposition 4.4, we have

$$\lim_{N \rightarrow \infty} \frac{1}{N} \sum_{n=1}^N h(\bar{L}d(\lambda_n)) = \frac{1}{(2\pi)^B \epsilon} \int_{\mathbb{T}^B} \Phi_\epsilon^d(\mathbf{x}) \, d\mathbf{x},$$

where

$$\Phi^d(\mathbf{x}) = h(\bar{L}d(\mathbf{x})). \quad (37)$$

Now we use that $\bar{L}\Phi^\sigma(\mathbf{x}) - \Phi^d(\mathbf{x}) \rightarrow 0$ as $\Delta L \rightarrow 0$. This is proved in lemma 5.2 below, implying

$$\frac{\bar{L}}{(2\pi)^B \epsilon} \int_{\mathbb{T}^B} \Phi_\epsilon^\sigma(\mathbf{x}) \, d\mathbf{x} - \frac{1}{(2\pi)^B \epsilon} \int_{\mathbb{T}^B} \Phi_\epsilon^d(\mathbf{x}) \, d\mathbf{x} \rightarrow 0. \quad (38)$$

Since $\Phi^d(\mathbf{x})$ is clearly continuous in \mathbf{L} , the individual limits exist too, concluding the proof. \square

Lemma 5.2. *Let h be continuous. Then, for $\mathbf{x} \in \Sigma$ we have*

$$\frac{\sigma_1(\mathbf{x})}{L_{\max}} \leq d(\mathbf{x}) \leq \frac{\sigma_1(\mathbf{x})}{L_{\min}}, \quad (39)$$

and, therefore,

$$\bar{L}\Phi^\sigma(\mathbf{x}) - \Phi^d(\mathbf{x}) \rightarrow 0 \quad (40)$$

uniformly on Σ as $\Delta L = L_{\max} - L_{\min} \rightarrow 0$.

Proof. Estimate (39) follows from lemma 4.1. Indeed, $d(\mathbf{x})$ is the time required by $\hat{\theta}_1(\phi_t(\mathbf{x}))$ to reach 2π from its initial value of $2\pi - \sigma_1 + 0$ at the time $t = +0$, see Figure 3, and lemma 4.1 provides an estimate on the derivative of $\hat{\theta}_1$.

We can now write (39) as

$$\sigma_1(\mathbf{x}) \left(\frac{\bar{L}}{L_{\max}} - 1 \right) \leq \bar{L}d(\mathbf{x}) - \sigma_1(\mathbf{x}) \leq \sigma_1(\mathbf{x}) \left(\frac{\bar{L}}{L_{\min}} - 1 \right).$$

Since both d and σ_1 are bounded, we have $\bar{L}d(\mathbf{x}) - \sigma_1(\mathbf{x}) \rightarrow 0$ uniformly in \mathbf{x} as the spread of the lengths decreases. The function h is continuous on a compact set, therefore it is uniformly continuous and $h(\sigma_1(\mathbf{x})) - h(\bar{L}d(\mathbf{x})) \rightarrow 0$ uniformly in \mathbf{x} . Finally, the denominator in the definition of Φ^σ , see equation (36), is bounded by L_{\min} and L_{\max} by lemma 4.1 and thus converges to \bar{L} . All of the above put together imply (40). \square

5.3 Discontinuities of Φ^σ and Φ^d

When defining the function Φ in Section 5.1 and the functions Φ^σ and Φ^d in Section 5.2 we implicitly assumed that they satisfy condition (22) on the set of their discontinuities. In this section we explain why can we expect it in general and how to rectify the situation when the definitions of function Φ produce too many discontinuities.

The surface Σ is a C -analytic set, see [42, Definition 6, Chapter V]. Thus we can apply [42, Proposition 18, Chapter V], to it, which splits Σ into an analytic manifold of dimension $B - 1$ and the remainder \mathcal{U} . The remainder has a smaller dimension and obviously satisfies condition (22).

Consider a connected piece of the $(B - 1)$ -dimensional manifold. If on this piece the zero of the defining equation

$$\det[e^{i\phi_t(\mathbf{x}_0)}S_0 - I] = 0$$

is simple, there is a unique eigenvector $\phi_{\mathbf{x}}$ (see Section 5.1), continuous with respect to \mathbf{x} on the manifold. The function Φ is well defined.

The situation when on all $(B - 1)$ -dimensional manifolds the eigenvalues are simple is expected to be generic. However, a proof exists only for a special case of graphs with Kirchhoff matching conditions [43]. Proving the simplicity (in a generic sense) of the solutions to

$$\det[e^{i\mathbf{x}}S_0 - I] = 0$$

for general S_0 thus remains an important open question. To complicate the picture, there are counter-examples with persistent eigenvalues of multiplicity two: these are provided by graphs with a looping bond separated from the rest of the graph. Moreover, there are

indications that the first-order perturbation used in [43] will not produce the result for general S_0 .

Fortunately, when the multiplicity is greater than one on a $(B - 1)$ -dimensional sub-manifold of Σ , we can still make the functions Φ continuous. First we note that the multiplicity must be constant on the whole manifold. For simplicity we assume the multiplicity is two. The eigenspace of the eigenvalue 1 of the matrix $e^{i\phi_t(\mathbf{x}_0)}S_0$ is continuous and we can choose a continuous basis $\phi_{\mathbf{x},1}$ and $\phi_{\mathbf{x},2}$. The function Φ of Section 5.1 can be then defined as

$$\Phi(\mathbf{x}) = G(\phi_{\mathbf{x},1}) + G(\phi_{\mathbf{x},2})$$

on the problematic manifold.

The function Φ^d of Section 5.2 can be simply defined as $h(\bar{L}d(\mathbf{x})) + h(0)$. To define function Φ^σ in a continuous and meaningful manner we note that if $\hat{\theta}_1(\mathbf{x}) = \hat{\theta}_2(\mathbf{x}) = 2\pi$, then the phases also coincided before the flow hit Σ , i.e. for small negative t , $\hat{\theta}_1(\phi_t(\mathbf{x})) = \hat{\theta}_2(\phi_t(\mathbf{x}))$. Thus the derivative in the denominator of equation (36) does not depend on which $\hat{\theta}$ we take and one can set

$$\Phi^\sigma(\mathbf{x}) = \frac{h(\sigma_1(\mathbf{x})) + h(0)}{\left. \frac{d}{dt}\hat{\theta}_1(\phi_t(\mathbf{x})) \right|_{t=0}},$$

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