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Isospectral discrete and quantum graphs with the same flip counts and nodal counts

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Abstract

The existence of non-isomorphic graphs which share the same Laplace spectrum (to be referred to as isospectral graphs) leads naturally to the following question: what additional information is required in order to resolve isospectral graphs? It was suggested by Band, Shapira and Smilansky that this might be achieved by either counting the number of nodal domains or the number of times the eigenfunctions change sign (the so-called flip count) (Band et al 2006 J. Phys. A: Math. Gen. 39 13999–4014; Band and Smilansky 2007 Eur. Phys. J. Spec. Top. 145 171–9). Recent examples of (discrete) isospectral graphs with the same flip count and nodal count have been constructed by Ammann by utilising Godsil–McKay switching (Ammann private communication). Here, we provide a simple alternative mechanism that produces systematic examples of both discrete and quantum isospectral graphs with the same flip and nodal counts.

Keywords: spectral theory, nodal domains, graph theory

(Some figures may appear in colour only in the online journal)

1. Introduction

One of the traditional means for studying the structure of eigenfunctions of the Laplacian on a large variety of domains is the counting of their nodal domains—the connected subsets where the eigenfunction has a constant sign. The systematic study begins by ordering the spectrum in a monotonically non-decreasing sequence, and associating with the nth eigenfunction the corresponding nodal domain number ν_n . For domains in one dimension, Sturm's oscillation theorem states that $\nu_n = n$. For higher dimensions Courant's theorem provides the upper bound $\nu_n \leq n$ [4]. Studies of nodal domains have yielded many new and surprising insights into

various branches of physics and mathematics (see e.g. [5] for a collection of relevant papers). In particular, it became apparent that the nodal sequence $\{\nu_n\}_{n=1}^{\infty}$ stores information about the domain on which the Laplacian is defined, such as its boundaries or metric, which does not overlap with the information stored in the spectrum [6]. Therefore, since the answer to Kac's famous question [7] 'can one hear the shape of a drum?' was shown to be 'no' (examples of pairs of isospectral³ planar domains were first obtained by Gordon, Webb and Wolpert [8]), this led Gnutzmann, Smilansky and others [9, 10] to ask 'can one *count* the shape of a drum?' More specifically, given two isospectral domains or manifolds, is the knowledge of the nodal count enough to distinguish the two? Brüning and Fajman [11] showed this is not the case for certain flat tori, however it seems to be positive in some particular classes of domains [12].

In the present article we address this question in the context of both discrete and quantum graphs. Studying the Laplacian in these simple, yet non-trivial, systems has proven to be remarkably insightful because many properties are shared with their higher-dimensional counterparts. For instance, it is known that for tree-graphs the Sturm result holds [13], and more generally Courant's theorem also applies in this context [14]. In addition, recent results connecting the stability of eigenvalues under small perturbations to nodal quantities were first born out of discoveries in graphs [15–18], before their application to planar domains [19]. Counting nodal domains in chaotic billiards [6, 20] is also highly related to analogous studies in *d*-regular graphs, which were carried out numerically [21] and analyzed theoretically [22] within a random wave model. We also point the reader to the review article [23] which provides further motivation and developments in the subject.

In [1, 2] a number of examples of pairs of isospectral quantum graphs were constructed, which were analogous of previous isospectral domains in \mathbb{R}^2 [8, 24–27] obtained using Sunada's method [28]. In all of the examples the nodal count was able to distinguish these pairs, leading the authors to conjecture that this could resolve isospectrality. Note that in the case of quantum graphs it was shown that knowing the spectrum is enough to distinguish between quantum graphs, provided the lengths of the edges are all incommensurate [29]. In the context of discrete graphs it was shown that if the so-called *weighted Laplacian* was used then one can find an example of isospectral graphs that are *not* distinguished by the nodal count [30], but the same could not be said of the standard Laplacian. Recently, Ammann has used the method of Godsil–McKay switching [31] to provide examples of discrete graphs in which both the flip count and nodal count of the Laplacian is the same [3]. Inspired by her results we show here that one can use an alternative simple mechanism for constructing pairs of both discrete and quantum graphs that are isospectral that have the same flip and nodal counts.

The article is presented as follows: in the remainder of the introduction we recount the necessary properties of both discrete graphs, quantum graphs and their respective nodal and flip counts. In section 2 we explain a simple mechanism for obtaining isospectral graphs and then go on to show that from this the flip counts and nodal counts will be the same. We also show in section 2.1 that one can find non-isospectral examples of discrete graphs for which the flip and nodal counts coincide. In section 3 we adapt the mechanism to the quantum graph setting and give analogous examples. Finally, in section 4 we offer some concluding remarks and possible further directions.

1.1. Discrete graphs

A discrete graph $G = (\mathcal{V}, \mathcal{E})$ is given by a set of vertices \mathcal{V} and (undirected) edges \mathcal{E} , meaning $(i,j) = (j,i) \in \mathcal{E}$ if the vertices i and j are connected (we also use the notation $i \sim j$ to denote

³ The term 'cospectral' is used in place of 'isospectral' by some other authors.

that i is connected to j). The number of vertices and edges are denoted $V = |\mathcal{V}|$ and $E = |\mathcal{E}|$, respectively. In the present context (unless otherwise stated) we assume G to be connected and simple, meaning there are no parallel edges or self loops (i.e. edges of the form e = (i, i)). The connectivity of G is encoded in the $V \times V$ adjacency matrix A(G) whose (i, j) and (j, i) entries are 1 if $(i, j) \in \mathcal{E}$ and 0, otherwise. The degree d_i of a vertex i is the number of vertices that are connected to it. We can extract this quantity from A using $d_i = \sum_j A_{ij}$ and in turn use this to construct the diagonal degree matrix $D(G) = \operatorname{diag}(d_1, \ldots, d_V)$. Combining these two matrices forms the discrete Laplacian $L(G) : \mathbb{R}^V \to \mathbb{R}^V$ given by

$$L(G) = D(G) - A(G). \tag{1}$$

The Laplacian is real, symmetric and positive-definite. It therefore has V non-negative eigenvalues $\lambda_1 \leq \lambda_2 \leq \ldots \leq \lambda_V$ and associated real eigenvectors $\boldsymbol{f}_n = (f_n(i), \cdots, f_n(V))^T$. We will also use the notation $\sigma(G) = \{\lambda_1, \ldots, \lambda_n\}$ to denote the spectrum of the Laplacian of G.

In the following we shall investigate the nodal properties. However eigenvectors that possess zeros present difficulties that must be avoided. It is therefore important to restrict the investigation to eigenvectors of the following type.

Definition 1.1 (Genericity in discrete graphs). Let f be an eigenvector of L with eigenvalue λ . Then f is called generic if the eigenvalue λ is non-degenerate and $f(i) \neq 0$ for all $i \in \mathcal{V}$.

1.2. Quantum graphs

Here we give a brief overview of the construction of quantum graphs. One should consult [32, 33] for a more detailed exposition.

A metric graph is obtained from a discrete graph $G = (\mathcal{V}, \mathcal{E})$ by endowing each edge $e = (i,j) \in \mathcal{E}$ with a finite length l_e , which in turn facilitates a position. Specifically, if we choose $o(e) = o((i,j)) = \min(i,j)$ to be the origin and $t(e) = \max(i,j)$ to be the terminus of the edge then we specify $x_e \in [0,l_e]$ to be the distance from the origin o(e). We will denote by $\Gamma = (G,l_1,\ldots,l_E)$ the corresponding metric graph. The establishment of a metric means we may construct functions $\psi(x)$ that are supported on the graph. We do this by restricting the function to each edge and we denote this by $\psi^e(x_e)$, where $x_e \in [0,l_e]$. To align with the notation in the discrete setting we will write $\psi^e(i)$ to denote $\psi^e(0)$ if i = o(e) and $\psi^e(l_e)$ if i = t(e).

Given this metric graph we may then consider operators acting on appropriate spaces of functions that are supported on the graph. In our present context we shall choose the free one-dimensional Schrödinger operator (the negative Laplacian) acting on each edge

$$L: \psi^e(x_e) \mapsto -\frac{\mathrm{d}^2 \psi^e}{\mathrm{d} x_e^2}(x_e)$$

and the correct function space (see e.g. [32] for details) is given by

$$H^2(\Gamma):=\bigoplus_{e\in\mathcal{E}}H^2([0,l_e]),$$

where $H^2([0, l_e])$ denotes the Sobolev space on the edge e of real one-dimensional functions $\psi \in L^2([0, l_e])$ whose weak-derivatives up to order two are square integrable.

The final step is to make the operator self-adjoint with respect to the following inner product

$$\langle \psi, \phi \rangle := \sum_{e \in \mathcal{E}} \int_0^{l_e} \psi(x)\phi(x) dx.$$
 (2)

This requires introducing vertex conditions that match the function and its derivative on each edge emanating from a vertex. A complete classification of conditions has been obtained [34], however here we will restrict ourselves to so-called Neumann (also referred to as Kirchoff) vertex conditions. If we let $\mathcal{E}_u = \{e \in \mathcal{E} : o(e) = u \text{ or } t(e) = u\}$ denote the set of edges incident to the vertex u then these conditions are specified by endowing the functions ψ at every vertex $u \in \mathcal{V}$ with the following two properties:

(i) the function ψ is continuous:

$$\psi^{e}(u) = \psi^{e'}(u) \qquad \forall \, e, e' \in \mathcal{E}_u \tag{3}$$

(ii) the sum of outgoing derivatives is zero:

$$\sum_{e \in \mathcal{E}_u} \frac{\mathrm{d}\psi^e}{\mathrm{d}x_e}(u) = 0,\tag{4}$$

where the derivatives are taken in the directions outgoing from the vertex u.

The function $\psi(x)$ is an eigenfunction of Γ (with eigenvalue λ) if $L\psi=\lambda\psi$ and the conditions (3) and (4) are satisfied. Moreover, since we shall only consider compact graphs, the spectrum of the operator L is a countable sequence of non-negative real numbers with no accumulation points. Thus we can number the eigenvalues $\lambda_1 \leq \lambda_2 \leq \ldots$ with corresponding eigenfunctions $\psi_n(x)$, which form a basis for $L^2(\Gamma)$ —the space of square integrable functions with respect to the inner product (2) and satisfying the boundary conditions (3) and (4). Again, we say the eigenvalue λ is simple if it is non-degenerate and use the notation $\sigma(\Gamma) = \{\lambda_1, \lambda_2 \ldots\}$ for the spectrum of our quantum graph.

In the quantum graphs setting there is an analogous version on definition 1.1 for generic eigenfunctions, which will be needed in order to avoid ambiguity over nodal properties.

Definition 1.2 (Genericity in quantum graphs). An eigenfunction ψ of L_{Γ} is called *generic* if it is non-zero on all vertices and the corresponding eigenvalue λ_n is simple.

1.3. The flip count and nodal count

The definition of generic eigenvectors (in the discrete case) and generic eigenfunctions (in the quantum case) allows us to proceed, without ambiguity, to defining the flip count and nodal (domain) count in each scenario⁴.

Definition 1.3 (Discrete graph flip count). Let f be a generic eigenvector of G. Then

$$\mathcal{F}_G(\mathbf{f}) := \{ (i, j) \in \mathcal{E}(G) : f_n(i) f_n(j) < 0 \}$$

denotes the set of (undirected) edges on the discrete graph G for which f changes sign (i.e. flips). $\mu_G(f) := |\mathcal{F}_G(f)|$ is then the number of flips of f.

⁴ Note that a number of other authors refer to our definition of the 'flip count' as the 'nodal (point) count', e.g. [17, 35]. We prefer this terminology in this context to emphasise the distinction between flips and nodal domains.

Definition 1.4 (Discrete graph nodal count). Let $\tilde{G} = (\mathcal{V}(G), \mathcal{E}(G) \setminus \mathcal{F}(f))$ be the graph formed by removing all edges on which a generic eigenvector f changes sign. The number of nodal domains of f on G is denoted $\nu_G(f)$ and is defined to be the number of connected components of \tilde{G} .

In the case of quantum graphs we have a completely analogous formalism. Note that due to the vertex conditions (3) and (4) we are guaranteed that the zeros of generic eigenfunctions ψ_n are points on the interior of the edges of the graphs.

Definition 1.5 (Quantum graph flip count). Let ψ be a generic eigenfunction of L_{Γ} and $\mathcal{Z}_{\Gamma}(\psi) := \{x \in \Gamma : \psi(x) = 0\}$ the associated zero set. Then the flip count is the number of times the eigenfunction changes sign on the edges, or

$$\mu_{\Gamma}(\psi) = \sum_{e \in \mathcal{E}} \int_{0}^{l_e} \delta_{\mathcal{Z}_{\Gamma}(\psi)}(x_e) \mathrm{d}x_e. \tag{5}$$

Definition 1.6 (Quantum graph nodal count). Let $\Gamma \setminus \mathcal{Z}_{\Gamma}(\psi)$ be the graph obtained by removing the zero set of ψ . Then the number of nodal domains $\nu_{\Gamma}(\psi)$ is the number of connected components of $\Gamma \setminus \mathcal{Z}_{\Gamma}(\psi)$.

In both discrete and quantum graphs the number of nodal domains $\nu_n = \nu_G(f_n)$ (resp. $\nu_n = \nu_\Gamma(\psi_n)$) of the *n*th eigenvector (resp. eigenfunction) are known to obey certain general bounds. An upper bound is given by Courant's theorem $\nu_n \leqslant n$, which was translated from the setting of domains to discrete graphs in [14] and to quantum graphs in [36]. A lower bound was established for both discrete and quantum graphs by Berkolaiko [13], so that for generic eigenvectors we have

$$n - \beta \leqslant \nu_n \leqslant n . \tag{6}$$

Here $\beta = E - V + 1$ is the first Betti number, which counts the number of fundamental cycles, or the minimum number of edges one must remove in order for the graph to become a tree. For the flip count we have

$$n-1 \leqslant \mu_n \leqslant n-1+\beta \ . \tag{7}$$

The lower bound was also proved in [13], the upper bound follows from the fact that $\mu_n \leq \nu_n - 1 + \beta$. The two bounds imply immediately that trees (6) and (7) reduce to the Sturm oscillation relation $\nu_n = \mu_n + 1 = n$, which means tree graphs cannot be distinguished via their flip or nodal counts. It has also been proved, conversely, that all graphs with flip counts that follow the integer sequence from 1 to V must be trees [35]. However, interestingly, the analogous statement about the nodal count remains illusive.

We would also like to highlight that, although the flip count and nodal count are obviously related (see [23] for further discussion on this relation), the two contain different types of information. The flip count is *local*, as the sign changes of eigenvectors or eigenfunctions occur across small distances, however the nodal count is truly a *global* quantity, as nodal domains can stretch across significant proportions of the graph. For this reason the flip count is often a much easier quantity to obtain, both numerically and analytically [23], than the nodal count.

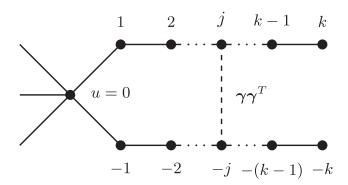


Figure 1. A graph G containing a k-leaf-pair connected to some root vertex u=0, the graph \bar{G} is formed by inserting the edge (j,-j) which can be achieved via the rank one matrix $[\gamma \gamma^T]_{ik} = (\delta_{i,j} - \delta_{i,-j})(\delta_{k,j} - \delta_{k,-j})$.

2. Discrete graphs

In this section we present a mechanism for constructing both isospectral and non-isospectral pairs of graphs with the same flip count and nodal count. It is based upon the idea of inserting edges between dangling bonds, or leaves, of a graph. To begin we introduce the following definition.

Definition 2.1. A leaf is a vertex i such that $d_i = 1$. A k-leaf is a set of k connected vertices such that k-1 have degree 2 and one has degree 1. A k-leaf-pair consists of two k-leaves joined together at a root vertex (see e.g. figure 1).

In other words, a k-leaf is a line graph of length k in which one end is connected to some base graph.

The basic premise of this mechanism will be that if we have a *k*-leaf-pair connected to the rest of the graph at some root vertex, *u* say, then there exists eigenvectors which are only non-zero on these leaves. If an edge is inserted appropriately, only these eigenvectors will change, whereas the rest will be left unaltered with the same eigenvalues.

Lemma 2.1. Let G_1 and G_2 be two graphs, which each contain a k-leaf-pair. Let \bar{G}_1 and \bar{G}_2 be the respective graphs obtained by inserting an edge connecting the jth vertex from the root in each k-leaf. Then $\sigma(G_1) = \sigma(G_2) \Leftrightarrow \sigma(\bar{G}_1) = \sigma(\bar{G}_2)$.

Proof. For convenience, let us number the vertices in G_1 and \bar{G}_1 in the following manner $\mathcal{V} := \{-k, -(k-1), \ldots, -1, 0, 1, \ldots, V-k-1\}$ and denote the subset $\mathcal{V}_{\text{leaves}} := \{-k, \ldots, k\}$ such that the two k-leaf ends are k and -k and are joined to the rest of the graph at a root vertex u = 0, as illustrated in figure 1. Suppose we insert the edge at the point (j, -j) for some $j \in \mathcal{V}_{\text{leaves}}$ then we can introduce the vector γ which takes the values $\gamma(i) = \delta_{i,j} - \delta_{i,-j}$,

$$L(\bar{G}_1) = L(G_1) + \gamma \gamma^T$$
.

Now, let $\pi : \mathbb{R}^V \to \mathbb{R}^V$ be the operator that exchanges the two leaves, whilst the rest of the graph remains invariant, i.e.

$$[\pi \mathbf{f}](\mathbf{i}) = \begin{cases} f(-\mathbf{i}) & \mathbf{i} \in \mathcal{V}_{\text{leaves}} \\ f(\mathbf{i}) & \mathbf{i} \in \mathcal{V} \setminus \mathcal{V}_{\text{leaves}}. \end{cases}$$
(8)

Since $\pi^2 = I_V$ we can decompose our space into those vectors which are even (+) and odd (-) under this transformation,

$$S_{\pm} := \{ f : \pi f = \pm f \} \tag{9}$$

and $\mathbb{R}^V \cong \mathcal{S}_+ \oplus \mathcal{S}_-$. Furthermore, if $f \in \mathcal{S}_+$ then $\langle \gamma, f \rangle := \gamma^T f = 0$ and thus, if it is an eigenvector of $L(G_1)$, we have

$$L(\bar{G}_1)f = L(G_1)f + \gamma \gamma^T f = \lambda f, \tag{10}$$

meaning it is also an eigenvector of $L(\bar{G}_1)$ with the same eigenvalue.

Now, since $[\pi, L(G_1)] = [\pi, L(\bar{G}_1)] = 0$ (both Laplacians are symmetric under the action of π) we can choose a basis in which all eigenvectors f_n are either even or odd. The corresponding spectra we denote by $\sigma^{\pm}(G_1)$ such that $\sigma(G_1) = \sigma^+(G_1) \cup \sigma^-(G_1)$ and similarly for \bar{G}_1 . All the above holds similarly for $L(G_2)$ and $L(\bar{G}_2)$. Hence, since $\sigma^+(G_1) = \sigma^+(\bar{G}_1)$ and $\sigma^+(G_2) = \sigma^+(\bar{G}_2)$, we have

$$\sigma^{+}(G_1) = \sigma^{+}(G_2) \Leftrightarrow \sigma^{+}(\bar{G}_1) = \sigma^{+}(\bar{G}_2). \tag{11}$$

It thus remains to show that $\sigma^-(G_1) = \sigma^-(G_2) \Leftrightarrow \sigma^-(\bar{G}_1) = \sigma^-(\bar{G}_2)$. If $f \in \mathcal{S}_-$ then the action (8) and decomposition (9) imply that for all $i \in \{0\} \cup (\mathcal{V} \setminus \mathcal{V}_{leaves})$ we have $[\pi f](i) = f(i) = -f(i)$, i.e. f(i) = 0. Therefore, if $f \in \mathcal{S}_-$ (it is only non-zero on \mathcal{V}_{leaves}) is an eigenvector of $L(G_1)$ with eigenvalue λ it is also an eigenvector of $L(G_2)$ with the same eigenvalue and hence $\sigma^-(G_1) = \sigma^-(G_2)$. The same reasoning gives us that $\sigma^-(\bar{G}_1) = \sigma^-(\bar{G}_2)$, which completes the result. However note that $\sigma^-(G_1) \neq \sigma^-(\bar{G}_1)$, in contrast to the even part of the spectrum.

Theorem 2.2. Let G_1 and G_2 be two graphs satisfying $\sigma(G_1) = \sigma(G_2)$ in which each graph contains a k-leaf-pair. Let us denote the respective eigenvectors of G_1 and G_2 by \boldsymbol{f}_n and \boldsymbol{g}_n and suppose that $\mu_{G_1}(\boldsymbol{f}_n) = \mu_{G_2}(\boldsymbol{g}_n)$ and $\nu_{G_1}(\boldsymbol{f}_n) = \nu_{G_2}(\boldsymbol{g}_n)$ for all generic n. If \bar{G}_1 and \bar{G}_2 are the graphs, with associated eigenvectors $\bar{\boldsymbol{f}}_n$ and $\bar{\boldsymbol{g}}_n$, obtained by inserting an edge between the two corresponding vertices in each k-leaf. Then

- (i) $\sigma(\bar{G}_1) = \sigma(\bar{G}_2)$ (they are isospectral)
- (ii) For all generic eigenvectors $\mu_{\bar{G}_1}(\bar{f}_n) = \mu_{\bar{G}_2}(\bar{g}_n)$ (they have the same flip count)
- (iii) For all generic eigenvectors $\nu_{\bar{G}_1}(\bar{f}_n) = \nu_{\bar{G}_2}(\bar{g}_n)$ (they have the same nodal count)

Proof. Part (i) is simply restating the result of lemma 2.1.

To show part (ii), using the reasoning from the proof of lemma 2.1, we know that if f is a generic eigenvector of $L(G_1)$ with eigenvalue λ then it must belong to $f \in \mathcal{S}_+$ and, hence, is also an eigenvector of $L(\bar{G}_1)$ with the same eigenvalue. In addition, if $(j,-j)=\mathcal{E}(\bar{G}_1)\setminus\mathcal{E}(G_1)$ is the edge inserted to make \bar{G}_1 then f(j)=f(-j). Therefore we have $\mu_{G_1}(f)=\mu_{\bar{G}_1}(f)$ since f does not change sign across the edge (j,-j). The same argument applies to give $\mu_{G_2}(g)=\mu_{\bar{G}_2}(g)$. Finally, by the isospectrality result of lemma 2.1, we know that if f and g are the mth eigenvectors in G_1 and G_2 then they must occupy the same position in the spectrum, say the nth, in \bar{G}_1 and \bar{G}_2 and so $\mu_{\bar{G}_1}(\bar{f}_n)=\mu_{G_1}(f_m)=\mu_{G_2}(g_m)=\mu_{\bar{G}_2}(\bar{g}_n)$ for all generic n.

In order to prove part (iii) we require more information about the eigenvectors than their value at the vertices j and -j. If k denotes the endpoint of the k-leaf, then by the eigenvalue equation $L(G_1)f = \lambda f$ we have

$$\lambda f(k) = f(k) - f(k-1) \implies f(k) = \frac{1}{(1-\lambda)} f(k-1).$$
 (12)

Thus f(k) depends only on the eigenvalue λ and the value of f at the vertex preceding it. Similarly $\lambda f(k-1) = 2f(k-1) - f(k) - f(k-2)$, which, using (12) gives

$$f(k-1) = \left((2-\lambda) - \frac{1}{(1-\lambda)} \right)^{-1} f(k-2),$$

so, again, we see that f(k-1) can be constructed by simply knowing λ and the preceding value f(k-2). The recursive nature therefore implies that on the leaves the vector takes the form $f(i) = F_i(\lambda) f(0)$ for some function $F_i(\lambda)$ (it's exact nature is not important here, only that it depends on λ).

By inserting the edge (j,-j) we therefore find $\nu_{\bar{G}_1}(f) = \nu_{G_1}(f) + \chi(\lambda,j)$, where $\chi(\lambda,j)$ (which only depends on λ and the inserted edge (j,-j)) is either 0 (the vertices j and -j belong to the same nodal domain of f), or -1 (the vertices j and -j belong to different nodal domains of f). Applying the same arguments to a generic eigenvector g of G_2 with the same eigenvalue λ gives $\nu_{\bar{G}_2}(f) = \nu_{G_2}(f) + \chi(\lambda,j)$ and so, by the isospectrality condition and the equality of nodal domains in G_1 and G_2 we find $\nu_{\bar{G}_2}(\bar{f}_n) = \nu_{G_1}(f_m) + \chi(\lambda,j) = \nu_{G_2}(g_m) + \chi(\lambda,j) = \nu_{\bar{G}_2}(\bar{g}_n)$ for all generic n.

The main issue to highlight is that, although all the generic eigenvectors themselves do not change between G and \bar{G} , some of their positions in the spectrum will. Therefore, the isospectrality condition ensures that they will change in the same manner in both G and \bar{G} , ensuring the flip count μ_n of the associated nth eigenvectors is the same.

More importantly, we do not preclude in theorem 2.2 that the graphs G_1 are G_2 are isomorphic. In fact, the easiest way to obtain examples to illustrate this theorem comes from taking $G_1 = G_2$ but containing multiple sets of k-leaf pairs. Adding edges to different pairs then makes it possible to create a \bar{G}_1 and \bar{G}_2 that are non-isomorphic, but are still isospectral, which is how the isospectral pair in figure 2 are created.

2.1. Removing the isospectrality condition

So far we have presented examples of mechanisms which are able to create families of isospectral graphs with the same flip count and nodal count. One may ask whether this condition is always needed. In the following we show this is not the case and present a way of constructing non-isospectral graphs with the same flip count and also the same nodal count. This is born out of lemma 2.1 and the observation that all trees have a flip count $\mu_n = n - 1$ and nodal count $\nu_n = n$.

Theorem 2.3. Let G be a graph containing a k-leaf-pair of length k = 1 and \bar{G} the graph obtained by inserting an edge between the ends of these leaves. If we denote f_n to be the nth eigenvector of G then the flip count of the nth eigenvector \bar{f}_n of \bar{G} is given (provided f_n is generic) by

$$\mu_{\bar{G}}(\bar{f}_n) = \begin{cases} \mu_G(f_{n+1}) & \text{if } 1 < \lambda_n < 3\\ \mu_G(f_n) & \text{otherwise} \end{cases}$$
 (13)

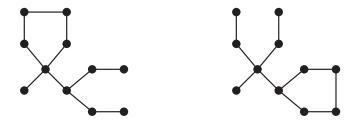


Figure 2. A pair of isospectral graphs with the same flip count and nodal count which originate by adding edges to trees.

and the nodal count by

$$\nu_{\bar{G}}(\bar{f}_n) = \begin{cases} \nu_G(f_n) & \text{if } \lambda_n < 1\\ \nu_G(f_{n+1}) - 1 & \text{if } 1 < \lambda_n < 3\\ \nu_G(f_n) - 1 & \text{if } \lambda_n > 3 \end{cases}$$
(14)

Proof. The statement (13) follows almost immediately from lemma 2.1. In this case our leaves are of length 1 and so the subspace S_- is spanned entirely by γ (given by $\gamma(i) = \delta_{i,1} - \delta_{i,-1}$). Thus, since γ is a non generic eigenvector of L(G) with eigenvalue 1 we have

$$L(\bar{G})\gamma = L(G)\gamma + \gamma\langle\gamma,\gamma\rangle = 3\gamma.$$

The rank 1 perturbation γ induces a shift of one eigenvalue from 1–3, while all other eigenvalues remain the same. Therefore, by lemma 2.1 we have for all eigenvectors, except γ ,

$$\bar{f}_n = \begin{cases} f_{n+1} & \text{if } 1 < \lambda_n < 3 \\ f_n & \text{otherwise} \end{cases}$$
 (15)

and so (13) follows by the fact that $\bar{f} \in S_+$ and thus $\langle \gamma, \bar{f} \rangle = 0 \Rightarrow \bar{f}(1) = \bar{f}(-1)$, i.e. \bar{f} does not change sign across the inserted edge (1, -1).

To establish (14) requires more information, specifically the sign of f(0) in comparison to f(1) = f(-1). Evaluating the Laplacian of G at the vertex 1 we get

$$[L(G)f](1) = \lambda f(1) = f(1) - f(0) \Rightarrow (1 - \lambda) = \frac{f(0)}{f(1)}.$$

Hence, for $\lambda < 1$, $\operatorname{sgn}(f(0)) = \operatorname{sgn}(f(1)) = \operatorname{sgn}(f(-1))$ and inserting an edge does not increase the number of nodal domains, whereas for $\lambda > 1$ the opposite is true. Combining this with (15) leads to (14).

As a consequence of theorem 2.3 we are able to get the following corollary, which enables us to generate pairs of non-isospectral graphs with the same flip count.

Corollary 2.4. Let G_1 and G_2 be graphs each containing a k-leaf-pair of length k=1 with eigenvectors \mathbf{f}_n and \mathbf{g}_n respectively. Suppose that for all generic eigenvectors we have $\mu_{G_1}(\mathbf{f}_n) = \mu_{G_2}(\mathbf{g}_n)$ and $\nu_{G_1}(\mathbf{f}_n) = \nu_{G_2}(\mathbf{g}_n)$ and they have the same number of eigenvalues in the ranges $0 \le \lambda < 1$, $1 \le \lambda < 3$ and $\lambda \ge 3$. Then, if \bar{G}_1 and \bar{G}_2 are the graphs obtained by inserting an edge between each leaf, then $\mu_{\bar{G}_1}(\bar{\mathbf{f}}_n) = \mu_{\bar{G}_2}(\bar{\mathbf{g}}_n)$ and $\nu_{\bar{G}_1}(\bar{\mathbf{f}}_n) = \nu_{\bar{G}_2}(\bar{\mathbf{g}}_n)$ for all generic n.

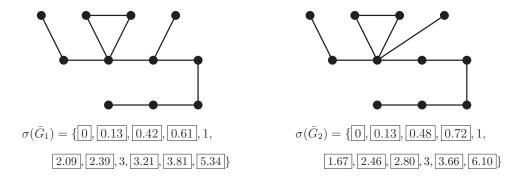


Figure 3. An example of two non-isospectral graphs in which all generic eigenvectors have the same flip count, given by $\mu_{\overline{G}_1} = \mu_{\overline{G}_2} = \{0, 1, 2, 3, 6, 7, 8, 9, 10\}$ and nodal count $\nu_{\overline{G}_1} = \nu_{\overline{G}_2} = \{1, 2, 3, 4, 6, 7, 8, 9, 10\}$. The spectrum is presented under each graph and eigenvalues associated to generic eigenvectors are marked in boxes.

Corollary 2.4 states that, via this mechanism, we are required to find non-isospectral graphs G_1 and G_2 with the same flip count in order to generate another pair of non-isospectral graphs \bar{G}_1 and \bar{G}_2 with the same flip count. At first sight this may seem like a pointless search, however it turns out to be very fruitful, as it allows us to go from tree-graphs (with trivial topologies) to non-tree-graphs, which no longer have trivial topologies. Examples of graphs \bar{G}_1 and \bar{G}_2 generated in this way are given in figure 3.

3. Quantum graphs

Definition 3.1. In the case of a metric graph we define a *l*-leaf to be a leaf with edge length *l*. In addition, we define a *l*-leaf-pair to be two *l*-leaves connected via some root vertex.

Remark 3.1. On a quantum graph, a vertex of degree 2 with Neumann vertex conditions (a so-called dummy vertex) does not alter any of the spectral properties [32]. Therefore we are free to add such vertices on leaves at any position we desire (see e.g. figure 4).

In the previous section we introduced the mechanism of inserting an edge between a pair of leaves. Our aim is to introduce a similar mechanism for quantum graphs, however the process of inserting an edge would increase the overall length of the graph, which could have dramatic consequences for the spectrum. The solution we find is thus to glue the leaves together at the same point, which alters the topology of the graph but retains the same overall length. This process leads us to theorem 3.2 below, which is the counterpart to theorem 2.2 in section 2. However, to begin, we start with the following lemma.

Lemma 3.1. Let Γ_1 and Γ_2 be two graphs each containing a l-leaf-pair. Let $\bar{\Gamma}_1$ and $\bar{\Gamma}_2$ be the respective graphs obtained by gluing the leaves in each pair together at the same point. Then $\sigma(\Gamma_1) = \sigma(\Gamma_2) \iff \sigma(\bar{\Gamma}_1) = \sigma(\bar{\Gamma}_2)$.

Proof. The proof proceeds in analogous manner to the discrete case given in lemma 2.1. Let us first administer some notation. In Γ_1 let u denote the root vertex which joins the two leaves, with v_{\pm} the ends of these leaves. Let us introduce two dummy vertices w_{\pm} the same distance away from the root on these respective leaves. Thus we have four edges which we denote



Figure 4. The process of gluing the leaves of a quantum graph Γ together at the dummy vertices w_+ and w_- to form a new quantum graph $\bar{\Gamma}$ with vertex w of degree 4. These dummy vertices are the same distance from the root, u, so $l_{(w_+,u)} = l_{(w_-,u)} = l_1$, and $l_{(w_+,v)} = l_{(w_-,v)} = l_2$.

 $e_{\pm 1} = (w_{\pm}, u)$ and $e_{\pm 2} = (w_{\pm}, v_{\pm})$, with lengths $l_{e_{+1}} = l_{e_{-1}} = l_1$ and $l_{e_{+2}} = l_{e_{-2}} = l_2$, as illustrated in figure 4. Thus our edge set consists of the edges $\mathcal{E} = \{e_{-2}, e_{-1}, e_1, e_2, e_3, \dots, e_{|\mathcal{E}|-2}\}$ and $\mathcal{E}_{\text{leaves}} := \{e_{-2}, e_{-1}, e_1, e_2\}$. Note that here $|\mathcal{E}|$ is the number of edges after we have inserted the dummy vertices w_{\pm} .

We now introduce the operator $\pi: L^2(\Gamma_1) \to L^2(\Gamma_1)$ that interchanges the two edges, i.e. for functions $\psi \in L^2(\Gamma_1)$ we have

$$[\pi\psi](x_{e_i}) = \begin{cases} \psi(x_{e_{-i}}) & i = -2, -1, 1, 2\\ \psi(x_{e_i}) & i = 3, \dots, |\mathcal{E}| - 2. \end{cases}$$
(16)

Again, since $\pi^2 = I$, the identity, we can decompose our Hilbert space into those functions which are even (+) and odd (-) under exchange of the two leaves

$$L_{+}^{2}(\Gamma_{1}) := \{ \psi \in L^{2}(\Gamma_{1}) : \pi \psi = \pm \psi \}, \tag{17}$$

with $L^2(\Gamma_1) = L^2_+(\Gamma_1) \oplus L^2_-(\Gamma_1)$. Moreover, if $\psi \in L^2_+(\Gamma_1)$ and is an eigenvector of L_{Γ_1} with eigenvalue λ then it is also an eigenvector of $L_{\bar{\Gamma}_1}$ with the same eigenvalue. To see this, note that if $L_{\Gamma_1}\psi = \lambda \psi$ then $-d^2\psi(x_e)/dx_e^2 = \lambda \psi(x_e)$ on all edges $e \in \mathcal{E}(\bar{\Gamma}_1)$ and thus it remains to check the vertex conditions at w_\pm are satisfied.

- (i) **Continuity:** by the vertex continuity at w_{\pm} on Γ_1 and the fact that ψ is even we have $\psi_{e_{+1}}(w_+) = \psi_{e_{+2}}(w_+) = \psi_{e_{-2}}(w_-) = \psi_{e_{-1}}(w_-)$, which is precisely the condition required at w on $\bar{\Gamma}_1$.
- (ii) **Derivatives:** on Γ_1 the (outgoing) derivatives at w_\pm satisfy $\psi'_{e_{+1}}(w_+) + \psi'_{e_{+2}}(w_+) = 0$ and $\psi'_{e_{-1}}(w_-) + \psi'_{e_{-2}}(w_-) = 0$ respectively. Adding these relations together gives $\psi'_{e_{+1}}(w_+) + \psi'_{e_{+2}}(w_+) + \psi'_{e_{-1}}(w_-) + \psi'_{e_{-2}}(w_-) = 0$, which again is the condition required for the derivatives of ψ at w on $\bar{\Gamma}_1$.

In addition, since π preserves the eigenspaces of Γ_1 we can choose a basis of eigenfunctions ψ_n such that they are either even or odd and we denote the corresponding spectra (including multiplicities) by $\sigma^{\pm}(\Gamma_1)$, so that $\sigma(\Gamma_1) = \sigma^+(\Gamma_1) \cup \sigma^-(\Gamma_1)$ and similarly for $\bar{\Gamma}_1$.

The same result holds for Γ_2 and $\bar{\Gamma}_2$. Hence, since $\sigma^+(\Gamma_1) = \sigma^+(\bar{\Gamma}_1)$ and $\sigma^+(\Gamma_2) = \sigma^+(\bar{\Gamma}_2)$, we have

$$\sigma^+(\Gamma_1) = \sigma^+(\Gamma_2) \iff \sigma^+(\bar{\Gamma}_1) = \sigma^+(\bar{\Gamma}_2).$$

It thus remains to show the same for the odd subspaces. We note that if $\psi \in L_-(\Gamma_1)$ then (16) and (17) imply that $\psi(x)=0$ for all points x which are not on the leaves of Γ_1 and similarly for Γ_2 . Therefore, $\psi \in L_-(\Gamma_1)$ is an eigenfunction of Γ_1 with eigenvalue λ if and only if it is an eigenfunction of Γ_2 with the same eigenvalue and so $\sigma^-(\Gamma_1)=\sigma^-(\Gamma_2)$. The same reasoning implies that $\sigma^-(\bar{\Gamma}_1)=\sigma^-(\bar{\Gamma}_2)$, which completes the result.

Theorem 3.2. Let Γ_1 and Γ_2 be two graphs each containing an l-leaf-pair and satisfying $\sigma(\Gamma_1) = \sigma(\Gamma_2)$. Let us denote the respective eigenfunctions by ψ_n and ϕ_n and suppose that $\mu_{\Gamma_1}(\psi_n) = \mu_{\Gamma_1}(\phi_n)$ and $\nu_{\Gamma_1}(\psi_n) = \nu_{\Gamma_2}(\phi_n)$ for all generic n. Let also $\bar{\Gamma}_1$ and $\bar{\Gamma}_2$ be the respective graphs obtained by gluing the leaves together at points w_{\pm} in the fashion of lemma 3.1 and $\bar{\psi}_n$ and $\bar{\phi}_n$ be the respective eigenfunctions. Then

- (i) $\sigma(\bar{\Gamma}_1) = \sigma(\bar{\Gamma}_2)$ (the graphs are isospectral).
- (ii) For all generic eigenvectors $\mu_{\bar{\Gamma}_1}(\bar{\psi}_n) = \mu_{\bar{\Gamma}_2}(\bar{\phi}_n)$ (they have the same flip count).
- (iii) For all generic eigenvectors $\nu_{\bar{\Gamma}_1}(\bar{\psi}_n) = \nu_{\bar{\Gamma}_2}(\bar{\phi}_n)$ (they have the same nodal count).

Remark 3.2. Depending on the choice of w_{\pm} it may be the case that eigenfunctions that are generic in Γ_1 (without the dummy vertices inserted) are no longer generic in $\bar{\Gamma}_1$, since they may be zero at w_{\pm} . However the combined zero set of all generic eigenfunctions forms a countable sequence of points on the edges of the leaves. Therefore, as this set is of zero measure, we can choose w_{\pm} almost everywhere on the leaves such that all generic eigenfunctions of Γ_1 are also generic on $\bar{\Gamma}_1$. The same holds for Γ_2 and $\bar{\Gamma}_2$.

Proof of theorem 3.2. Part (i) is simply restating lemma 3.1.

For part (ii) we note that if ψ is a generic eigenfunction of Γ_1 with eigenvalue λ , then $\psi \in L^2_+(\Gamma_1)$ and hence, by the argument in the proof of lemma 3.1 it is an eigenfunction of $\bar{\Gamma}_1$ with the same eigenvalue. If ψ is the mth eigenfunction ψ_m of Γ_1 and the nth eigenfunction $\bar{\psi}_n$ of $\bar{\Gamma}_1$ then $\mu_{\Gamma_1}(\psi_m) = \mu_{\bar{\Gamma}_1}(\bar{\psi}_n)$, since the process of gluing the edges together does not induce any more zeros. For the same reason $\mu_{\Gamma_2}(\phi_r) = \mu_{\bar{\Gamma}_2}(\bar{\phi}_n)$ when ϕ is generic and the nth (resp. rth) eigenfunction of Γ_2 (resp. $\bar{\Gamma}_2$). Thus lemma 3.1 ensures that, since $\bar{\Gamma}_1$ and $\bar{\Gamma}_2$ are isospectral, we have m=r and thus $\mu_{\bar{\Gamma}_1}(\bar{\psi}_n) = \mu_{\bar{\Gamma}_2}(\bar{\phi}_n)$ for all generic n.

For part (iii) we need to deduce some more information about the eigenfunctions. Firstly, if ψ is an eigenfunction of Γ_1 we know that on each edge it must be of the form

$$\psi(x) = A_1 \sin(\sqrt{\lambda}x) + B_1 \cos(\sqrt{\lambda}x).$$

Now, let $x \in [0, l]$ denote the position on one of the leaves with the point x = 0 giving the position at the end of the leaf and x = l the point of the root vertex u. Since all the vertices obey Neumann conditions we find that

$$\frac{\mathrm{d}\psi}{\mathrm{d}x}(0) = A_1 \sqrt{\lambda} \cos(0) - B_1 \sqrt{\lambda} \sin(0) = A_1 \sqrt{\lambda} = 0.$$

Thus $\psi(x) = B_1 \cos(\sqrt{\lambda}x)$. For the same reasoning we have on the graph $\Gamma_2 \phi(x) = B_2 \cos(\sqrt{\lambda}x)$, for some other constant B_2 . Gluing the edges together at the points w_\pm we either have that the number of nodal domains is the same $\nu_{\Gamma_1}(\psi) = \nu_{\bar{\Gamma}_1}(\psi)$ (the points w_\pm belong to the same nodal domain of ψ on Γ_1) or it decreases by one, i.e. $\nu_{\bar{\Gamma}_1}(\psi) = \nu_{\Gamma_1}(\psi) - 1$ (the points w_\pm belong to different nodal domains of ψ on Γ_1). However the same must be true for ϕ since

 $\psi(x)/\phi(x)$ is constant for all $x \in \mathcal{E}_{leaves}$. Therefore $\nu_{\bar{\Gamma}_1}(\bar{\psi}_n) = \nu_{\bar{\Gamma}_2}(\bar{\phi}_n)$ and the isospectrality of lemma 3.1 ensures they must occupy the same position in the spectrum.

We also comment that one could, in principle, obtain a pair of non-isospectral quantum graphs with the same flip and nodal counts in an analogous manner to section 2.1. The process would involve taking two tree graphs Γ_1 and Γ_2 , both containing a l-leaf-pair, and then gluing together the leaves to obtain $\bar{\Gamma}_1$ and $\bar{\Gamma}_2$, as outlined above. Γ_1 will have the same eigenvalues in the odd part of the spectrum as Γ_2 (i.e. $\lambda_n^{\text{odd}}(\Gamma_1) = \lambda_n^{\text{odd}}(\Gamma_2)$) and, similarly, $\bar{\Gamma}_1$ the same (odd) eigenvalues as $\bar{\Gamma}_2$ (i.e. $\lambda_n^{\text{odd}}(\bar{\Gamma}_1) = \lambda_n^{\text{odd}}(\bar{\Gamma}_2)$).

These odd eigenvalues can be explicitly calculated. They correspond to the eigenvalues of a line graph with Dirichlet conditions at one end, Neumann at the other and Neumann (resp. Dirichlet) for Γ (resp. $\bar{\Gamma}$) at a central vertex a distance l_1 from the end with Dirichlet conditions. This means the associated eigenvalues are strictly interlacing, i.e. $\lambda_n^{\rm odd}(\Gamma_1) < \lambda_n^{\rm odd}(\bar{\Gamma}_1) < \lambda_{n+1}^{\rm odd}(\Gamma_1)$ (see e.g. theorem 3.1.8 in [32]).

Since Γ_1 and Γ_2 are trees, they have the same flip and nodal counts. The even eigenvalues of Γ_1 are the same as $\bar{\Gamma}_1$ (similarly for Γ_2 and $\bar{\Gamma}_2$). Thus, if the positions in the spectrum (not necessarily the values) of these eigenvalues are the same—i.e. Γ_1 and Γ_2 have the same number of *even* eigenvalues in each interval $(\lambda_1^{\text{odd}}, \bar{\lambda}_1^{\text{odd}}), (\bar{\lambda}_1^{\text{odd}}, \lambda_2^{\text{odd}})$ etc—then the flip counts (although not necessarily the nodal counts) of $\bar{\Gamma}_1$ and $\bar{\Gamma}_2$ will coincide. However, due to the fact that there are an infinite number of eigenvalues for quantum graphs, this cannot be checked numerically. Thus, at present, we are unsure about the existence of such a pair of quantum graphs.

4. Conclusions

The work presented here outlines a simple mechanism for constructing both discrete and quantum isospectral graphs with the same flip and nodal count. Thus presenting a family of counter-examples to the conjecture that pairs of isospectral (non-tree) graphs may be distinguished by their nodal properties [1, 2, 30]. In addition, we have also shown that certain non-isospectral (discrete) graphs share the same flip count and nodal count. These results afford the existence of both isospectral and non-isospectral graphs with either the same or different flip/nodal counts, hence knowledge of whether the flip/nodal counts are the same or different is not enough to deduce whether two graphs are isospectral or not.

We believe this work highlights a number of previous questions and raises yet more. For instance, what is the likelihood of finding isospectral graphs and quantum graphs with the same flip/nodal count? Numerical simulations by Oren suggest these may be extremely rare in the cases such as random regular graphs [37]. With our methods, we can create graphs with very different topology that are isospectral and have identical flip counts and nodal counts. What properties unite all of these examples? And is there a criterion we can point to that tells us whether isospectral graphs and quantum graphs will have the same flip/nodal count, or are these examples all coincidental? Perhaps recent advances in our understanding of nodal and flip counts in connection with the stability of eigenvalues [15–18] may provide answers, as this makes connections with topological properties of the graph. Progress in this respect would be highly applicable to graph-theoretical problems looking at distinguishing non-isomorphic graphs and may also indicate how to proceed in the case of bounded domains.

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