Abstract. In this paper we propose a spectral flow for graph Laplacians, and prove that it counts the number of nodal domains for a given Laplace eigenvector. This extends work done for Laplacians on $\mathbb{R}^n$ to the graph setting. We mention some open problems relating the topology of a graph to the analytic behaviour of its Laplace eigenvectors, and include numerical examples illustrating our flow.

Key words. graph Laplacians, spectral theory, nodal deficiency, nodal domains

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A GRAPH SPECTRAL FLOW FOR COMPUTING NODAL DEFICIENCIES

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1. Introduction. The goal of this paper is to relate the analytic and topological properties of a weighted, combinatorial graph. In particular, we show that if $\phi_k$ is an eigenvector of the graph Laplacian $L$, then the number of nodal domains of $\phi_k$ can be counted via a family of perturbed graph Laplacians, the ideas of which we outline below. This provides a direct graph analogue of the continuum version in which Laplace eigenfunctions are considered, and provides an alternative proof of the counts obtained by Berkolaiko and Colin de Verdiere in [3] and [9] respectively.

Given a connected, weighted graph $G = (V,E,w)$, with adjacency matrix $A = (w_{ij})_{i,j \in V}$, we define the graph Laplacian as $L = D - A$, $D = \left( \sum_{(i,j) \in E} w_{ij} \right)_{ii}$. For an eigenvalue/eigenvector pair $(\lambda_k, \phi_k)$ of $L$, we construct a new graph $G_{\phi_k,\sigma}$ by 1) placing ghost vertices on each edge of $G$ where $\phi_k$ changes sign, and 2) adding a $\sigma$ dependence on all edge weights in such a way that, as $\sigma \to \infty$, the only edges that have non-zero weight are those edges attached to ghost vertices and edges of $G$ for which $\phi_k$ did not change sign. The graph Laplacian for $G_{\phi_k,\sigma}$ is written $L_{\phi_k,\sigma}$. Next, we define a bilinear form $B_\sigma$ for functions on $G_{\phi_k,\sigma}$ whose spectrum, as $\sigma \to \infty$, counts the number of nodal domains of $\phi_k$. In particular, we define

$$B_\sigma(u, v) = \langle u, L_{\phi_k,\sigma} v \rangle + \sigma \langle u, v \rangle_{\chi V_0} + \sigma \langle u, v \rangle_{\chi V_{gh}},$$

where $V_0$ consists of all vertices on which $\phi_k$ is 0, and $V_{gh}$ consists of all the ghost points; the inner product used is the standard vector dot product, though other graph inner products also work. Our main result is Theorem 3.4, along with its corollary, which together roughly state:

**Theorem 1.1.** As $\sigma \to \infty$, 
1. there are $k - \nu(\phi_k) + |E_0|$ eigenvalues which cross $\lambda_k$, where $E_0$ is the collection of edges over which $\phi_k \neq 0$ and changes sign, 
2. the number of eigenvalues of $B_\sigma$ that converge to $\lambda_k$ is exactly the number of nodal domains $\nu(\phi_k)$ of $\phi_k$.

In the rest of this section, we provide the context and motivation for this result in the continuum and graph settings. Namely, we start by reviewing what is known about nodal domains and nodal deficiencies for Laplace eigenfunctions, and then discuss similar graph eigenvector results.

1.1. The Continuum Spectral Flow. Consider a connected, bounded domain $\Omega \subset \mathbb{R}^n$ with Lipschitz boundary. The eigenvalues of the Laplacian $\Delta$ restricted to $\Omega$, 

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with Dirichlet boundary conditions, form an increasing sequence $0 < \lambda_0 \leq \lambda_1 \leq \cdots$; call their corresponding eigenfunctions $\phi_0, \phi_1, \ldots$. The **nodal set** of an eigenfunction $\phi_k$ are the connected components of $\{\phi_k \neq 0\} =: \Gamma$, the **nodal domains** are the connected components of $\Omega \setminus \Gamma$, and the number of nodal domains is denoted $\nu(\phi_k)$.

The **nodal deficiency** of an eigenfunction $\phi_k$ corresponding to a simple eigenvalue $\lambda_k$ is defined as

$$\delta(\phi_k) = k - \nu(\phi_k);$$

if $\lambda_k$ is not simple, we set $k_* = \inf \{s : \lambda_s = \lambda_k\}$ and set

$$\delta(\phi_k) = k_* - \nu(\phi_k).$$

When $n = 1$ and $\Omega$ is a bounded, connected interval, the classical Sturm-Liouville theory states that the nodal deficiency is always 0:

**Theorem 1.2.** Let $\Omega = [0, 1]$ and consider the Dirichlet eigenvalue problem

$$\partial_{xx}u(x) = \lambda u(x) \text{ for } x \in (0, 1) \text{ and } u(0) = u(1) = 0.$$ 

Sort the eigenvalues $0 < \lambda_0 \leq \lambda_1 \leq \cdots$, and call the corresponding eigenfunctions $\phi_0, \phi_1, \ldots$. Then $\phi_k$ has exactly $k$ zeros in $(0, 1)$.

For a modern discussion of this result, see [15, Chapter XIII].

In higher dimensions the situation is significantly more difficult. One early result was Courant’s nodal theorem, which provides an upper bound on the nodal deficiency:

**Theorem 1.3.** Let $\Omega \subset \mathbb{R}^n, n \geq 2$, be a bounded, connected domain with Laplaceian $\Delta$, and let $0 < \lambda_1 \leq \lambda_2 \leq \cdots$ be the ordered eigenvalues for the Dirichlet eigenvalue problem

$$\begin{cases} 
\Delta u = \lambda u & \text{in } \Omega, \\
u = 0 & \text{on } \partial \Omega.
\end{cases}$$

If $\phi_1, \phi_2, \ldots$ are the associated eigenfunctions, then $k \geq \nu(\phi_k)$.

For a full proof of this theorem see [7, Chapter 1.5]; for more on Dirichlet eigenvalue problems, see [10, Chapter 6.4]. We mention, in particular, a corollary of Courant’s nodal theorem:

**Proposition 1.4 ([7, Cor. 2]).** With the same terminology as in Theorem 1.3,

- $\phi_1$ has constant sign;
- $\lambda_1$ has multiplicity 1;
- $\lambda_1$ is characterized as being the only eigenvalue with eigenfunction of constant sign.

In our work, we use this as a lemma towards proving the graph-based Courant’s nodal theorem; compare to Proposition 3.1.

The upper bound in Courant’s theorem can only be attained finitely many times, as shown by Pleijel through an explicit construction in [14]. On the other hand, there exist examples of eigenfunctions with arbitrarily large index that have just two nodal domains: take a rectangle and a Laplace eigenfunction for this domain. By perturbing the Laplace operator by an appropriate potential, the perturbed eigenfunction will have adjacent nodal domains merge, leading to a (possibly much) larger nodal deficiency than what we started with.

This discussion suggests that counting nodal deficiencies is in general difficult, even in low dimensions. A step towards resolving these difficulties is presented in
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[4], where the nodal deficiency is reinterpreted as the Morse index of the Dirichlet-to-Neumann operator. Through this interpretation, they are able to count the nodal deficiency as the spectral flow of a bilinear form that combines the Dirichlet energy for a domain with a kind of Dirac mass on the eigenfunction’s nodal line. Their main result is the following.

**Theorem 1.5.** The nodal deficiency of \( \phi_k \) is precisely the number of eigenvalues of the bilinear form

\[
B_\sigma(u,v) := \int_\Omega \nabla u \cdot \nabla v d\mu + \sigma \int_{\Gamma} uv dS
\]

that cross \( \lambda_k + \epsilon \) for \( \epsilon > 0 \) small, as \( \sigma \to \infty \). Equivalently, the number of nodal domains of \( \phi_k \) is exactly the multiplicity of the first Dirichlet eigenvalue on \( \Omega \setminus \Gamma \), which are precisely the eigenvalues of the limiting bilinear form \( B_\infty \).

The proof is straightforward after the right framework is introduced, and many of the results and proofs in this paper are direct graph analogues of the continuum results. In our formulation, the domain \( \Omega \) is replaced by a weighted graph \( G \), \( \Delta \) is replaced by the graph Laplacian \( L \) on \( G \), and the nodal set \( \Gamma \) is replaced by the edges over which a graph Laplacian eigenvector either 1) changes sign, or 2) has a zero. **Theorem 3.4** shows that our graph spectral flow is able to count the nodal deficiency of a graph Laplacian eigenvector, just as the continuum spectral flow does.

Naturally, one could ask what happens when the graph spectral flow is constructed on a graph built from a point cloud sampled from \( \Omega \subset \mathbb{R}^n \); as we sample more points and construct “denser and denser” graphs, do the graph spectral flows converge to the continuum spectral flow? This question will be the subject of future work.

**1.2. Nodal deficiencies of graph Laplacian eigenvectors.** One of the implicit themes in this work is connecting analytic properties of the graph Laplacian to topological properties of the underlying graph. Similar ideas can be found in some of the early work of Fiedler (see, for example, [11, Theorem (2,3)]). Here we highlight the monograph [5], along with some more recent work due to Berkolaiko in [2],[3], and shortly after by Colin De Verdiere [9].

While graph Laplacians have been studied since the 20th century, nodal domain theorems for graph Laplacians have appeared relatively recently. In particular, [5] contains a fairly complete overview of what is currently known. Since graph functions are discrete, the notion of “nodal domain” is a little less precise. Two possibilities are the weak nodal domains \( \{ x : |f(x)| > 0 \} \) and the strong nodal domains \( \{ x : |f(x)| \geq 0 \} \). One of the main results is

**Theorem 1.6 ([5, Theorem 3.1]).** For any graph \( G \), the \( k \)th eigenfunction \( f_k \) of the graph Laplacian \( L \) has at most \( k \) weak nodal domains and at most \( k + r - 1 \) strong nodal domains, where \( r \) is the multiplicity of \( \lambda_k \).

The proof given utilizes matrix-theoretic methods, and is actually stated for a larger class of operators called generalized graph Laplacians. In our work, we are able to combine the two bounds by, roughly speaking, considering both weak and strong nodal domains in the same framework. In particular, we start with a weak nodal domain \( S \) of the original graph \( G \), embed \( S \) into a subdivided version of \( G \), and find the maximal strong nodal domain containing the embedded subgraph \( S \). Moreover, our methods have a distinct spectral theoretic flavour; this is due to the continuum analogue our construction is based off of.
We next highlight recent contributions by Berkolaiko and Colin de Verdiere, whose proofs are closer in spirit to the current work. Given a graph $G = (V,E)$, define the 1st Betti number $\beta_1$ of $G$ to be the number if linearly independent cycles in $G$; this number can be interpreted in the sense of simplicial homology, or as the minimum number of edges that need to be removed from $E$ to turn $G$ into a tree. Let $L$ be the graph Laplacian of $G$, and $\phi_k$ the eigenvector of the $k$th eigenvalue $\lambda_k$ of $L$.

**Theorem 1.7 ([3, Theorem 1.1]).** If $\lambda_k$ is simple and $\phi_k$ is never zero, then the number of edges $\nu$ along which $\phi_k$ changes sign satisfies $n - 1 \leq \nu \leq n - 1 + \beta$.

Moreover, the nodal deficiency $\delta(\phi_k) = k - \nu$ is the Morse index (number of negative eigenvalues) of the operator $\Lambda_k : B \to \lambda_k(B)$.

As described in [9], $B$ is a map associating unitary maps to each directed edge of $G$, and has an associated Schrödinger operator

$$q_B(f) = -\frac{1}{2} \sum_{(i,j) \in \overrightarrow{E}} -w_{ij}|f_i - e^{\alpha_{ij}}\sqrt{-1}f_j|^2 + \sum_{i \in V} V_i|f_i|^2,$$

where $V_i = \sum_{(i,j) \in E} -w_{ij}$, $\overrightarrow{E}$ is the collection of oriented edges, and $\alpha : \overrightarrow{E} \to \mathbb{R}$ is any alternating function.

A corollary of the above theorem is that, under the same assumptions, $k - \beta \leq \nu(\phi_k) \leq k$, where $\nu(\phi_k)$ is the number of nodal domains of the graph function $\phi_k$. As mentioned above, proofs of these results can be found in [3], [2], and [9]. This paper provides an alternative proof of these bounds utilizing Dirichlet eigenvalues of graphs.

**1.3. Organization of paper.** Section 2 details the graph subdivision process, and construction of the perturbed family of graph Laplacians, central to the graph spectral flow procedure. Some basic properties of the flow, like non-negativity, are also shown. Section 3 relates the subdivision process to the theory of Dirichlet eigenvalue problems on graphs. Through this framework we are able to prove our main result Theorem 3.4. We then give a simplified spectral flow procedure, and finally present some numerical examples in Section 4.

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**2. The Graph Spectral Flow.** In this section we define the graph spectral flow corresponding to an eigenvector of the graph Laplacian as a discrete version of the spectral flow in [4]. We will show some basic properties of this flow, and in the following section finish the proof that this graph spectral flow computes the nodal deficiency for graph eigenvectors.

Throughout the rest of this paper, we will assume that $G = (V,E,w)$ denotes a fixed weighted graph without multiple edges. Vertices will generally be represented by natural numbers, edges will be 2-tuples of vertices and may be denoted as either $(i,j)$ or $e_{ij}$ or just $e$, and edge weights correspond to the value of $w$ on an edge $e$, namely $w(e); w(e) = 0$ means the edge $e$ is not present in the graph. When $e = (i,j)$, we may also write $w_{ij}$. The adjacency matrix of $G$ is the $|V| \times |V|$ matrix $W = (w_{ij})_{(i,j) \in E}$, and
the degree matrix is the diagonal $|V| \times |V|$ matrix $D = (\sum_{j} w_{ij})_{i \in V}$. The spectrum of $G$ will be the spectrum of the graph Laplacian $L = D - W$; in particular, we are not considering the normalized graph Laplacian in this paper, nor are we considering the spectrum of adjacency matrices. For more on graph Laplacians and their spectra, see [8] or [6].

Given a graph $G = (V, E, w)$, its graph Laplacian $L$ is positive semi-definite, and so its spectrum consists of real eigenvalues $0 = \lambda_1 \leq \lambda_2 \leq \cdots \leq \lambda_n$. For each $k = 1, 2, \ldots$, consider the eigenvalue/eigenvector pair $(\lambda_k, \psi_k)$. We will usually have a fixed index $k$ in mind, and refer to a fixed pair $(\lambda_k, \psi_k)$ as $(\lambda, \psi)$ or $(\lambda_k, \psi)$. In what follows, we will interpret these (and other) vectors as functions on the graph $G$ through their values on vertices: if $u : V \to \mathbb{R}$ is one such function, the value of $u$ on vertex $i$ will be written as $u(i)$ or $u_i$.

**Definition 1.** Given an eigenvector $\psi$ of the graph Laplacian, interpreted as a function $\psi : V \to \mathbb{R}$, we define
- the zero vertices $V_0 \subset V$ as those vertices $i$ with $\psi_i = 0$;
- the zero edges $E_0 \subset E$ as those edges $(i, j)$ with $\psi_i \psi_j = 0$;
- the sign-change edges $E_0 \subset E$ as those edges $(i, j)$ such that $\psi_i \psi_j < 0$;
- the ghost vertices $V_{gh}$ that replace sign-change edges, defined by

$$V_{gh} = \{0_{ij} : (i, j) \in E_0\}.$$

**Definition 2.** The $\psi$-subdivision graph of $G$ is a new graph

$$G_{\psi, \sigma} = (V_\psi, E_\psi, w_{\psi, \sigma}),$$

depending on a parameter $\sigma \in [0, \infty)$, with
- $V_\psi := V \cup V_{gh}$,
- $E_\psi := E \cup \{(i, 0_{ij}), (0_{ij}, j) : (i, j) \in E_0\}$, and
- $w_{\psi, \sigma}(e) = \begin{cases} w(e), & e \in E \setminus E_0, \\ \frac{1}{1 + \sigma} w(e), & e \in E_0, \\ \frac{\sigma}{1 + \sigma} w(\tilde{e})(1 + q_{ji}), & e = (\tilde{i}, 0_{ij}), \tilde{e} = (i, j), q_{ji} := \frac{\psi_j}{\psi_i} > 0. \end{cases}$

The idea is that if $\psi$ changes sign across the edge $e = (i, j)$, then interpolating $\psi$ over $e$ should determine the location of a zero $0_{ij}$; these zero vertices are precisely the ghost vertices $V_{gh}$ defined above. The edge weights for $G_{\psi, \sigma}$ are chosen in the following manner. Initially we may want the weights of new edges $(i, 0_{ij}), (0_{ij}, j)$ to determine the location of the zero $0_{ij}$ along $(i, j)$. In practice we will use these numbers to interpolate functions on $G$ to functions on $G_{\psi, \sigma}$, but we need slightly different edge weights to give us the correct spectral properties we want for the graph spectral flow. Explicitly, letting the ($\sigma$ independent) edge weights of $(i, 0_{ij})$ and $(0_{ij}, j)$ be $a_{ij}$ and $a_{ji}$ respectively, we want

$$a_{ij} + a_{ji} = 1, \quad a_{ij} \psi_i + a_{ji} \psi_j = 0; \quad (2.1)$$

$a_{ij}, a_{ji}$ give the proportions along the edge $(i, j)$ at which we can find a zero of $\psi$. Here $a_{ij}$ should be interpreted as starting at vertex $i$ and walking for length $a_{ij} w_{ij}$ to reach $\psi$’s zero.

Solving (2.1) for $a_{ij}$ and $a_{ji}$ gives $a_{ij} = \frac{1}{1 + q_{ji}}$ and $a_{ji} = \frac{1}{1 + q_{ij}}$. Since these constants tell us where the zero of $\psi$ is relative to $i$ and $j$, we use these constants to interpolate from functions on $G$ to functions on $G_{\psi, \sigma}$. 

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Definition 3. Given a function \( f \) on \( G \), we extend \( f \) to a function \( \tilde{f} \) on \( G_{\psi,\sigma} \) by setting \( \tilde{f}_i = f_i \) for \( i \in V \), and \( \tilde{f}_{0ij} = a_{ij} f_i + a_{ji} f_j \).

By (2.1) we have \( \tilde{\psi}_{0ij} = a_{ij} \psi_i + a_{ji} \psi_j = 0 \), as expected.

Note that when \( \sigma = 0 \), \( G_{\psi,\sigma} \) simplifies to the original graph \( G \), plus a single disjoint vertex for each \( e \in E_0 \); the graph Laplacian \( L_{\psi,\sigma} \) simplifies to \( L_{\psi,0} = L \oplus 0_{|E_0|} \) with \( 0 \) an \( m \times m \) matrix of zeros. Thus, each eigenvalue/eigenvector pair of \( L_{\psi,0} \) after interpolation, and the zero eigenvalue of \( L_{\psi,0} \) has multiplicity \( 1 + |E_0| \) with corresponding eigenvectors the characteristic function for \( G \), and a characteristic function for each \( 0_{ij} \).

Before exploring properties of these subdivision graphs and their Laplacians, we explicitly describe the subdivision process for the complete graph on three vertices \( K_3 \), i.e. the three vertex graph with a single edge between every possible pair of vertices; other examples are provided in the last section. The adjacency and Laplacian matrices of \( K_3 \) are

\[
A = \begin{pmatrix} 0 & 1 & 1 \\ 1 & 0 & 1 \\ 1 & 1 & 0 \end{pmatrix} \quad \text{and} \quad L = \begin{pmatrix} 2 & -1 & -1 \\ -1 & 2 & -1 \\ -1 & -1 & 2 \end{pmatrix}.
\]

We have \( \text{Spec}(L) = \{0, 3, 3\} \) with associated eigenvectors \((1,1,1), (1,-1,0), (1,0,-1)\) respectively. Set \( \psi = (1,-1,0) \). If we denote the vertices of \( K_3 \) by \( \{1,2,3\} \), the eigenvector \( \psi \) has just one sign change over the edge \((1,2)\), and \( q_{12} = q_{21} = 1 \). The subdivision graph \( G_{\psi,\sigma} \) thus has vertex set \( \{1,2,3,0_{12}\} \), and the edges/edge weights can be read from the adjacency and Laplacian matrices of \( G_{\psi,\sigma} \):

\[
A_{\psi,\sigma} = \begin{pmatrix} 0 & 1 & 2\sigma \\ 1 & 0 & 2\sigma \\ 2\sigma & 2\sigma & 0 \end{pmatrix} \quad \text{and} \quad L_{\psi,\sigma} = \begin{pmatrix} 2\sigma+1 & 1 & -1 \\ -1 & 2\sigma+1 & -1 \\ -1 & -1 & 2 \end{pmatrix}.
\]

See Figure 2.1 for an illustration of \( K_3 \) and \( G_{\psi,\sigma} \).

In particular, we reiterate that \( L_{\psi,0} = L \oplus 0_{V_{gh}} = L \oplus 0_1 \).
Notice that, in general, Definition 2 tells us to give edges of the form \((i,0_{ij})\) edge weight \(w_{ij}(1 + q_{ji})\) and not \(w_{ij}\frac{1}{1+q_{ji}} = w_{ij}a_{ij}\) (ignoring the \(\sigma\) dependence), which one might expect from the equality \(a_{ij}w_{ij} + a_{ji}w_{ij} = w_{ij}\). The reason for this is spectral, as the proof of the next proposition shows.

**Proposition 2.1.** Suppose \((\lambda_k, \psi)\) is an eigenvalue/eigenvector pair for the graph \(G\), i.e. \(L\psi = \lambda_k\psi\). Then \(L\psi,\sigma\tilde{\psi} = \lambda_k\tilde{\psi}\) for all \(\sigma\).

**Proof.** This is a straightforward computation. Because \(\tilde{\psi}\) is an eigenvector with eigenvalue \(\lambda_k\), we have

\[
(L\psi)_i = \sum_{(i,j) \in E} w_{ij}(\psi_i - \psi_j) = \lambda_k\psi_i.
\]

If the vertex \(i\) is not in \(0_{gh}\), then

\[
(L\psi,\sigma\tilde{\psi})_i = \sum_{(i,j) \in E_\psi} w_{ij,\sigma}(\psi_i - \psi_j)
\]

\[
= \sum_{(i,j) \in E \setminus E_0} w_{ij}(\psi_i - \psi_j) + \sum_{(i,j) \in E_0} \frac{1}{1+\sigma}w_{ij}(\psi_i - \psi_j)
\]

\[
+ \sum_{(i,0_{ij}) \in E_\psi \setminus E} \frac{\sigma}{1+\sigma}w_{ij}(1 + q_{ji})(\psi_i - \psi_{0_{ij}})
\]

\[
= \sum_{(i,j) \in E \setminus E_0} w_{ij}(\psi_i - \psi_j)
\]

\[
+ \sum_{(i,j) \in E_0} w_{ij} \left[ \frac{1}{1+\sigma}(\psi_i - \psi_j) + \frac{\sigma}{1+\sigma}(1 + q_{ji})\psi_i \right]
\]

\[
= \sum_{(i,j) \in E \setminus E_0} w_{ij}(\psi_i - \psi_j)
\]

\[
+ \sum_{(i,j) \in E_0} w_{ij} \left[ \frac{1}{1+\sigma}(\psi_i - \psi_j) + \frac{\sigma}{1+\sigma}(\psi_i - \psi_j) \right]
\]

\[
= \sum_{(i,j) \in E} w_{ij}(\psi_i - \psi_j) = \lambda_k\tilde{\psi}_i = \lambda_k\psi_i.
\]

Otherwise,

\[
(L\psi,\sigma\tilde{\psi})_{0_{ij}} = \frac{\sigma}{1+\sigma}w_{ij}(1 + q_{ji})(\psi_{0_{ij}} - \psi_i) + \frac{\sigma}{1+\sigma}w_{ij}(1 + q_{ij})(\psi_{0_{ij}} - \psi_j)
\]

\[
= -\frac{\sigma w_{ij}}{1+\sigma}((1 + q_{ji})\psi_i + (1 + q_{ij})\psi_j)
\]

\[
= 0 = \lambda_k\tilde{\psi}_{0_{ij}},
\]

and so \(L\psi,\sigma\tilde{\psi} = \lambda_k\tilde{\psi}\).

We can now define the graph spectral flow.

**Definition 4.** Define the family of bilinear forms \(B_\sigma\) on \(G_\psi\) by

\[
B_\sigma(u, v) = \langle u, L\psi, \sigma v \rangle + \sigma \langle u, v \rangle_{\chi_{0_{gh}}} = \sigma \chi_{V_0} + \sigma \langle u, v \rangle_{\chi_{V_{gh}}}.
\]

Here, \(\chi_{V_0}\) is the indicator function for \(V_0\) in \(G_\psi\) and \(\langle u, v \rangle_{\chi_{V_0}}\) is the inner product for \(G_\psi\) weighted by \(\chi_{V_0}\), i.e. the inner product restricted to \(V_0\). When \(\langle u, v \rangle = u^t v\), \(\langle u, v \rangle_{\chi_{V_0}} = u^t \text{diag}(\chi_{V_0}) v\).
Written out in full,

\[ B_\sigma(u, v) = \sum_{(i,j) \in \mathcal{E} \setminus \mathcal{E}_0} w_{ij} (u_i - u_j)(v_i - v_j) \]

\[ + \sum_{(i,j) \in \mathcal{E}_0} w_{ij} \frac{1}{1 + \sigma} (u_i - u_j)(v_i - v_j) \]

\[ + \sum_{(i,j) \in \mathcal{E}_0} w_{ij} \frac{\sigma}{1 + \sigma} \left[ (1 + q_{ji})(u_i - u_{0,i})(v_i - v_{0,i}) \right. \]

\[ + (1 + q_{ij})(u_j - u_{0,j})(v_j - v_{0,j}) \]

\[ + \sigma \sum_{i \in V_0} u_i v_i + \sigma \sum_{i \in V_{\emptyset}} u_i v_i \cdot \]

For functions \( \hat{u} \) and \( \hat{v} \) that are extensions of functions \( u, v \) on \( G \), we have

\[ u_{0,i} = a_{ij} u_i + a_{ji} u_j = \frac{1}{1 + q_{ij}} u_i + \frac{1}{1 + q_{ji}} u_j, \]

so the last term of \( B_\sigma(\hat{u}, \hat{v}) \) becomes

\[ \sum_{(i,j) \in \mathcal{E}_0} a_{ij}^2 u_i v_i + a_{ij} a_{ji} u_i v_j + a_{ij} a_{ji} u_j v_i + a_{ji}^2 u_j v_j \]

\[ = \sum_{(i,j) \in \mathcal{E}_0} a_{ij} a_{ji} (\sqrt{q_{ji}} u_i + \sqrt{q_{ij}} u_j)(\sqrt{q_{ji}} v_i + \sqrt{q_{ij}} v_j) \]

\[ = \sum_{(i,j) \in \mathcal{E}_0} u^T p_{ij} v. \]

Here \( p_{ij} \) is the matrix with zeros except at the \( i, j \) submatrix, taking the form

\[ p_{ij} = \begin{pmatrix} a_{ij}^2 & a_{ij} a_{ji} & a_{ji}^2 \\ a_{ij} a_{ji} & 1 & q_{ij} \end{pmatrix} = a_{ij} a_{ji} P_{ij}. \]

We also see that

\[ \sum_{(i,j) \in \mathcal{E}_0} w_{ij} \frac{\sigma}{1 + \sigma} \left[ (1 + q_{ji})(u_i - u_{0,i})(v_i - v_{0,i}) + (1 + q_{ij})(u_j - u_{0,j})(v_j - v_{0,j}) \right] \]

\[ = \sum_{(i,j) \in \mathcal{E}_0} w_{ij} \frac{\sigma}{1 + \sigma} \left[ (1 + q_{ji})(1 - a_{ij}) u_i - a_{ji} u_j)((1 - a_{ij}) v_i - a_{ji} v_j) \right. \]

\[ + (1 + q_{ij})(1 - a_{ji}) u_j - a_{ij} u_i((1 - a_{ji}) v_j - a_{ij} v_i)] \]

\[ = \sum_{(i,j) \in \mathcal{E}_0} w_{ij} \sigma \frac{\sigma}{1 + \sigma} \left[ a_{ji} (u_i - u_j)(v_i - v_j) + a_{ij} (u_j - u_i)(v_j - v_i) \right] \]

\[ = \sum_{(i,j) \in \mathcal{E}_0} w_{ij} \sigma \frac{\sigma}{1 + \sigma} (u_i - u_j)(v_i - v_j), \]

since \( a_{ij} + a_{ji} = 1 \) and \( \frac{a_{ij}}{1 + a_{ji}} = 1 \). If \( V_0 = \emptyset \), we conclude
\[ B_\sigma(u,v) = \sum_{(i,j) \in E \setminus E_0} w_{ij}(u_i - u_j)(v_i - v_j) + \sum_{(i,j) \in E_0} w_{ij} \frac{1}{1 + \sigma}(u_i - u_j)(v_i - v_j) \]
\[ + \sum_{(i,j) \in E_0} w_{ij} \frac{\sigma}{1 + \sigma}((1 + \sigma)(u_i - u_{0_{ij}})(v_i - v_{0_{ij}})) \]
\[ + (1 + q_{ij})(u_j - u_{0_{ij}})(v_j - v_{0_{ij}})) + \sigma \sum_{i \in V_0} u_iv_i \]
\[ = \sum_{(i,j) \in E \setminus E_0} w_{ij}(u_i - u_j)(v_i - v_j) + \sum_{(i,j) \in E_0} w_{ij} \frac{1}{1 + \sigma}(u_i - u_j)(v_i - v_j) \]
\[ + \sum_{(i,j) \in E_0} w_{ij} \frac{\sigma}{1 + \sigma}(u_i - u_j)(v_i - v_j) + \sigma \sum_{i \in V_0} u_iv_i \]
\[ = \sum_{(i,j) \in E} w_{ij}(u_i - u_j)(v_i - v_j) \]
\[ + \sigma \sum_{(i,j) \in E_0} a_{ij}a_{ji}(\sqrt{q_{ij}}u_i + \sqrt{q_{ji}}u_j)(\sqrt{q_{ij}}v_i + \sqrt{q_{ji}}v_j) \]
\[ = \langle u, Lv \rangle + \sigma \sum_{(i,j) \in E_0} a_{ij}a_{ji}\langle u, P_{ij}v \rangle. \]

When \( V_0 \neq \emptyset \), we just need to add \( \sigma \sum_{i \in V_0} u_iv_i = \sigma \sum_{i \in V_0} \langle u, E_{ii}v \rangle \) to the last line above, with \( E_{ii} \) the zero matrix with a 1 at the \( i \)th entry.

In summary, we have shown the following proposition:

**Proposition 2.2.** Suppose \( \tilde{u}, \tilde{v} : G_{\psi, \sigma} \rightarrow \mathbb{R} \) are extensions of functions \( u, v \) on \( G \). Then

\[ B_\sigma(\tilde{u}, \tilde{v}) = \langle u, Lv \rangle + \sigma \sum_{(i,j) \in E_0} a_{ij}a_{ji}\langle u, P_{ij}v \rangle + \sigma \sum_{i \in V_0} \langle u, E_{ii}v \rangle. \]

Proposition 2.2 motivates a simplified spectral flow, where the constructed flow is based off of edges only and does not require ghost points added. We call this construction the edge-based flow and discuss it in the next section, in relation to the Dirichlet graph eigenvalue problem. We note that by changing the constants in the sums involving \( P_{ij} \) and \( E_{ii} \), we are able to compute the same spectral information without evaluating the flow as \( \sigma \rightarrow \infty \). This suggests quick methods for numerically computed spectral flows, and thus nodal deficiencies.

An important aspect of the (continuum) spectral flow is that each eigenvalue of \( B_\sigma \) is non-decreasing in \( \sigma \), and that whenever such an eigenvalue crosses the line \( \lambda_k + \epsilon \), the slope of the eigenvalue branch is strictly positive. Moreover, the eigenvalues of \( B_\sigma \) are analytic curves branching from the spectrum of \( L \); this is a standard result in perturbation theory, c.f. [13, Chapter 2]. The next proposition establishes the non-negativity of the spectral flow.

**Proposition 2.3.** The eigenvalues of \( B_\sigma \) are non-decreasing eigenvalue branches of \( \lambda_i \), \( 0 \leq i \leq k \).

**Proof.** Suppose \( (\lambda, u) = (\lambda_\sigma, u_\sigma) \) is an eigenvalue/eigenvector pair of \( B_\sigma \) with \( \langle u, u \rangle = 1 \), so that

\[ B_\sigma(u, v) = \lambda\langle u, v \rangle \quad \forall v \in \mathbb{R}^{|V_0|}. \]
As mentioned, these are analytic branches in terms of $\sigma$, branching from the eigenvalue/eigenvector pairs of $L_{\psi,0} = L + 0_{E_0}$.

Differentiating with respect to $\sigma$ gives

$$B_\sigma(u, v)' = B'_\sigma(u, v) + B_\sigma(u', v),$$

and $(\lambda(u, v))' = \lambda'(u, v) + \lambda(u', v)$.

By the variational formulation for eigenvalues, we must have $B_\sigma(u, u') = \lambda(u, u')$, and so

$$\lambda'(u, u) + \lambda(u', u) = B'_\sigma(u, u) + B_\sigma(u', u),$$

which in turn gives

$$\lambda' = B'_\sigma(u, u) = \langle u, L'_{\psi, \sigma} u \rangle + \langle u, u \rangle_{\chi_{V_0}} + \langle u, u \rangle_{\chi_{V_{gh}}}.$$

Since $\langle u, u \rangle_{\chi_{V_0}}, \langle u, u \rangle_{\chi_{V_{gh}}} \geq 0$, all that remains is to show that $\langle u, L'_{\psi, \sigma} u \rangle \geq 0$.

For arbitrary $v \in \mathbb{R}^{|V_0|}$, we have

$$\langle v, L'_{\psi, \sigma} v \rangle = \sum_{(i,j) \in E_0} w'_{ij}(v_i - v_j)^2$$

$$= \sum_{(i,j) \in E_0} \left( \frac{1}{1 + \sigma} \right)' w_{ij} (v_i - v_j)^2$$

$$+ \sum_{(i,j) \in E_0 \setminus E} \left( \frac{\sigma}{1 + \sigma} \right)' w_{ij} (1 + q_{ji})(v_i - v_{0_{ji}})^2$$

$$= \sum_{(i,j) \in E_0} \left( \frac{1}{1 + \sigma} \right)' w_{ij} (v_i - v_j)^2 + \left( \frac{\sigma}{1 + \sigma} \right)' w_{ij} (1 + q_{ji})(v_i - v_{0_{ji}})^2$$

$$+ \left( \frac{\sigma}{1 + \sigma} \right)' w_{ij} (1 + q_{ji})(v_j - v_{0_{ji}})^2$$

$$= \sum_{(i,j) \in E_0} \frac{w_{ij}}{(1 + \sigma)^2} \left( - (v_i - v_j)^2 + (1 + q_{ji})(v_i - v_{0_{ji}})^2 \right)$$

$$+ \left( 1 + q_{ij} \right)(v_j - v_{0_{ij}})^2;$$

all of the $w_{ij}, q_{ij}$ are positive, establishing the non-negativity of $\lambda'_{\sigma}$. \[ \Box \]

Later, we will show that the only eigenvectors that satisfy $\lambda'_{\sigma} = 0$ are those that are zero on $V_0 \cup V_{ph}$, and therefore must satisfy $\lambda_{\sigma}|_{\sigma = 0} \geq \lambda_k$. The proper framework for this result is via Dirichlet eigenvalue problems on graphs, which is the subject of the next section.

3. The Relation to Dirichlet Eigenvalues. Our results on the graph spectral flow involve the limiting behaviour of $B_{\sigma}$ and $L_{\psi, \sigma}$ as $\sigma \to \infty$. For such a statement like $L_{\psi, \infty} u = \lambda u$ to make sense, we need $u|_{V_0 \cup V_{gh}} = 0$; for the rest of this paper, we use the convention that $0 \cdot \infty = 0$. Thus, the limiting eigenvalue problem asks for a function $u$ with $L_{\psi, \infty} u = \lambda u$ and $u|_{V_0 \cup V_{gh}} = 0$. This is reminiscent of a Dirichlet
boundary value condition, so we begin by recalling the basic definitions and properties of Dirichlet eigenvalues for graphs. Afterwards we return to the graph spectral flow, and finish the proof that the spectral flow counts the nodal deficiency of a graph eigenvector. For a complete introduction to Dirichlet eigenvalues on graphs, see [8, Chapter 8].

**Definition 5.** For a graph \( G = (V, E, w) \) and a subset of vertices \( S \), we define:
- the vertex boundary \( \partial V S \) as the vertices in \( V \setminus S \) that are adjacent to some vertex in \( S \), and
- the edge boundary \( \partial E S \) as the edges in \( E \) that connect a vertex in \( \partial V S \) to a vertex in \( S \).

The space of graph functions \( u: V \to \mathbb{R} \) that are zero on \( \partial V S \subset V \) is denoted \( D^* S \) or just \( D^* \) when \( S \) is clear, i.e.
\[
D^* = \{ u: V \to \mathbb{R}: u|_S = 0 \}.
\]

Finally, the **Dirichlet subgraph induced by** \( S \), or the **D-subgraph induced by** \( S \), denoted \( S(D) \), is the subgraph of \( G \) induced by the vertices in \( S \), together with the vertices of \( \partial V S \) and edges of \( \partial E S \); explicitly, the induced subgraph is \((S \cup \partial V S, E|_{S \cup \partial E S}, w|_{E|_{S \cup \partial E S}})\).

This notion of vertex boundaries allows us to impose Dirichlet/zero boundary conditions on problems involving the graph Laplacian. In this work, \( S \) will usually be a strong nodal domain of \( G \).

**Definition 6.** The **first Dirichlet eigenvalue** of a graph \( G \), corresponding to \( S \), is
\[
\lambda_1(D) = \inf_{u \neq 0} \sum_{u \in D^*} \frac{w_{ij}(u_i - u_j)^2}{\sum_{i \in S} u_i^2} = \inf_{u \neq 0} \sum_{(i,j) \in \partial E S} \frac{\langle u, L(D)u \rangle_S}{\langle u, u \rangle_S} = \inf_{u \neq 0} \sum_{(i,j) \in \partial E S} \frac{\langle u, L(D)u \rangle_S}{\langle u, u \rangle_S} = \inf_{u \neq 0} \sum_{(i,j) \in \partial E S} \frac{\langle u, L(D)u \rangle_S}{\langle u, u \rangle_S}.
\]

The operator \( L(D) \) is the graph Laplacian of \( G \) with the rows and columns corresponding to vertices in \( \partial V S \) removed.

**Higher order eigenvalues are found inductively via the Courant-Fischer/Min-max theorem (see, for example, [13, Chapter 1, §10]):** after determining \( \lambda_1(D), \ldots, \lambda_k(D) \), and associated eigenvectors \( \phi_1, \ldots, \phi_k \), we have
\[
\lambda_{k+1}(D) = \inf_{u \neq 0, \langle u, u \rangle = 1} \sum_{(i,j) \in E(S(D))} w_{ij}(u_i - u_j)^2.
\]

Right away we see that \( \lambda_1(D) > 0 \). In fact, if the induced subgraph \( S(D) \) is connected (modulo zero vertices, to be made precise), then the corresponding eigenvector is signed. This result is used to show that the first Dirichlet eigenvalue of a connected subgraph is simple, which is then used to show that higher eigenvectors cannot be signed.

**Definition 7.** Given a graph \( G = (V, E) \) and a subset of vertices \( S \), we call the induced D-subgraph of \( S \) **Dirichlet disconnected** if there are subgraphs \( S_1, S_2 \) of \( G \)
such that \( S^{(D)} = S_1^{(D)} \cup S_2^{(D)} \) and \( S_1 \cap S_2 \subset \partial V S \). Otherwise, \( S \) is \textbf{Dirichlet connected} if \( S \) is not Dirichlet disconnected and both \( S_1 \) and \( S_2 \) are connected subgraphs of \( G \). We will write this last term as \( D \)-connected.

An equivalent characterization for an induced \( D \)-subgraph \( S^{(D)} \) to be \( D \)-connected is that any two vertices are path-connected in \( S^{(D)} \), where the path cannot pass through \( \partial V S \).

**Proposition 3.1.** Suppose that the subgraph \( S^{(D)} \) is \( D \)-connected. Then
1. the eigenvector \( \phi_1 \) corresponding to \( \lambda_1^{(D)} \) is signed,
2. \( \lambda_1^{(D)} \) is simple, and
3. higher index eigenvectors \( \phi_i \) cannot be signed, implying a signed eigenvector must correspond to the first Dirichlet eigenvalue.

For a graph function \( u: G \to \mathbb{R} \), we write \( u \geq 0 \) to mean \( u_i \geq 0 \) for each vertex \( i \in S \). This result is a direct graph analogue of the theorem for Dirichlet eigenvalues for the Laplacian acting on a connected, bounded domain; see [7, §1.5, Corollary 2].

**Proof.** Claims 1. and 2. are described in [5, Lemma 6.1], with their \( V^o \cup \partial V \) corresponding to our \( S^{(D)} \).

For claim 3., since \( \phi_k \) minimizes \( \sum_{(i,j) \in E(S^{(D)})} w_{ij} (u_i - u_j)^2 \) over all \( u \) with \( \langle u, u \rangle = 1, u \neq 0, u \in D^* \), and \( u \perp \phi_i \) for \( 1 \leq i \leq k - 1 \), we have in particular that \( \langle \phi_k, \phi_1 \rangle = 0 \). We already have that \( \phi_1 \) is signed, and so if \( \phi_k \) was signed as well, assuming both eigenvectors positive gives \( \langle \phi_1, \phi_k \rangle > 0 \). Thus a higher signed eigenvector cannot be orthogonal to \( \phi_1 \), forcing \( \phi_k \) to change sign within \( S \).

**Proposition 3.2.** Given a graph \( G \) and a Laplace eigenvector \( \psi \) with eigenvalue \( \lambda \), decompose the (weak) nodal domains \( S = \{ i : \psi_i > 0 \} \cup \{ i : \psi_i < 0 \} \) of the \( \psi \)-subdivision \( G_{\psi, \infty} \) into \( D \)-connected graphs \( S_1, S_2, ..., S_n \). Then the restriction of \( \psi \) to each \( S_l \), \( \psi|_{S_l} \), is a Dirichlet eigenvector of \( S^{(D)} \) with eigenvalue \( \lambda \). Moreover, \( \psi|_{S_l} \) is signed, and so \( \lambda \) is the first Dirichlet eigenvalue for each \( S_l \).

Note that each of the \( S_l \) are maximally connected, strong nodal domains of \( G_{\psi, \infty} \).

**Proof.** Recall that \( G_{\psi, \infty} \) contains the original vertices of \( G \) together with ghost points \( 0_{ij} \) for each \( (i, j) \in E_0 \), and each edge \( (i, j) \in E_0 \) is replaced by two edges \( (i, 0_{ij}) \) and \( (0_{ij}, j) \), with respective edge weights \( (1 + q_{ji}) \) and \( (1 + q_{ij}) \), in \( G_{\psi, \infty} \).

For a \( D \)-connected component \( S_l \), define

\[
\psi|_{S_l} = \begin{cases} 
\psi_i, & i \in S_l, \\
0, & i \notin S_l,
\end{cases}
\]

which is the restriction of \( \psi \) to \( S_l \), followed by an extension by zero to the rest of the graph. We claim that \( \psi|_{S_l} \) is an eigenvector of \( L_{\psi, \infty} \) restricted to \( S_l \), which implies that \( \psi|_{S_l} \) is also a Dirichlet eigenvector of \( S_l \).

In general, for any function \( u \) that is zero on \( V_0 \cup V_{\phi h} \) we have

\[
(L_{\psi, \infty} u)_i = \sum_{(i,j) \in E \setminus E_0} w_{ij} (u_i - u_j) + \sum_{(i,j) \in E_0} w_{ij} (1 + q_{ji}) (u_i - u_{0_{ij}})
\]
For \( i \in S_l \),
\[
(L_{\psi, \infty} \psi|S_l)_i = \sum_{(i,j) \in E \setminus E_0} w_{ij}((\psi|S_l)_i - (\psi|S_l)_j) + \sum_{(i,j) \in E_0} w_{ij}(1 + q_{ji})(|\psi|_{S_l})_i
\]
\[
= \sum_{(i,j) \in E \setminus E_0} w_{ij}(\psi_i - \psi_j) + \sum_{(i,j) \in E_0} w_{ij}(1 + q_{ji})\psi_i
\]
\[
= \sum_{(i,j) \in E \setminus E_0} w_{ij}(\psi_i - \psi_j) + \sum_{(i,j) \in E_0} w_{ij}(\psi_i - \psi_j)
\]
\[
= \sum_{(i,j) \in E} w_{ij}(\psi_i - \psi_j) = \lambda i = \lambda(\psi|S_l)_i,
\]
where \( E_0 \) can be empty or not depending on if \( i \) has neighbors in \( V_{gh} \). This shows each \( \psi|S_l \) is a Dirichlet eigenvector of \( S_l \) with eigenvalue \( \lambda \). Moreover, each \( S_l \) is a D-connected subgraph of \( G_{\psi, \infty} \) corresponding to a nodal domain \( \{i: \psi_i > 0\} \) or \( \{i: \psi_i < 0\} \), and so each \( \psi|S_l \) is signed.

Thus we have constructed signed Dirichlet eigenvectors for \( \lambda \) on each of the D-connected components of \( S^{(D)} \), establishing that \( \lambda \) is the first Dirichlet eigenvalue for each \( S_l \).

\[ \square \]

Recall that if \( (\lambda_\sigma, u_\sigma) \) is a branch of eigenvalue/eigenvector pairs for the spectral flow \( B_\sigma \), then \( \lambda' \geq 0 \). A key ingredient of the nodal deficiency count, both in the continuum and graph cases, is that whenever an eigenvalue crossing occurs, the slope of the crossing branch is positive. This ensures that eigenvalues can only limit to \( \lambda_k \) as \( \sigma \to \infty \), and any crossing does indeed contribute to the nodal deficiency of \( \lambda_k \).

PROPOSITION 3.3. If \( \lambda_{\sigma^*} = \lambda_k \) and \( \lambda_{\sigma^*} = 0 \) for some \( \sigma^* \in (0, \infty) \), then the corresponding eigenvector \( u \) for \( \lambda_{\sigma^*} \) is a constant multiple of \( \psi \). This implies that if \( \lambda_{\sigma^*} < \lambda_k \) and \( \lambda_{\sigma^*} = \lambda_k \), then \( \lambda'_{\sigma^*} > 0 \).

Proof. Fix an eigenvector branch \( u = u_\sigma \) corresponding to \( \lambda = \lambda_\sigma \). Then
\[
\lambda' = \langle u, L_{\psi, \sigma} u \rangle + \langle u, u \rangle V_{gh} + \langle u, u \rangle V_0
\]
\[
0 = \langle u, L_{\psi, \sigma} u \rangle + \langle u, u \rangle V_{gh} + \langle u, u \rangle V_0.
\]
Since each term is non-negative, we conclude that
\[
\langle u, L_{\psi, \sigma} u \rangle = \langle u, u \rangle V_{gh} = \langle u, u \rangle V_0 = 0.
\]
The last two equalities almost imply that \( u \) is a Dirichlet eigenvector of \( S^{(D)} = (\{i: \psi_i > 0\} \cup \{i: \psi_i < 0\})^{(D)} \) at \( \sigma^* \), since there may still be interaction between vertices in different nodal domains; this is rectified by the other equality \( \langle u, L_{\psi, \sigma} u \rangle = 0 \), which implies \( q_{ji} u_i + u_j = 0 \). This, together with the fact that \( u \) is an eigenvalue of \( L_{\psi, \sigma^*} \), shows that, for \( i \notin V_0 \cup V_{gh} \),
\[
(L_{\psi, \sigma^*} u)_i = \sum_{(i,j) \in E_0} w_{ij}(1 + q_{ji}) u_i + \sum_{j \in V_{gh}} w_{ij} u_i + \sum_{(i,j) \in E \setminus (E_0 \cup E_{V_0})} w_{ij}(u_i - u_j)
\]
\[
= \lambda_k u_i.
\]
\[ \square \]
In fact, we see that $L_{\psi,\sigma} u = L_{\psi,\infty} u_{\sigma^*} = \lambda_k u_{\sigma^*}$ as well, showing $u_{\sigma^*}$ is a Dirichlet eigenvector of $S^{(D)}$. The $\lambda_k$ eigenspace of $L_{\psi,\sigma^*}$ is generated by the first Dirichlet eigenvectors $\psi|_{S_i}$ of the D-connected components of $S^{(D)}$, and each of the $\psi|_{S_i}$ generate the one dimensional eigenspace for the first Dirichlet eigenvalue on $S^{(D)}_i$. Our strategy to show $u = cv \psi$ is to establish this equality for one of the components $S_i$, and then use what we know about $u$ to extend the equality to neighboring components $S_j$. The D-connectedness of $S^{(D)}$ ensures we can extend the equality to each of the D-connected components. We note that our strategy mimics the proof of the discrete nodal theorem from [5, Section 3.2].

Explicitly, we start by choosing any $i \in S_l$ with $(i, j) \in E_0, j \in S_l$, so that $S^{(D)}_l \cap S^{(D)}_j \subset V_0 \cup V_{gh}$. Next we find the constant $c$ giving $u_i = cv_i$, which determines $u|_{S_l} = cv|_{S_l}$. Since $u_j = -cq_i u_i = c \psi_j$, we get $u|_{S^{(D)}_j} = c\psi|_{S^{(D)}_j}$, and the D-connectedness of $S^{(D)}$ gives $u = c\psi$ on $S$. Finally, $u$ and $\psi$ are zero on $V_\psi \setminus S$, so indeed $u = c\psi$ at $\sigma^*$. For the second claim, note that if $\lambda_{\sigma} \neq \lambda_k$, then $u_{\sigma}$ and $\psi$ are orthogonal owing to the self-adjointness of $L_{\psi,\sigma}$: in particular, $\langle u_{\sigma}, \psi \rangle = 0$ for $\sigma \in [0, \sigma^*)$. $\sigma^* = \sup \{ \sigma: \lambda_{\sigma} < \lambda_k \}$. If the eigenvalue branch $\lambda_{\sigma}$ crosses $\lambda_k$ at $\sigma^*$ and $\lambda_{\sigma}^* = 0$, then $u_{\sigma^*} = cv$ and $\langle u_{\sigma^*}, \psi \rangle = c(\psi, \psi)$. The eigenvectors $u_{\sigma^*}$ and $\psi$ are non-trivial, so $c \neq 0$, and thus $\langle u_{\sigma^*}, \psi \rangle \neq 0$. But the inner products $\langle u_{\sigma}, \psi \rangle$ are analytic in $\sigma$ and therefore cannot have a discontinuity at $\sigma^*$. This proves the claim, that $\lambda_{\sigma}^* > 0$.

At this stage we can prove our main result: the graph spectral flow computes the nodal deficiency of a graph Laplacian eigenvector. Afterwards we present a few refinements and simplifications to the construction that allow for quick numerical implementations.

**Theorem 3.4.** As $\sigma \to \infty$, the eigenvalues of $B_\sigma$ converge to the Dirichlet eigenvalues of the D-subgraph $S^{(D)} = \{ \{ i: \psi > 0 \} \cup \{ i: \psi < 0 \} \}^{(D)}$. The number of D-connected components of $S^{(D)}$ is the multiplicity of $\lambda_k$ for $B_\infty$. 

**Proof.** Fix an eigenvalue $\lambda_k$ of the Laplacian $L$ of $G$, and call the corresponding eigenvector $\psi$.

By Propositions 2.3 and 3.1, the eigenvalue branches $\lambda_{\sigma}$ are all non-decreasing in $\sigma$, and so must either cross the line $\lambda_k$ for some finite $\sigma^*$ ($\lambda_k = \lambda_{\sigma^*}$) or approach $\lambda_k$ from below ($\lambda_{\sigma} \not\nearrow \lambda_k$ as $\sigma \to \infty$). If there is a crossing, then $\lambda_{\sigma^*} > 0$ and this eigenvalue branch converges to either a higher Dirichlet eigenvalue of $S^{(D)}$, or $\infty$. Otherwise $\lambda_{\sigma} \not\nearrow \lambda_k$, and as $\sigma \to \infty$, the eigenvectors of $B_\sigma$ have zero boundary conditions imposed on $V_0 \cup V_{gh}$. Note that this last set is precisely the vertex boundary of $\{ \psi_i > 0 \} \cup \{ \psi_i < 0 \}$. Since these eigenvectors each have eigenvalue $\lambda_k$ in the $\sigma$ limit, they must be a linear combination of the eigenvectors $\psi|_{S_i}$ for each D-connected component of $S^{(D)}$. This shows that $\lambda_k$ is the first Dirichlet eigenvalue for each $S_i$, establishing the theorem.

Our main result is a simple corollary of the theorem:

**Corollary 3.5.** The number of nodal domains of an eigenvector $\psi$ is the multiplicity of the eigenvalue $\lambda_k$ for $B_\infty$.

Recall that the nodal deficiency $\delta(\psi)$, when $\lambda_k$ is simple, is $k - \nu(\psi)$, the number of nodal domains of $\psi$. The corollary implies that each eigenvalue branch that crosses $\lambda_k$ contributes $+1$ to $\delta(\psi)$, so we expect $\delta(\psi) + |V_{gh}|$ eigenvalue branches to cross $\lambda_k$. Of course when $\lambda_k$ is repeated, $\delta(\psi) = k_* - \nu(\psi)$, with $k_* = \inf \{ s: \lambda_s = \lambda_k \}$.

**3.1. A modified spectral flow.** In the continuum spectral flow, the bilinear form $B_\sigma$ corresponds to a rank-1 perturbation of the Laplacian via a Dirac delta mass
localized to the nodal line. Here, we show how this interpretation motivates a different candidate for the graph spectral flow, which we then relate to our vertex-based flow.

To construct a graph analogue of these rank-1 perturbations, we want to perturb the Laplacian by an operator that

1. is localized to the nodal line,
2. annihilates the given eigenfunction $\psi$, and
3. is symmetric.

For simplicity we assume that $\psi$ is non-zero on every vertex; if this is not the case, perturb $\psi$ by a small amount of noise. For requirement 1), we construct $E_0$ as above and define a rank-1 family of matrices whose non-zero entries are localized to the edge indices for each $(i, j) \in E_0$. The candidate perturbation (with the required symmetry from 3)) is now $P_{ij} = \begin{pmatrix} a & b \\ b & d \end{pmatrix}$, where the indicated entries are in the $2 \times 2$ block of the $|V| \times |V|$ zero matrix. If the given eigenvector is $\psi$, requirement 2) imposes the conditions

$$\begin{cases} a\psi_i + b\psi_j = 0, \\ b\psi_i + d\psi_j = 0. \end{cases}$$

Solving this system gives $a = bq_{ji}$ and $b = dq_{ji}$. Choosing $d = q_{ij}$ results in $P_{ij} = \begin{pmatrix} q_{ji} & 1 \\ 1 & q_{ij} \end{pmatrix}$. The graph spectral flow is then the bilinear form corresponding to $L + \sigma \sum_{(i,j) \in E_0} w_{ij} P_{ij}$. Note the resemblance to Proposition 2.2.

We can construct a similar looking spectral flow that does not require an everywhere non-zero eigenfunction by focusing on the similarity to the Dirichlet boundary value problem. Based on Proposition 2.1, and the discussion after Proposition 2.2, we can compute $\nu(\lambda_k)$ without evaluating the spectral flow for $\sigma \to \infty$. The idea is that since the limiting graph should have Dirichlet boundary conditions, we impose these conditions in the original graph Laplacian in such a way that when $\sigma = 1$, the spectrum of a (simpler) bilinear form encodes the nodal deficiency. We do this in the following way: for $i \in S_l$ and $u : D^* \to \mathbb{R}$, we write the action of $L_{\psi,\infty}$ on $u$ as

$$(L_{\psi,\infty}u)_i = \sum_{(i,j) \in E \setminus (E_0 \cup E_{V_0})} w_{ij}(u_i - u_j) + \sum_{(i,j) \in E_0} w_{ij}(1 + q_{ji})u_i + \sum_{(i,j) \in E_{V_0}} w_{ij}u_i,$$

the second sum corresponds to edges that meet a ghost vertex, while the third sum corresponds to edges that meet a zero vertex of $\psi$. The Dirichlet eigenvalues of $S^{(D)}$ are the eigenvalues of $L_{\psi,\infty}$ with the columns and rows corresponding to $V_{gh}$ and $V_0$ removed. We can construct this same matrix by: taking the original graph Laplacian $L$, deleting the rows and columns corresponding to $V_0$, zeroing the entries $L_{ij}$ for $(i, j) \in E_0$ and $(i, j) \in E_{V_0}$, and finally adding the diagonal matrix $(\sum_{(i,j) \in E_0} w_{ij}q_{ji})_{ii}$. Note that this only constructs an edge-based version of $L_{\psi,\infty}$, and not any of the graph Laplacians for finite $\sigma$. For the sake of plotting the spectral flow, we add dependence on $\sigma$ through the matrices $P_{ij} = \begin{pmatrix} q_{ji} & 1 \\ 1 & q_{ij} \end{pmatrix}$ for $(i, j) \in E_0$ and $P'_{ij} = \begin{pmatrix} 0 & 1 \\ 1 & 0 \end{pmatrix}$ for $(i, j) \in E_{V_0}$. The edge based flow is then completely determined by the matrix

$$L + \sigma \sum_{(i,j) \in E_0} w_{ij} P_{ij} + \sigma \sum_{(i,j) \in E_{V_0}} w_{ij} P'_{ij},$$
Fig. 3.1. In the original graph configuration, we suppose $\psi$ is a Laplace eigenvector, $\psi_1 > 0 > \psi_2$, and $\psi_3 = 0$. The effective configuration that the edge-based Laplacian from Theorem 3.6 sees is indicated on the right.

from which we delete the rows and columns corresponding to $V_0$ and then compute the spectrum, for various $\sigma \in [0, 1]$. The corresponding bilinear form (with the $V_0$ columns and rows implicitly removed) is

$$B_\sigma(u, v) = \langle u, Lv \rangle + \sigma \sum_{(i,j) \in E_0} \langle u, w_{ij} P_{ij} v \rangle + \sigma \sum_{(i,j) \in E_{V_0}} \langle u, w_{ij} P'_{ij} v \rangle.$$ 

We summarize this construction in the next theorem.

**Theorem 3.6.** The number of nodal domains of an eigenvector $\phi_k$ with eigenvalue $\lambda_k$ is multiplicity of $\lambda_k$ in the spectrum of

$$L + \sum_{(i,j) \in E_0} w_{ij} P_{ij} + \sum_{(i,j) \in E_{V_0}} w_{ij} P'_{ij},$$

with the rows and columns corresponding to $V_0$ removed.

In Figure 3.1, we illustrate the effective edges that the operator in Theorem 3.6 sees. Restating Corollary 3.5 in this modified framework, we obtain the upper bound in Theorem 1.7.

**Corollary 3.7.** If $\phi_k \neq 0$, then $\nu(\phi_k) \leq k$.

**Proof.** Since $\phi_k \neq 0$, $V_0 = \emptyset$ and no rows or columns are removed from $L + \sum_{(i,j) \in E_0} w_{ij} P_{ij}$. This implies that this matrix has shape $|V| \times |V|$, and since $\lambda_k$ was the $k$th eigenvector, there are exactly $k$ other eigenvalues $\lambda_i \leq \lambda_k$. These eigenvalues will either flow to $\lambda_k$ or a limit strictly larger than $\lambda_k$ as $\sigma \to 1$, so the multiplicity of $\lambda_k$ in the spectrum of $L + \sum_{(i,j) \in E_{V_0}} w_{ij} P'_{ij}$ must be $\leq k$. Since the multiplicity of $\lambda_k$ is precisely $\nu(\phi_k)$, the corollary is established. \[\square\]

As an illustration of this last construction, consider again the graph $K_3$ with eigenvector $(1, -1, 0)$ from Figure 2.1. The original graph Laplacian is

$$L = \begin{pmatrix} 2 & -1 & -1 \\ -1 & 2 & -1 \\ -1 & -1 & 2 \end{pmatrix}.$$ 

Deleting the rows corresponding to $V_0 = \{3\}$, zeroing the entries $L_{ij}$ for $(i,j) \in E_0 = \{(1,2)\}$, and adding the corresponding diagonal matrix $\begin{pmatrix} 1 & 0 \\ 0 & 1 \end{pmatrix}$, gives $\begin{pmatrix} 3 & 0 \\ 0 & 3 \end{pmatrix}$. The
multiplicity of eigenvalue 3 in this last matrix is 2, which is precisely the number of nodal domains of \((1, -1, 0)\).

We chose \(K_3\) for this example to illustrate some key aspects of the construction. In the next section we provide some more complex examples showcasing the behaviour of the graph spectral flow for a variety of graphs.

### 3.2. Nodal deficiency and ghost vertices.

One feature about our vertex-based flow is that the eigenvalue branches which converge to \(\lambda_*\) almost always correspond to ghost vertices: since the flow is non-decreasing, and ghost vertices are in the kernel of \(L_{\psi,0}\), the eigenvalue branches \(\lambda_\sigma\) that converge to \(\lambda_*\) almost always satisfy \(\lambda_0 = 0\). Of course if there are more nodal domains than ghost vertices, then some of the non-zero eigenvalues will also converge to \(\lambda_*\).

This observation suggests that the topology of a graph \(G\), and in particular the collection of sign-change edges \(E_0\) and zero edges \(E_{V_0}\) for an eigenvector \(\psi\), play an important role in determining the nodal domains of \(G\).

**Open Problem.** How do the sign-change and zero edges contribute to the nodal domain counts? For each eigenvalue branch converging to \(\lambda_*\), the corresponding eigenvector will converge to a linear combination of first Dirichlet eigenvectors for each \(D\)-connected domain of \(G\): what do the eigenvectors tell us about the nodal domains, and how does the graph topology determine which sign-change and zero edges give rise to eigenvectors of \(L_{\psi,\infty}\)?

### 4. Examples.

In this section we provide some examples of both the subdivision process and spectral flow for some common types of graphs. For some of these graphs we can explicitly state what the spectrum is, and we state these without proof; see [6] for details.

#### 4.1. Complete graphs.

For a complete graph on \(n\) vertices, denoted \(K_n\), we label the vertices \(\{1, 2, ..., n\}\) and add in all edges \((i, j), 1 \leq i < j \leq n\). The spectrum of the graph Laplacian is \(\{0, n, ..., n\}\), with \(n\) repeated \(n - 1\) times, and the (complex valued) eigenvectors are \((1, \xi, \xi^2, ..., \xi^{n-1})\) for roots of unity \(\xi^n = 1\), both facts due to the graph Laplacian being circulant; see any text on matrix analysis, such as [1, Chapter 12], for details.

In Figure 4.1, we display the eigenvectors and spectral flows corresponding to \(\lambda_2\) and \(\lambda_3\). The top row shows the second Laplace eigenvector for \(K_5\), followed by the edge-based and vertex-based flows. The first plot shows the eigenvector’s values on each vertex. The next two plots show the spectral flow for the edge-based and vertex-based flows, respectively. We show all eigenvalue branches for the sake of illustration, but of particular note is the fact that only two of the branches converge to 5, and the rest quickly diverge from the line \(\lambda_k = 5\). For the vertex-based flow, we have eigenvalue branches corresponding to the original vertices as well as the ghost vertices; one of the two branches that limits to 5 originated as a zero eigenvalue, corresponding to one of the ghost vertices. In Figure 4.1 we display the same plots using the third Laplace eigenvector.

#### 4.2. Cyclic graphs.

The cyclic graph on \(n\) vertices, denoted \(C_n\), has vertices \(\{1, 2, ..., n\}\), and edges \((i, i + 1)\) for \(1 \leq i < n\), and \((n, 1)\). The spectrum of \(C_n\) is \(\{2 - 2 \cos\left(\frac{2\pi j}{n}\right)\}_{j=0}^{n-1}\). Accordingly, each eigenvalue has multiplicity 2.

In Figure 4.2, we show the second Laplace eigenvector for \(C_5\), the cyclic graph on five vertices. In the edge-based flow plot (middle), we show the flow of all five eigenvalues branches for \(C_5\), as well as the vertex-based flow (right). Examining the
Fig. 4.1. The second (top row) and third (bottom row) eigenvector of the graph Laplacian for $K_5$, along with their edge-based (middle column) and vertex-based (right column) spectral flows. Note that in the edge-based flow for the second eigenvector (middle top row), only four eigenvalue branches appear. This is because we delete the row and column corresponding to the zero of the eigenvector. In the edge-based flow for the third eigenvector (middle bottom), only three eigenvalue branches appear; the other two are hidden by the eigenvalue branch above $\lambda_3$.

Fig. 4.2. The edge-based (middle) and vertex-based (right) spectral flows for an eigenvector of the graph Laplacian for $C_5$ (left).

function plot suggests this eigenvector has 2 nodal domains, which is verified in the spectral flows via 2 eigenvalue branches converging to the second eigenvalue.

In Figure 4.3 (top left), we consider the cyclic graph on 31 vertices and compute the number of nodal domains each eigenvector has. Since the eigenvectors all have the form $(1, \xi, \xi^2, ..., \xi^{30})$ with $\xi^{31} = 1$, taking the real and imaginary parts will produce two real valued eigenvectors with the same number of nodal domains. This can be seen explicitly in the scatter plot of nodal domains.

4.3. Petersen graphs. A generalized Petersen graph $GP(n, m)$ for $n \geq 3$ and $1 \leq m \leq \lfloor \frac{n-1}{2} \rfloor$ consists of $2n$ vertices $\{a_0, ..., a_{n-1}, b_0, ..., b_{n-1}\}$, with edges of the form $(a_i, a_{i+1})$, $(a_i, b_i)$, and $(b_i, b_{i+m})$ for $0 \leq i \leq n-1$, where the sums are considered modulo $n$. Some basic properties of these graphs are described in [12].

In Figure 4.4, we show the edge-based and vertex-based spectral flows for the 7th and 8th eigenvectors of $GP(7, 3)$. Examining the two plots of the eigenvectors (top row), we count 3 nodal domains for each. However, both the edge-based (middle column) and vertex-based (right column) spectral flows seem to suggest that there should be 4 nodal domains, since 4 eigenvalue branches converge to $\lambda_s \approx 2.915$. When we zoom in to the edge-based spectral flow of the 7th eigenvector near $\sigma = 1$.
Fig. 4.3. Black dots correspond to the number of nodal domains for each eigenvector of $C_{31}$ (top left), $GP(7, 3)$ (top right), $I_7$ (bottom left), $I_7, 5$ (bottom right), and black dots are connected by a line if they correspond to the same eigenvalue. The red line is the curve $y = x$; an eigenvector’s nodal deficiency is the vertical distance between the left-most black dot it is connected to, and the red line.

(Figure 4.5), we see that a crossing does in fact occur, causing the actual final nodal domain count to be correct; in the vertex-based flow, the crossing occurs near $\sigma = 600$. This example suggests that the interplay between the numerics and analysis of the spectral flow is more subtle than we might expect, since crossings in the edge-flow may occur close to the limit $\sigma = 1$. Also note that in the vertex-based flows, only eigenvalue branches coming from ghost points converge to $\lambda_3$ from below; all other eigenvalue branches, especially those from $\text{Spec}(L)$, cross $\lambda_3$. In general, we have that if $|E_0| > |V|$, then all of the limiting eigenvalues originate from ghost vertices. Otherwise, some of the limiting eigenvalues may be branches from eigenvalues of $L$, depending on the nodal count and $|E_0|$.

Finally, Figure 4.3 (top right) displays the nodal domain counts for each eigenvector of $GP(7, 3)$. Note that eigenvectors 7 and 8 have 3 nodal domains each, as verified by Figure 4.4.

4.4. 1- and 2-d intervals. In this section we consider interval graphs $I_n$, and graph analogues of rectangles $I_{n,m}$. The vertices of $I_n$ are \{1, 2, ..., $n$\}, and the edges are $(i, i+1)$ for $1 \leq i \leq n - 1$. For $I_{n,m}$, we have vertices \{$v_{1,1}, v_{1,n}, v_{2,1}, ..., v_{n,m}$\}, and edges of the form $(v_{i,j}, v_{i,1})$ and $(v_{i,j}, v_{i+,1})$ for all possible $i$ and $j$.

The spectrum of $I_n$ is well-known, and is $(2 - 2\cos(\frac{j\pi}{n}))_{j=0}^{n-1}$; a simple argument involving a “doubled” interval and the spectrum of $C_{2n}$ is given in [6]. In Figures 4.3 and 4.6 we display the nodal domain count of $I_7$ (bottom left), and the spectral flow for the third eigenvector of $I_7$, respectively. Note that, as suggested by the continuum Sturm-Liouville theory, the eigenvectors of $I_7$ have zero nodal deficiency, since three eigenvalue branches converge to $\lambda_3$. In the vertex-based flow, the two eigenvalue branches converging to $\lambda_3$ come from ghost points, and all other eigenvalue branches cross.

For the spectrum of $I_{n,m}$, we can take two eigenvectors $\phi_k, \psi_j$ of $I_k, I_j$, with corresponding eigenvalues $\lambda_k, \lambda_j$, and define a Laplace eigenvector $\phi_k \otimes \psi_j$ on $I_{n,m}$ with eigenvalue $\lambda_k \lambda_j$. These new eigenvectors are orthogonal to each other, and there are $nm$ of them, so we explicitly construct the eigenspaces of $I_{n,m}$’s Laplacian; that
we also get the corresponding eigenvalues as a bonus. Since the eigenvalues of \( I_{n,m} \) are all possible (outer) products of eigenvectors of \( I_n \) and \( I_m \), we cannot expect that the nodal deficiency is always zero. Figure 4.3 (bottom right) confirms this, which displays the number of nodal domains for each eigenvector of \( I_{7,5} \). In Figure 4.7, we display two views of the fifth eigenvector of \( I_{7,5} \), together with its spectral flows.

**4.5. Erdos-Renyi random graphs.** Erdos-Renyi graphs on \( n = 20 \) vertices were sampled with edge probabilities \( p = 0.1, 0.3, 0.5, 0.7, 0.9, 0.95 \), and the number of nodal domains for each sample’s eigenvectors were computed. Figure 4.8 displays some random graphs with the third eigenvector displayed (first row, third row), along with the scatter plots showing the corresponding number of nodal domains (second row, fourth row). The nodal domain plots suggest that for smaller edge probabilities the random graphs more closely resemble intervals, whereas for higher edge probabilities the random graphs more closely resemble complete graphs.

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Fig. 4.6. The spectral flow for the third eigenvector of the interval graph $I_7$. We display the eigenvector (left), along with its edge-based (middle) and vertex-based (right) spectral flows. The eigenvector graph shows three nodal domains, and each of the spectral flows have three eigenvalue branches converging to $\lambda_3 = 2(1 - \cos(\frac{2\pi}{7})) \approx 0.753$.

Fig. 4.7. The spectral flow for the fifth eigenvector of the interval graph $I_{7,5}$. The eigenvector is displayed (left) along with the edge-based (middle) and vertex-based (right) spectral flows. This eigenvector has three nodal domains, and both the edge- and vertex-based flows have 3 eigenvalues less than or equal to $\lambda_5$ in the limit.
Fig. 4.8. Various Erdos-Renyi random graphs with nodal domain counts for each eigenvector plotted below; the graphs correspond to edge probabilities (clockwise order) $p = 0.1, 0.3, 0.5, 0.7, 0.9, 0.95$. As the probability that an edge connects vertices increases, the spectral flow is able to detect that they are closer to being a complete graph than an interval.

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