

Spectral decimation of piecewise centrosymmetric Jacobi operators on graphs

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Abstract. We study the spectral theory of a class of piecewise centrosymmetric Jacobi operators defined on an associated family of substitution graphs. Given a finite centrosymmetric matrix viewed as a weight matrix on a finite directed path graph and a probabilistic Laplacian viewed as a weight matrix on a locally finite strongly connected graph, we construct a new graph and a new operator by edge substitution. Our main result proves that the spectral theory of the piecewise centrosymmetric Jacobi operator can be explicitly related to the spectral theory of the probabilistic Laplacian using certain orthogonal polynomials. Our main tools involve the so-called spectral decimation, known from the analysis on fractals, and the classical Schur complement. We include several examples of self-similar Jacobi matrices that fit into our framework.

1. Introduction

The aim of this paper is to introduce and study the spectral theory of a new class of Jacobi operators on substitution graphs, inspired by B. Simon et al. [17, 31]. Our main results include the determination of the spectrum, spectral gaps, the type of the spectral measures, and the eigenvalue counting function for a large new class of finite and infinite substitution graphs. This class provides a new framework to study physically relevant graph Laplacians, e.g. self-similar versions of almost Mathieu-type operators [56]. In comparison to the previous literature, the appearance of orthogonal polynomials is a significant new idea in the context of the classical spectral decimation.

Our work is part of a long term study of mathematical physics on fractals and graphs, more specifically, quantum Hall systems with AMO and their topological

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quantum phases [1–6, 8–14, 27, 29, 33, 34, 37, 44, 54, 55, 59–62], in which novel features of physical systems can be associated with the unusual spectral and geometric properties of fractals and graphs compared to smooth manifolds.

Given a finite centrosymmetric matrix viewed as a weight matrix on a finite directed path graph and a probabilistic Laplacian viewed as a weight matrix on a locally finite strongly connected direct graph, we construct a new (possibly high dimensional, large or infinite) graph and a new operator that acts as a weight matrix on this graph. In a sense that will be made precise, this graph can be viewed as a result of a substitution procedure involving the initial graphs, and as such will be referred to as a substitution graph. Further, the new operator, which we call a piecewise centrosymmetric Jacobi operator acts on the space of square summable functions defined on the vertices of the substitution graph.

The construction of the substitution graphs allows us to show that these spectra are related to the spectra of the initial finite centrosymmetric matrices and can be determined using the spectral decimation method popularized in mathematical physics and analysis on fractals beginning with work of Rammal and Toulouse [63, 64]. This method is equivalent to the classical Dirichlet to Neumann map and Schur complement, see [12, 19, 23, 24, 27, 40, 50, 53, 54] and references therein. We make an explicit link between the classical spectral theory and the spectral decimation method through the analysis of families of orthogonal polynomials. We conclude the paper with several examples of one-dimensional graphs that fit into our framework. These self-similar graphs are obtained using a substitution method starting from a pair of initial graphs and this framework allows us to consider finite and infinite self-similar graphs defined in one or higher dimensions. The Jacobi operators are then defined so as to respect the adjacency relations in the resulting graph, and can be naturally viewed as weight matrices on the graphs. Thus, we say that a matrix $\mathbf{J} = (\mathbf{J}(x, y))$ is a *Jacobi matrix* if \mathbf{J} reflects the adjacency relations of the graph G , where $x, y \in V(G)$ and $G = (V(G), E(G))$ is a graph. For two different vertices $x, y \in V(G)$, we set $\mathbf{J}(x, y) = 0$, whenever x and y are not adjacent, i.e., $(x, y) \notin E(G)$; see [17] for a definition of Jacobi matrices on periodic trees.

We begin with previewing the substitution method to define the graphs of interest, and refer to Section 2 for more details. We first introduce the two initial inputs of the method: the *building block graph* G_{cs} and the *model graph* G_p .

(a) The building block graph G_{cs} . Let \mathbf{J}_{cs} be a finite tridiagonal matrix and assume that \mathbf{J}_{cs} is centrosymmetric, i.e. $\mathbf{J}_{cs} = R \mathbf{J}_{cs} R$, where R is an anti-diagonal identity

matrix

$$R = \begin{pmatrix} 0 & 0 & \dots & 0 & 0 & 1 \\ 0 & 0 & \dots & 0 & 1 & 0 \\ 0 & 0 & \dots & 1 & 0 & 0 \\ \vdots & \vdots & & \vdots & \vdots & \vdots \\ 0 & 1 & \dots & 0 & 0 & 0 \\ 1 & 0 & \dots & 0 & 0 & 0 \end{pmatrix}.$$

We regard \mathbf{J}_{cs} as the weight matrix of a finite directed path graph G_{cs} , in the sense that the diagonal and off-diagonal entries in \mathbf{J}_{cs} respectively denote the weights assigned to the vertices and edges of G_{cs} . We note that centrosymmetric matrices have a rich eigenstructure and appear in several applications [15, 18, 28, 32, 35, 52, 57, 58, 81, 86, 87]. Figure 1 shows an example of a building block graph G_{sc} associated with the centrosymmetric matrix \mathbf{J}_{cs} .

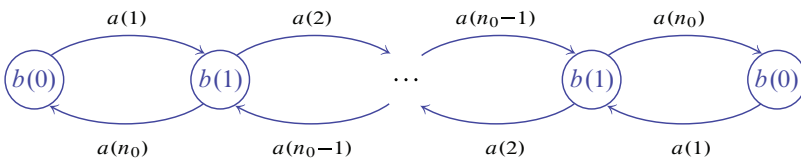


Figure 1. A finite directed weighted path graph G_{cs} . The weights associated with the edges and vertices are the entries of a centrosymmetric Jacobi matrix \mathbf{J}_{cs} .

(b) The model graph G_p . Let G_p be a locally finite connected directed graph. We consider a random walk on G_p and therefore assume that the weight matrix of G_p is given by a *probabilistic graph Laplacian*

$$\Delta_{\mathbf{p}} f(x) = f(x) - \sum_{y:(x,y) \in E(G_p)} p(x,y) f(y),$$

where $\mathbf{p} = \{p(x,y)\}_{(x,y) \in E(G_p)}$ is a given sequence of transition probabilities. Note that if we consider a symmetric random walk on G_p , then $\Delta_{\mathbf{p}}$ becomes the standard probabilistic graph Laplacian. Throughout this work, we fix G_p and assume that $\Delta_{\mathbf{p}}$ is a probabilistic graph Laplacian on G_p .

Using the building block graph G_{cs} and the model graph G_p we obtain the substitution graphs as follows.

(c) The substitution graphs. Given a building block G_{cs} and a model graph G_p , we construct a new graph $G = (V(G), E(G))$ by substituting copies of G_{cs} between adjacent vertices in G_p . Figure 2 shows an example of a substitution graph starting

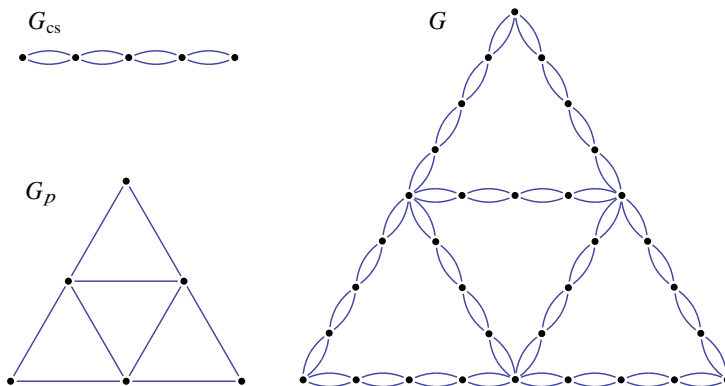


Figure 2. Let G_{cs} be a finite directed weighted path graph associated with a centrosymmetric Jacobi matrix \mathbf{J}_{cs} of Figure 1. Let G_p be a finite graph approximation of a Sierpinski lattice. We construct a new graph $G = (V(G), E(G))$ by substituting copies of the graph G_{cs} between adjacent vertices in G_p . The weight matrix of the graph G will be given by $\mathbf{J} := F_{G_p}(\Delta_p, \mathbf{J}_{cs})$ and is an example of a piecewise centrosymmetric Jacobi operator on G .

from the building block graph G_{cs} of Figure 1. For a choice of the probabilistic Laplacian Δ_p of G_p , the weight matrix of the newly constructed graph G is given by a *substitution operator*

$$(\Delta_p, \mathbf{J}_{cs}) \mapsto F_{G_p}(\Delta_p, \mathbf{J}_{cs}),$$

which will be formally introduced in Definition 2.5. The substitution operator assigns to each pair $(\Delta_p, \mathbf{J}_{cs})$ a Jacobi matrix on the graph G , which we denote by $\mathbf{J} := F_{G_p}(\Delta_p, \mathbf{J}_{cs})$ and refer to as a *piecewise centrosymmetric Jacobi operator* on G . That the substitution operator is well defined is a consequence of the symmetry assumption on \mathbf{J}_{cs} . In addition, as we will see later, this symmetry assumption is key in establishing many of our results.

The paper is organized as follows. In Section 2, we define the substitution graph and operator associated with a fixed graph G_p and a building block graph G_{cs} . We show that each element in the range of the latter can be identified with a piecewise centrosymmetric Jacobi operator. Proposition 2.8 summarizes some of the relevant properties of the substitution operator.

In Section 3 we begin the spectral analysis of the centrosymmetric matrix \mathbf{J}_{cs} and connects it to the analysis of a related family of polynomials and rational functions. This is summarized in our first main result, Theorem 3.3 which allows us to find a relatively simple formula for the Schur complement of \mathbf{J}_{cs} . Consequently, the spectral analysis of the piecewise centrosymmetric Jacobi operators $\mathbf{J} = F_{G_p}(\Delta_p, \mathbf{J}_{cs})$ can be investigated in the realm of the *spectral decimation method*, a standard framework in

the analysis on fractals. Developed in the 1980s [7, 21, 36, 63, 64], the spectral decimation method attracted considerable attention over the last decades [20, 42, 49, 67–69, 75, 77, 78, 82]. For an overview of some modern approach to the spectral decimation method, we refer to [48, 53, 76, 77, 80].

The framework for the spectral decimation method developed in [53] is the one that is most suited for the piecewise centrosymmetric Jacobi operators. Using it along with a set of assumptions (Assumption 4.4) we obtain one of our other main results, Theorem 4.7, which gives a description of the spectrum of $\mathbf{J} = F_{G_p}(\Delta_{\mathbf{p}}, \mathbf{J}_{cs})$. The essence of this result is that it relates the spectra $\sigma(\mathbf{J})$, $\sigma(\Delta_{\mathbf{p}})$, and an *exceptional set* $\mathcal{E}_{\mathbf{J}_{cs}}$ that appears naturally in the spectral decimation method. The link between these sets is obtained using a polynomial, *the spectral decimation function* $R_{\mathbf{J}_{cs}}$ that we are able to explicitly calculate. Furthermore, we prove that the resolvent operators of \mathbf{J} and $\Delta_{\mathbf{p}}$ satisfy the renormalization group identity given in (14). This result is related to [25, Theorem 2.2] and Bellissard's work on quasicrystals [21, Theorem 1], although we do not rely on them. However, the connections and differences between our framework and Bellissard's are elaborated in [56, Section 6].

Section 3 is divided into two parts. The first part deals with the spectral analysis of a centrosymmetric matrix \mathbf{J}_{cs} , to which is associated two families of polynomials. Using these polynomials, we compute in Theorem 3.3 the Schur complement of \mathbf{J}_{cs} , and identify the polynomial $R_{\mathbf{J}_{cs}}(z)$ as a spectral decimation function. Subsequently, the second part of Section 3 is devoted to an analysis of $R_{\mathbf{J}_{cs}}(z)$. In particular, we relate the preimages of the points $\{0, 2\}$ under $R_{\mathbf{J}_{cs}}$ to the exceptional set $\mathcal{E}_{\mathbf{J}_{cs}}$, determine the critical points of $R_{\mathbf{J}_{cs}}(z)$ thereby establishing the existence of the branches of the inverse $R_{\mathbf{J}_{cs}}^{-1}$ in the domain $[0, 2]$. These results are summarized in Theorem 3.6. Section 4 contains the main results on the spectra of piecewise centrosymmetric matrices. More specifically, in Proposition 4.6 we prove the spectral similarity between \mathbf{J} and $\Delta_{\mathbf{p}}$ and determine the exceptional set $\mathcal{E}_{\mathbf{J}_{cs}}$. We then prove our main result, Theorem 4.7 which gives a complete description of the spectrum of the piecewise centrosymmetric Jacobi operator \mathbf{J} . Finally, in Section 5, we illustrate our results by focussing on one-dimensional path graphs which corresponds to the classical Jacobi matrices.

2. Weighted substitution with centrosymmetric Jacobi matrices

This section introduces the main concepts of the paper, namely the definition of the substitution graph and operator.

2.1. Centrosymmetric Jacobi matrices

Suppose $G_{cs} = (V(G_{cs}), E(G_{cs}))$ is a finite directed weighted path graph with vertices $V(G_{cs})$ and edges $E(G_{cs})$. We assume that G_{cs} consists of $n_0 + 1$ vertices for $n_0 \geq 1$, and denote the vertices by $V(G_{cs}) = \{0, 1, \dots, n_0\}$. The set of edges is then given by $E(G_{cs}) = \{(i, i + 1) \mid i \in \{0, \dots, n_0 - 1\}\} \cup \{(i + 1, i) \mid i \in \{0, \dots, n_0 - 1\}\}$. We describe the weights assigned to the vertices and edges by the following $(n_0 + 1) \times (n_0 + 1)$ centrosymmetric Jacobi matrix

$$\mathbf{J}_{cs} := \begin{pmatrix} b(0) & a(1) & 0 & \dots & 0 \\ a(n_0) & b(1) & a(2) & \dots & 0 \\ 0 & a(n_0 - 1) & b(2) & \ddots & \vdots \\ \vdots & \vdots & \ddots & \ddots & a(n_0) \\ 0 & 0 & 0 & a(1) & b(0) \end{pmatrix}. \tag{1}$$

The boundary and interior vertices of G_{cs} are given by

$$\partial G_{cs} := \{0, n_0\} \quad \text{and} \quad V(G_{cs}) \setminus \partial G_{cs} = \{1, \dots, n_0 - 1\},$$

respectively. In the sequel, the class of centrosymmetric Jacobi matrices will be denoted by

$$\mathcal{CSJ} := \{\mathbf{J}_{cs} \mid \mathbf{J}_{cs} \text{ is centrosymmetric of the form (1), where } n_0 \geq 1\}.$$

2.2. Probabilistic graph Laplacians

Suppose $G_p = (V(G_p), E(G_p))$ is a locally finite (strongly) connected directed graph. Let $\{p(x, y)\}_{(x,y) \in E(G_p)}$ be a sequence of weights assigned to the directed edges. The edge (x, y) points from the vertex x to y and we regard $p(x, y)$ as a transition probability from x to y . We impose the following conditions:

$$\begin{cases} (x, y) \in E(G_p) \iff 0 < p(x, y) \leq 1, \\ (x, y) \notin E(G_p) \iff p(x, y) = 0, \\ \sum_{y:(x,y) \in E(G_p)} p(x, y) = 1 \quad \text{for all } x \in V(G_p). \end{cases} \tag{2}$$

Definition 2.1. Let $\mathbf{p} = \{p(x, y)\}_{(x,y) \in E(G_p)}$ be a given sequence of transition probabilities, i.e. \mathbf{p} satisfies the conditions in (2). The probabilistic graph Laplacian on the graph G_p associated to \mathbf{p} is defined by

$$\Delta_{\mathbf{p}} f(x) = f(x) - \sum_{y:(x,y) \in E(G_p)} p(x, y) f(y), \tag{3}$$

where $f \in \ell(G_p) := \{f: V(G_p) \rightarrow \mathbb{C}\}$ and $x \in V(G_p)$.

The collection of all probabilistic Laplacians on a fixed graph G_p is denoted by

$$\mathcal{L}_{G_p} := \{\Delta_{\mathbf{p}} \mid \Delta_{\mathbf{p}} \text{ defined in (3), } \mathbf{p} = \{p(x, y)\}_{(x,y) \in E(G_p)} \text{ satisfies (2)}\}.$$

Remark 2.2. The third equation in the conditions (2) arises naturally in different contexts and applications [38, 43, 46, 47]. It is related to the consistency condition in [78, equation (1.4)], where Strichartz utilizes the electrical network interpretation of the weights. This condition is also found in [57, Assumption 2.8], in the framework of Toda-lattices on fractal-type graphs as one of the sufficient conditions leading to the existence of static soliton solutions on such graph. This condition also makes it a Markov chain that later helps us to apply the Kolomogorov’s condition to establish operators of interest as self-adjoint.

Throughout the paper, we make the following assumption on G_p .

Assumption 2.3. We assume that if $(x, y) \in E(G_p)$, then, so is $(y, x) \in E(G_p)$ and we refer to $x, y \in V(G_p)$ as adjacent vertices. Note that in general, the transition probabilities $p(x, y)$ and $p(y, x)$ are not equal.

2.3. Weighted edge substitution operator

We construct a new graph $G = (V(G), E(G))$ by starting from G_p , then substituting copies of a graph G_{cs} between adjacent vertices in G_p . We refer to [78] for similar constructions. Now, recall that the vertices and boundary vertices of G_{cs} are given by $V(G_{cs}) = \{0, 1, \dots, n_0\}$ and $\partial G_{cs} = \{0, n_0\}$, respectively. Let $(x, y) \in E(G_p)$ (hence $(y, x) \in E(G_p)$) for some $x, y \in V(G_p)$. We replace the edges (x, y) and (y, x) in the graph G_p with a copy of G_{cs} , by identifying x with 0 and y with n_0 . Equivalently, we can identify x with n_0 and y with 0, due to the centrosymmetry assumption on G_{cs} and in either case, the resulting graph G is the same. We distinguish two types of vertices in the graph G . The vertices which we obtain from G_p and therefore being just $V(G_p)$ and the vertices that are obtained from G_{cs} through the substitution procedure. The edges of the graph G are exactly the edges in each copy of G_{cs} . We construct a Jacobi matrix on the graph G , and view it as the graph weight matrix. We refer to [17] for a similar definition.

Definition 2.4. A Jacobi matrix on a graph $G = (V(G), E(G))$ is a matrix $\mathbf{J} = (\mathbf{J}(x, y))_{x,y \in V(G)}$ indexed by the vertices $V(G)$, such that $\mathbf{J}(x, y) = 0$ whenever $(x, y) \notin E(G)$ and $x \neq y$. We denote the set of all Jacobi matrices on graphs by

$$\mathcal{J} := \{\mathbf{J} \mid \mathbf{J} \text{ is a Jacobi matrix on a graph}\}.$$

Note that there are no specific requirements on $J(x, y)$ in the cases $(x, y) \in E(G)$ or $x = y$, and $J(x, y)$ can be zero or not.

Definition 2.5 (Substitution operator). Fix a graph G_p as defined in Section 2.2. A substitution operator associated with G_p is the mapping F_{G_p} given by

$$F_{G_p}: \mathcal{L}_{G_p} \times \mathcal{CSJ} \rightarrow \mathcal{J}, \quad (\Delta_{\mathbf{p}}, \mathbf{J}_{cs}) \mapsto F_{G_p}(\Delta_{\mathbf{p}}, \mathbf{J}_{cs}),$$

where $F_{G_p}(\Delta_{\mathbf{p}}, \mathbf{J}_{cs})$ is defined as follows. Let G_{cs} be the graph associated to the centrosymmetric matrix \mathbf{J}_{cs} and $G = (V(G), E(G))$ is the resulting substitution graph. The substitution procedure naturally induces a *covering map*, which we denote by $\phi: V(G) \rightarrow V(G_{cs})$ (each vertex in G is in a copy of G_{cs} and hence corresponds naturally to a vertex in G_{cs}).

- (1) $J := F_{G_p}(\Delta_{\mathbf{p}}, \mathbf{J}_{cs})$ is a Jacobi matrix on the graph G . The diagonal entries are given by

$$\mathbf{J}(x, x) := \mathbf{J}_{cs}(\phi(x), \phi(x)), \quad x \in V(G).$$

- (2) Each $(x, y) \in E(G)$ is associated with an edge $(\phi(x), \phi(y))$ in a copy of G_{cs} and suppose that this copy replaced the edges between the vertices, say $u, v \in V(G_p)$. Then we set

$$\begin{cases} \mathbf{J}(x, y) := p(u, v) \mathbf{J}_{cs}(0, 1) & \text{if } x = u, \\ \mathbf{J}(x, y) := \mathbf{J}_{cs}(\phi(x), \phi(y)) & \text{if } x \notin V(G_p). \end{cases} \quad (4)$$

Remark 2.6. In the particular case $n_0 = 1$, we have $V(G_p) = V(G)$. Moreover, if we choose Δ_0 for the Jacobi matrix \mathbf{J}_{cs} , where

$$\Delta_0 := \begin{pmatrix} 1 & -1 \\ -1 & 1 \end{pmatrix}. \quad (5)$$

then the Substitution formula (4) gives $\mathbf{J} = \Delta_{\mathbf{p}}$. This implies that the graphs G and G_p are identical.

Definition 2.7. Let $\mathbf{J} \in \mathcal{J}$. If there exist a graph G_p , and a probabilistic Laplacian $\Delta_{\mathbf{p}} \in \mathcal{L}_{G_p}$ and $\mathbf{J}_c \in \mathcal{CSJ}$, such that $\mathbf{J} = F_{G_p}(\Delta_{\mathbf{p}}, \mathbf{J}_c)$, then we call \mathbf{J} a piecewise centrosymmetric Jacobi operator.

We end this section by summarizing the key properties of the substitution operator that will be needed in the sequel.

Proposition 2.8. *The following statements follow from the (4).*

- (1) $F_{G_p}(\Delta_{\mathbf{p}}, \Delta_0) = \Delta_{\mathbf{p}}$, (where Δ_0 is defined in (5)).
- (2) $F_{G_p}(\Delta_0, \mathbf{J}_{cs}) = \mathbf{J}_{cs}$.
- (3) $F_{G_p}(\Delta_{\mathbf{p}}, I) = I$, where the identity matrices I might be of different size.

(4) Let $\mathbf{J}_{\text{cs}}^{(1)}$ and $\mathbf{J}_{\text{cs}}^{(2)}$ be elements of $\mathcal{CS}\mathcal{J}$ and of the same size. Then for $\lambda, \mu \in \mathbb{C}$, we have

$$F_{G_p}(\Delta_{\mathbf{p}}, \lambda \mathbf{J}_{\text{cs}}^{(1)} + \mu \mathbf{J}_{\text{cs}}^{(2)}) = \lambda F_{G_p}(\Delta_{\mathbf{p}}, \mathbf{J}_{\text{cs}}^{(1)}) + \mu F_{G_p}(\Delta_{\mathbf{p}}, \mathbf{J}_{\text{cs}}^{(2)}).$$

3. Orthogonal polynomials and centrosymmetric Jacobi matrices

In this section we elaborate on the connection between the centrosymmetric Jacobi matrices and a family of orthogonal polynomials.

3.1. Schur complement of centrosymmetric Jacobi matrices

The connection between orthogonal polynomials and the spectral theory proved fruitful during the last few decades and generated considerable interest among various communities of researchers. Our reference list is by no means exhaustive, and we refer the reader for instance to Simon’s treatises and the references therein [22, 26, 39, 70–72, 85]. The objective of this section is to reinterpret concepts from the spectral decimation technique in terms of orthogonal polynomials. Because we are dealing with Jacobi matrices, orthogonal polynomials naturally arise through the associated three-term recurrence relations. For us, two cases are relevant, namely the three-term recurrence relations corresponding to the centrosymmetric Jacobi matrices \mathbf{J}_{cs} and the restriction of \mathbf{J}_{cs} to the interior vertices of G_{cs} , which we denote by \mathbf{J}_{cs}^D . Note that when dealing with \mathbf{J}_{cs}^D we assume $n_0 \geq 2$ as \mathbf{J}_{cs}^D is the interior block matrix of \mathbf{J}_{cs} ,

$$\mathbf{J}_{\text{cs}} = \left(\begin{array}{c|ccc|c} b(0) & a(1) & 0 & \dots & 0 \\ \hline \vdots & & \mathbf{J}_{\text{cs}}^D & & \vdots \\ \hline 0 & \dots & 0 & a(1) & b(0) \end{array} \right).$$

We regard \mathbf{J}_{cs} as a matrix acting on $\ell(V(G_{\text{cs}})) = \ell(\{0, 1, \dots, n_0\})$, where $\ell(I)$ denotes the linear space of \mathbb{C} -valued functions $\ell(I) := \{f: I \rightarrow \mathbb{C}\}$ for a set I . In particular, \mathbf{J}_{cs}^D acts on $\ell(\{1, \dots, n_0 - 1\})$. Throughout this section, we suppose that $\mathbf{J}_{\text{cs}} \in \mathcal{CS}\mathcal{J}$ is fixed for some $n_0 \geq 2$ and $a(k) \neq 0$ for each $k = 0, \dots, n_0 + 1$. We introduce a sequence of monic polynomials $P_0(z), P_1(z), \dots, P_{n_0+1}(z)$ corresponding to \mathbf{J}_{cs} as follows. We initialize $P_0(z) := 1$ and $P_1(z) := z - b(0)$. For $k \in \{2, \dots, n_0 + 1\}$, we define $P_k(z)$ to be the determinant of the leading principal

$k \times k$ submatrix of $zI - \mathbf{J}_{cs}$, i.e.,

$$P_k(z) := \det \begin{pmatrix} z - b(0) & -a(1) & 0 & \dots & 0 \\ -a(n_0) & z - b(1) & -a(2) & \dots & 0 \\ 0 & -a(n_0 - 1) & z - b(2) & \ddots & \vdots \\ \vdots & \vdots & \ddots & \ddots & -a(k - 1) \\ 0 & 0 & 0 & -a(n_0 + 2 - k) & z - b(k - 1) \end{pmatrix}.$$

Note that $P_{n_0+1}(z) = \det(zI - \mathbf{J}_{cs})$ is the characteristic polynomial of \mathbf{J}_{cs} whose eigenvalues are the zeros of $P_{n_0+1}(z)$. It can be easily shown that the sequence of polynomials $P_0(z), P_1(z), \dots, P_{n_0+1}(z)$ satisfies the following recurrence relations:

$$\begin{cases} P_0(z) = 1, & P_1(z) = z - b(0), \\ P_k(z) = (z - b(k - 1))P_{k-1}(z) - a(k - 1)a(n_0 + 2 - k)P_{k-2}(z), \end{cases} \tag{6}$$

for $k \in \{2, \dots, n_0 + 1\}$. Similarly, for the Jacobi matrix \mathbf{J}_{cs}^D , we initialize $P_0^D(z) := 1$ and $P_1^D(z) := z - b(1)$. For $k \in \{2, \dots, n_0 - 1\}$, we define $P_k^D(z)$ to be the determinant of the leading principal $k \times k$ submatrix of $zI - \mathbf{J}_{cs}^D$, i.e.,

$$P_k^D(z) := \det \begin{pmatrix} z - b(1) & -a(2) & 0 & \dots & 0 \\ -a(n_0 - 1) & z - b(2) & -a(3) & \dots & 0 \\ 0 & -a(n_0 - 2) & z - b(3) & \ddots & \vdots \\ \vdots & \vdots & \ddots & \ddots & -a(k) \\ 0 & 0 & 0 & -a(n_0 + 1 - k) & z - b(k) \end{pmatrix},$$

where in this case $P_{n_0-1}^D(z) = \det(zI - \mathbf{J}_{cs}^D)$ is the characteristic polynomial of \mathbf{J}_{cs}^D . The sequence $P_0^D(z), P_1^D(z), \dots, P_{n_0-1}^D(z)$ satisfies the recurrence relations

$$\begin{cases} P_0^D(z) = 1, & P_1^D(z) = z - b(1), \\ P_k^D(z) = (z - b(k))P_{k-1}^D(z) - a(k)a(n_0 + 1 - k)P_{k-2}^D(z), \end{cases} \tag{7}$$

for $k \in \{2, \dots, n_0 - 1\}$.

We first prove auxiliary lemmas.

Lemma 3.1. *The following identities hold:*

$$(1) \quad P_1^D(z)P_1(z) - P_0^D(z)P_2(z) = a(1)a(n_0);$$

(2) for $n_0 \geq 2$ and $k \in \{2, \dots, n_0\}$,

$$\begin{aligned} P_k^D(z)P_k(z) - P_{k-1}^D(z)P_{k+1}(z) \\ = a(n_0 + 1 - k)a(k)(P_{k-1}^D(z)P_{k-1}(z) - P_{k-2}^D(z)P_k(z)); \end{aligned}$$

(3) $P_{n_0-1}^D(z)P_{n_0-1}(z) - P_{n_0-2}^D(z)P_{n_0}(z) = a(n_0)a(1)(\prod_{i=2}^{n_0-1} a(i))^2$.

Proof. To prove (1) we use the recurrence relations (6), (7) and obtain

$$P_1^D(z)P_1(z) - P_0^D(z)P_2(z) = (z - b(1))P_1(z) - P_2(z) = a(1)a(n_0).$$

Similarly for (2), repeated application of the recurrence relations (6), (7) gives

$$\begin{aligned} P_k^D(z)P_k(z) - P_{k-1}^D(z)P_{k+1}(z) \\ = P_k^D(z)P_k(z) - P_{k-1}^D(z)((z - b(k))P_k(z) - a(k)a(n_0 + 1 - k)P_{k-1}(z)) \\ = (P_k^D(z) - P_{k-1}^D(z)(z - b(k)))P_k(z) + a(k)a(n_0 + 1 - k)P_{k-1}(z)P_{k-1}^D(z) \\ = -a(k)a(n_0 + 1 - k)P_{k-2}^D(z)P_k(z) + a(k)a(n_0 + 1 - k)P_{k-1}(z)P_{k-1}^D(z). \end{aligned}$$

To prove (3), we iterate the arguments in parts (1) and (2). ■

Lemma 3.2. *Let $n_0 \geq 2$. Then*

$$(P_{n_0}(z))^2 - \left(\prod_{i=1}^{n_0} a(i)\right)^2 = \det(zI - \mathbf{J}_{cs}) \det(zI - \mathbf{J}_{cs}^D).$$

Proof. We first compute $P_{n_0}(z)$ as a determinant and expand by the first row. Using the centrosymmetric assumption of \mathbf{J}_{cs}^D , we see that the cofactor of $a(1)$ is $-a(n_0)P_{n_0-2}^D(z)$, leading to

$$P_{n_0}(z) = (z - b(0)) \det(zI - \mathbf{J}_{cs}^D) - a(1)a(n_0)P_{n_0-2}^D(z).$$

Hence,

$$(z - b(0))P_{n_0-1}^D(z) = P_{n_0}(z) + a(1)a(n_0)P_{n_0-2}^D(z). \tag{8}$$

Repeated application of the recurrence relations (6), (7) gives

$$\begin{aligned} \det(zI - \mathbf{J}_{cs}) \det(zI - \mathbf{J}_{cs}^D) &= P_{n_0+1}(z)P_{n_0-1}^D(z) \\ &= (z - b(0))P_{n_0}(z)P_{n_0-1}^D(z) - a(n_0)a(1)P_{n_0-1}(z)P_{n_0-1}^D(z) \\ &= (P_{n_0}(z) + a(1)a(n_0)P_{n_0-2}^D(z))P_{n_0}(z) - a(n_0)a(1)P_{n_0-1}(z)P_{n_0-1}^D(z) \\ &= (P_{n_0}(z))^2 - a(n_0)a(1)(P_{n_0-1}^D(z)P_{n_0-1}(z) - P_{n_0-2}^D(z)P_{n_0}(z)), \end{aligned}$$

where the third equality holds by (8). The statement follows by Lemma 3.1 (3). ■

To state the main result of this section, we first establish some Schur complement computations for \mathbf{J}_{cs} . These computations will be relevant in Section 4 and used in the context of the spectral decimation method. We decompose \mathbf{J}_{cs} on $\ell(\partial G_{cs}) \oplus \ell(V(G_{cs}) \setminus \partial G_{cs}) = \ell(\{0, n_0\}) \oplus \ell(\{1, \dots, n_0 - 1\})$ in the block form

$$\begin{pmatrix} S_0 & \bar{X}_0 \\ X_0 & Q_0 \end{pmatrix} = \left(\begin{array}{cc|cccc} b(0) & 0 & a(1) & 0 & \dots & 0 \\ 0 & b(0) & 0 & 0 & \dots & a(1) \\ \hline a(n_0) & 0 & b(1) & a(2) & \dots & 0 \\ 0 & 0 & a(n_0 - 1) & b(2) & \ddots & \vdots \\ \vdots & \vdots & \vdots & \ddots & \ddots & a(n_0 - 1) \\ 0 & a(n_0) & 0 & 0 & a(2) & b(1) \end{array} \right). \tag{9}$$

We observe that S_0 is multiple of the identity matrix $b(0)I$ and that $Q_0 = \mathbf{J}_{cs}^D$. Let $z \in \rho(\mathbf{J}_{cs}^D)$, an element of the resolvent set of \mathbf{J}_{cs}^D , then the Schur complement of \mathbf{J}_{cs} with respect to the decomposition (9) is given by

$$\text{Schur}_{\ell(\partial G_{cs})}(\mathbf{J}_{cs}) := zI - S_0 - \bar{X}_0(zI - Q_0)^{-1}X_0.$$

Our first result states that the Schur complement of \mathbf{J}_{cs} can be expressed using the polynomials $P_{n_0}(z)$ and $P_{n_0-1}^D(z)$.

Theorem 3.3. *For each $z \in \rho(\mathbf{J}_{cs}^D)$ we have*

$$\text{Schur}_{\ell(\partial G_{cs})}(\mathbf{J}_{cs}) = \phi_{\mathbf{J}_{cs}}(z)(R_{\mathbf{J}_{cs}}(z)I - \Delta_0),$$

where Δ_0 is defined in (5) and the functions $R_{\mathbf{J}_{cs}}(z)$ and $\phi_{\mathbf{J}_{cs}}(z)$ are given by

$$R_{\mathbf{J}_{cs}}(z) := 1 - \frac{P_{n_0}(z)}{\prod_{i=1}^{n_0} a(i)}, \quad \phi_{\mathbf{J}_{cs}}(z) := -\frac{\prod_{i=1}^{n_0} a(i)}{P_{n_0-1}^D(z)}. \tag{10}$$

Remark 3.4. Note that $P_{n_0-1}^D(z) = \det(zI - \mathbf{J}_{cs}^D)$. In particular, the domain of $\phi_{\mathbf{J}_{cs}}(z)$ is given by $\rho(\mathbf{J}_{cs}^D)$.

Before proving this result, we first establish an auxiliary lemma.

Lemma 3.5. *Let \bar{X}_0 , Q_0 , and X_0 be the block matrices defined in (9) and $z \in \rho(\mathbf{J}_{cs}^D)$. The following identity holds:*

$$\bar{X}_0(zI - Q_0)^{-1}X_0 = -\frac{\prod_{i=1}^{n_0} a(i)}{P_{n_0-1}^D(z)} \begin{pmatrix} -\frac{P_{n_0-2}^D(z)}{\prod_{i=2}^{n_0-1} a(i)} & -1 \\ -1 & -\frac{P_{n_0-2}^D(z)}{\prod_{i=2}^{n_0-1} a(i)} \end{pmatrix}.$$

In particular, this implies $\text{Schur}_{\ell(\partial G_{cs})}(\mathbf{J}_{cs}) \in \mathcal{CSJ}$ for all $z \in \rho(\mathbf{J}_{cs}^D)$.

Proof. Recall that Q_0 is the Jacobi matrix \mathbf{J}_{cs}^D . We invert the matrix $(zI - \mathbf{J}_{cs}^D)$ using Cramer's rule and restrict the computations to the relevant entries in the adjugate matrix, i.e. $(zI - Q_0)^{-1}$ is equal

$$\frac{1}{P_{n_0-1}^D(z)} \begin{pmatrix} P_{n_0-2}^D(z) & * & \dots & * & (-1)^{n_0}(-1)^{n_0-2} \prod_{i=2}^{n_0-1} a(i) \\ * & * & \dots & * & * \\ \vdots & \vdots & \vdots & \vdots & \vdots \\ * & * & \dots & * & * \\ (-1)^{n_0}(-1)^{n_0-2} \prod_{i=2}^{n_0-1} a(i) & * & \dots & * & P_{n_0-2}^D(z) \end{pmatrix}.$$

For X_0 and \bar{X}_0 , we have

$$X_0 = \begin{pmatrix} a(n_0) & 0 \\ 0 & 0 \\ \vdots & \vdots \\ 0 & a(n_0) \end{pmatrix}, \quad \bar{X}_0 = \begin{pmatrix} a(1) & 0 & \dots & 0 \\ 0 & 0 & \dots & a(1) \end{pmatrix}.$$

A direct computation gives

$$\bar{X}_0(zI - Q_0)^{-1} X_0 = \frac{a(1)a(n_0)}{P_{n_0-1}^D(z)} \begin{pmatrix} P_{n_0-2}^D(z) & \prod_{i=2}^{n_0-1} a(i) \\ \prod_{i=2}^{n_0-1} a(i) & P_{n_0-2}^D(z) \end{pmatrix}. \quad \blacksquare$$

Proof of Theorem 3.3. By Lemma 3.5 and (10), we have

$$\begin{aligned} \bar{X}_0(zI - Q_0)^{-1} X_0 &= \phi_{\mathbf{J}_{cs}}(z) \begin{pmatrix} -\frac{P_{n_0-2}^D(z)}{\prod_{i=2}^{n_0-1} a(i)} & -1 \\ -1 & -\frac{P_{n_0-2}^D(z)}{\prod_{i=2}^{n_0-1} a(i)} \end{pmatrix} \\ &= \phi_{\mathbf{J}_{cs}}(z) \begin{pmatrix} 1 & -1 \\ -1 & 1 \end{pmatrix} - \phi_{\mathbf{J}_{cs}}(z) \left(1 + \frac{P_{n_0-2}^D(z)}{\prod_{i=2}^{n_0-1} a(i)}\right) \begin{pmatrix} 1 & 0 \\ 0 & 1 \end{pmatrix}. \end{aligned}$$

Recall that S_0 is multiple of the identity matrix $b(0)I$, hence

$$\begin{aligned} \text{Schur}_{\ell(\partial G_{cs})}(\mathbf{J}_{cs}) &= zI - S_0 - \bar{X}_0(zI - Q_0)^{-1} X_0 \\ &= \phi_{\mathbf{J}_{cs}}(z) \left(\frac{z - b(0)}{\phi_{\mathbf{J}_{cs}}(z)} + 1 + \frac{P_{n_0-2}^D(z)}{\prod_{i=2}^{n_0-1} a(i)} \right) I - \phi_{\mathbf{J}_{cs}}(z) \Delta_0. \end{aligned}$$

Using (10) and the identity (8), we compute

$$\begin{aligned} \frac{z - b(0)}{\phi_{\mathbf{J}_{cs}}(z)} + 1 + \frac{P_{n_0-2}^D(z)}{\prod_{i=2}^{n_0-1} a(i)} &= -\frac{(z - b(0))P_{n_0-1}^D(z)}{\prod_{i=1}^{n_0} a(i)} + 1 + \frac{a(1)a(n_0)P_{n_0-2}^D(z)}{\prod_{i=1}^{n_0} a(i)} \\ &= 1 - \frac{P_{n_0}(z)}{\prod_{i=1}^{n_0} a(i)} = R_{\mathbf{J}_{cs}}(z). \quad \blacksquare \end{aligned}$$

3.2. Main technical tools

This section is devoted to analyzing the polynomial $R_{\mathbf{J}_{cs}}(z)$. In Section 4 we will see that $R_{\mathbf{J}_{cs}}(z)$ is a *spectral decimation function*, which represents a significant tool in the spectral analysis on fractals and self-similar graphs. The following theorem is the main result of this section and summarizes the relevant features of $R_{\mathbf{J}_{cs}}(z)$ when investigating spectral properties of Jacobi matrices on graphs.

Theorem 3.6. *The following statements hold.*

(1) *For all $z \in \mathbb{C}$, we have*

$$\det(zI - \mathbf{J}_{cs}) \det(zI - \mathbf{J}_{cs}^D) = \left(\prod_{i=1}^{n_0} a(i) \right)^2 R_{\mathbf{J}_{cs}}(z)(R_{\mathbf{J}_{cs}}(z) - 2).$$

In particular, $z \in \sigma(\mathbf{J}_{cs}) \cup \sigma(\mathbf{J}_{cs}^D)$ if and only if $R_{\mathbf{J}_{cs}}(z) \in \{0, 2\}$.

(2) *If $z \in \sigma(\mathbf{J}_{cs}) \cap \sigma(\mathbf{J}_{cs}^D)$, then z is a critical point of $R_{\mathbf{J}_{cs}}$, i.e. $R'_{\mathbf{J}_{cs}}(z) = 0$.*

(3) *Let z be a critical point of $R_{\mathbf{J}_{cs}}(z)$; then $R_{\mathbf{J}_{cs}}(z) \notin (0, 2)$. In particular, there exist n_0 branches of the inverse $R_{\mathbf{J}_{cs}}^{-1}$, that are defined and continuous in the domain $[0, 2]$.*

To prove this result, we make the following elementary observation.

Lemma 3.7. *The polynomial $P_{n_0}(z)$ has n_0 simple real roots. The critical points of $P_{n_0}(z)$ are also real and interlaced between its roots. Moreover, if z_c is a critical point of $P_{n_0}(z)$, then we have*

$$P_{n_0}(z_c)P''_{n_0}(z_c) < 0.$$

We now have all the tools needed to prove the main result of this section.

Proof of Theorem 3.6. It is assumed that $n_0 \geq 2$ and $a(k) \neq 0$ for each $k = 0, \dots, n_0 + 1$ (see Section 3.1), and therefore $P_{n_0}(z)$ is a polynomial of order at least 2. Theorem 3.3 implies: $P_{n_0}(z) = 0$ if and only if $R_{\mathbf{J}_{cs}}(z) = 1$.

(1) Use Lemma 3.2 and the following computation:

$$\begin{aligned} \frac{1}{\left(\prod_{i=1}^{n_0} a(i)\right)^2} \left[(P_{n_0}(z))^2 - \left(\prod_{i=1}^{n_0} a(i)\right)^2 \right] &= \left(\frac{P_{n_0}(z)}{\prod_{i=1}^{n_0} a(i)} - 1 \right) \left(\frac{P_{n_0}(z)}{\prod_{i=1}^{n_0} a(i)} + 1 \right) \\ &= R_{\mathbf{J}_{cs}}(z)(R_{\mathbf{J}_{cs}}(z) - 2), \end{aligned}$$

where in the last equality, we used the definition of the $R_{\mathbf{J}_{cs}}$ given in (10).

Statement (2) follows from differentiating the identity in part (1):

$$\begin{aligned}
 & 2R_{\mathbf{J}_{cs}}(z)R'_{\mathbf{J}_{cs}}(z) - 2R'_{\mathbf{J}_c}(z) \\
 &= \frac{[\det(zI - \mathbf{J}_{cs})]' \det(zI - \mathbf{J}_{cs}^D) + \det(zI - \mathbf{J}_{cs})[\det(zI - \mathbf{J}_{cs}^D)]'}{(\prod_{i=1}^{n_0} a(i))^2}. \tag{11}
 \end{aligned}$$

In (3), if the critical point z_c is in $\sigma(\mathbf{J}_{cs}) \cup \sigma(\mathbf{J}_{cs}^D)$, then the first part of the statement holds by part (1). We assume $z_c \notin \sigma(\mathbf{J}_{cs}) \cup \sigma(\mathbf{J}_{cs}^D)$ and define

$$D(z) := \frac{\det(zI - \mathbf{J}_{cs}) \det(zI - \mathbf{J}_{cs}^D)}{(\prod_{i=1}^{n_0} a(i))^2}.$$

Note that the polynomial $D(z)$ is of degree $2n_0$ and the roots of $D(z)$ are given by the eigenvalues $\sigma(\mathbf{J}_{cs}) \cup \sigma(\mathbf{J}_{cs}^D)$. By (11), we see that z_c is also a critical point of $D(z)$. Moreover, z_c lies between two roots of $D(z)$ due to the assumption $z_c \notin \sigma(\mathbf{J}_{cs}) \cup \sigma(\mathbf{J}_{cs}^D)$. Using Lemma 3.2, we compute

$$D''(z) = \frac{2(P'_{n_0}(z))^2 + 2P_{n_0}(z)P''_{n_0}(z)}{(\prod_{i=1}^{n_0} a(i))^2}.$$

By (10), we have $P'_{n_0}(z_c) = 0$ and Lemma 3.7 implies that z_c is a local maximum of $D(z)$, i.e.,

$$D''(z_c) = \frac{2P_{n_0}(z_c)P''_{n_0}(z_c)}{(\prod_{i=1}^{n_0} a(i))^2} < 0.$$

In particular, we have $D(z_c) > 0$. We rewrite the identity in part (1),

$$(R_{\mathbf{J}_{cs}}(z_c) - 1)^2 = R_{\mathbf{J}_{cs}}(z_c)^2 - 2R_{\mathbf{J}_{cs}}(z_c) + 1 = D(z_c) + 1,$$

which gives $R_{\mathbf{J}_{cs}}(z_c) = 1 \pm \sqrt{D(z_c) + 1} \notin (0, 2)$. ■

4. Spectral decimation of piecewise centrosymmetric Jacobi matrices on graphs

We start by recalling some facts about of the spectral decimation method following the framework set forth in [53], as it is the best suited for our results. Let \mathcal{H} and \mathcal{H}_0 be Hilbert spaces, and $U: \mathcal{H}_0 \rightarrow \mathcal{H}$ be an isometry. Suppose H and H_0 are bounded linear operators on \mathcal{H} and \mathcal{H}_0 , respectively, and that ϕ, ψ are complex-valued functions. We call the operator H *spectrally similar* to the operator H_0 with functions ϕ and ψ if [53, Definition 2.1]

$$U^*(H - zI)^{-1}U = (\phi(z)H_0 - \psi(z)I)^{-1}, \tag{12}$$

for all $z \in \mathbb{C}$ such that the two sides of (12) are well defined. Note, in particular, that for z in the domain of both ϕ and ψ and satisfying $\phi(z) \neq 0$ we have $z \in \rho(H)$ (the resolvent set of H) if and only if $R(z) = \frac{\psi(z)}{\phi(z)} \in \rho(H_0)$. We call $R(z)$ the *spectral decimation function*. The functions $\phi(z)$ and $\psi(z)$ are difficult to determine directly from the structure of the considered fractal or graph, but they can be computed effectively using a Schur complement (several examples may be found in [19, 20]). Identifying \mathcal{H}_0 with a closed subspace of \mathcal{H} via U , let \mathcal{H}_1 be the orthogonal complement and decompose H on $\mathcal{H} = \mathcal{H}_0 \oplus \mathcal{H}_1$ in the block form

$$H = \begin{pmatrix} S & \bar{X} \\ X & Q \end{pmatrix}. \tag{13}$$

Lemma 4.1 ([53, Lemma 3.3]). *For $z \in \rho(H) \cap \rho(Q)$ the operators H and H_0 are spectrally similar if and only if the Schur complement of H (with respect to the decomposition (13)), given by $\text{Schur}_{\mathcal{H}_0}(H) := zI - S - \bar{X}(zI - Q)^{-1}X$, satisfies*

$$\text{Schur}_{\mathcal{H}_0}(H) = \psi(z)I - \phi(z)H_0.$$

The following set plays a crucial role in the spectral decimation method.

Definition 4.2. The *exceptional set* of H is given by

$$\mathcal{E}_H := \{z \in \mathbb{C} \mid z \in \sigma(Q) \text{ or } \phi(z) = 0\}.$$

Proposition 4.3 ([53, Theorem 3.6]). *Let H be spectrally similar to H_0 with functions ϕ and ψ and $z \notin \mathcal{E}_H$. Then*

- (1) $R(z) \in \rho(H_0)$ if and only if $z \in \rho(H)$;
- (2) $R(z)$ is an eigenvalue of H_0 if and only if z is an eigenvalue of H . Moreover, there is a one-to-one map

$$f_0 \mapsto f := f_0 - (zI - Q)^{-1}Xf_0$$

from the eigenspace of H_0 corresponding to $R(z)$ onto the eigenspace of H corresponding to z .

We now apply this framework of the spectral decimation method to the substitution graph G and operator $\mathbf{J} = F_{G_p}(\Delta_p, \mathbf{J}_{cs})$ obtained from a graph G_p equipped with a probabilistic Laplacian Δ_p , and a graph G_{cs} be a finite path graph associated to a centrosymmetric weight matrix \mathbf{J}_{cs} .

Assumption 4.4. We assume that

- (1) there exists a Hilbert space of \mathbb{C} -valued functions on $V(G_p)$, which we denote by $\ell^2(G_p, d\pi_p)$, such that the probabilistic graph Laplacian Δ_p is bounded and self-adjoint;

- (2) there exists a Hilbert space of \mathbb{C} -valued functions on $V(G)$, which we denote by $\ell^2(G, d\pi_J)$, such that \mathbf{J} is bounded and self-adjoint;
- (3) there exists an isometry $U: \ell^2(G_p, d\pi_p) \rightarrow \ell^2(G, d\pi_J)$.

Remark 4.5. The self-adjointness assumption is by no means necessary. In fact, the results in [53] hold for more general operators. Section 5 shows how to construct such Hilbert spaces in the one-dimensional path graphs case, for which Assumption 4.4 holds. The key idea is to equip the set of vertices $V(G_p)$ and $V(G)$ with a measure satisfying a Kolmogorov’s cycle type condition, see (15) for more details.

We also note that Assumption 4.4 combined with Perron–Frobenius theorem implies that $\sigma(\Delta_{\mathbf{p}}) \subset [0, 2]$, as $\Delta_{\mathbf{p}}$ is a stochastic matrix (with spectrum in $[-1, 1]$) shifted by the identity, see also [53, Remark 5.9].

Proposition 4.6. *The following statements hold.*

- (1) For the exceptional set, we have $\mathcal{E}_{\mathbf{J}_{cs}} = \sigma(\mathbf{J}_{cs}^D)$.
- (2) \mathbf{J}_{cs} is spectrally similar to Δ_0 (given in (5)) with the functions $\phi_{\mathbf{J}_{cs}}(z)$ defined in (10), and $\psi_{\mathbf{J}_{cs}}(z) := \phi_{\mathbf{J}_{cs}}(z)R_{\mathbf{J}_{cs}}(z)$, where $R_{\mathbf{J}_{cs}}(z)$ is given by (10). In particular, $R_{\mathbf{J}_{cs}}(z)$ is the corresponding spectral decimation function.
- (3) $\mathbf{J} = F_{G_p}(\Delta_{\mathbf{p}}, \mathbf{J}_{cs})$ is spectrally similar to $\Delta_{\mathbf{p}}$ with the same functions $\phi_{\mathbf{J}_{cs}}(z)$ and $\psi_{\mathbf{J}_{cs}}(z)$ as in part (2). The associated spectral decimation function and exceptional set coincide with $R_{\mathbf{J}_{cs}}(z)$ and $\mathcal{E}_{\mathbf{J}_{cs}}$, respectively.

Proof. Statement (1) follows by Definition 4.2 and $\phi_{\mathbf{J}_{cs}}(z) \neq 0$ (see (10) and recall the assumption $a(i) \neq 0$). Statement (2) follows by Lemma 4.1 and Theorem 3.3. Statement (3) is an immediate consequence of Lemma [53, Lemma 3.10] and its main idea can be sketched as follows. Using the isometry U , we decompose \mathbf{J} on $\ell^2(G, d\pi_J) = U(\ell^2(G_p, d\pi_p)) \oplus U(\ell^2(G_p, d\pi_p))^\perp$ in the block form (13) and denote the Schur complement of \mathbf{J} with respect to the decomposition (13) by $\text{Schur}_{\ell(V(G_p))}(\mathbf{J}) := zI - S - \bar{X}(zI - Q)^{-1}X$. The Schur complement is preserved under the substitution operator F_{G_p} , in the sense

$$F_{G_p}(\Delta_{\mathbf{p}}, \text{Schur}_{\ell(\partial G_{cs})}(\mathbf{J}_{cs})) = \text{Schur}_{\ell(V(G_p))}(\mathbf{J}).$$

Proposition 2.8, Theorem 3.3, and Lemma 4.1 imply the last statements:

$$\begin{aligned} \text{Schur}_{\ell(V(G_p))}(\mathbf{J}) &= \phi_{\mathbf{J}_{cs}}(z) F_{G_p}(\Delta_{\mathbf{p}}, R_{\mathbf{J}_{cs}}(z)I - \Delta_0) \\ &= \phi_{\mathbf{J}_{cs}}(z)(R_{\mathbf{J}_{cs}}(z)F_{G_p}(\Delta_{\mathbf{p}}, I) - F_{G_p}(\Delta_{\mathbf{p}}, \Delta_0)) \\ &= \phi_{\mathbf{J}_{cs}}(z)(R_{\mathbf{J}_{cs}}(z)I - \Delta_{\mathbf{p}}). \end{aligned} \quad \blacksquare$$

The main result of this section is the following theorem.

Theorem 4.7. *The following statements hold.*

- (1) $R_{\mathbf{J}_{cs}}^{-1}(\sigma(\Delta_{\mathbf{p}}) \setminus \{0, 2\}) \subset \sigma(\mathbf{J}) \subset R_{\mathbf{J}_{cs}}^{-1}(\sigma(\Delta_{\mathbf{p}}) \cup \{0, 2\})$.
- (2) *The resolvent operators satisfy the following renormalization identity:*

$$U^*(zI - \mathbf{J})^{-1}U = -\frac{P_{n_0-1}^D(z)}{\prod_{i=1}^{n_0} a(i)}(R_{\mathbf{J}_{cs}}(z)I - \Delta_{\mathbf{p}})^{-1} \tag{14}$$

for $z \in \rho(\mathbf{J})$ and $z \notin \mathcal{E}_{\mathbf{J}_{cs}} = \sigma(\mathbf{J}_{cs}^D)$.

- (3) *The polynomial $R_{\mathbf{J}_{cs}}$ preserves the types of the spectral measures of the operators \mathbf{J} and $\Delta_{\mathbf{p}}$ outside of the finite exceptional set $R_{\mathbf{J}_{cs}}^{-1}(\{0, 2\})$.*

Proof. Theorem 3.6 asserts that $\mathcal{E}_{\mathbf{J}_{cs}} \subset R_{\mathbf{J}_{cs}}^{-1}\{0, 2\}$. Statements (1) and (2) follow by Proposition 4.3 and Proposition 4.6. Statement (3) is proved following the same lines as [80, Theorem 2.3]. We use (14), (12), and the Schur complement in Lemma 4.1 with the block decomposition (13). Using the standard general theory [65, Section VIII.7] or [84, Chapter 3], for a self-adjoint operator H on a Hilbert space \mathcal{H} the spectral measure μ_ψ of $\psi \in \mathcal{H}$ is uniquely defined by the Herglotz function $F_\psi(z)$, a Borel transform of a finite Borel measure, $F_\psi(z) = \langle \psi | (H - z)^{-1} \psi \rangle_{\mathcal{H}} = \int_{\mathbb{R}} \frac{1}{\lambda - z} d\mu_\psi(\lambda)$, $z \in \mathbb{C} \setminus \mathbb{R}$. The measure μ_ψ is unique by the Stieltjes inversion formula, which implies the result. In particular, if $** \in \{\text{pp, sc, ac}\}$ stands for *pure point, singular continuous, absolutely continuous* spectrum, then, for $z \notin \mathcal{E}_{\mathbf{J}_{cs}}$, we have $R(z) \in \sigma_{**}(\Delta_{\mathbf{p}})$ if and only if $z \in \sigma_{**}(\mathbf{J})$. ■

Remark 4.8. Theorem 4.7 can be extended to a formula for the spectral projections and the spectral resolution of the identity, similarly to [80, Theorem 2.3], using the general theory of Schur complement for self-adjoint operators, see [19, 50, 51, 65, 73, 74, 79, 82]. Useful resolvent estimates are given in [45, 66].

Corollary 4.9. *If the points 0 and 2 are limit points of $\sigma(\Delta_{\mathbf{p}})$, then*

$$\sigma(\mathbf{J}) = R_{\mathbf{J}_{cs}}^{-1}(\sigma(\Delta_{\mathbf{p}})).$$

Proof. Theorem 3.6 asserts the existence and continuity of the branches of the inverse $R_{\mathbf{J}_{cs}}^{-1}$ on the interval $[0, 2]$. We conclude

$$\begin{aligned} R_{\mathbf{J}_{cs}}^{-1}(\sigma(\Delta_{\mathbf{p}})) &= \overline{R_{\mathbf{J}_{cs}}^{-1}(\sigma(\Delta_{\mathbf{p}}) \setminus \{0, 2\})} \subset \sigma(\mathbf{J}) \subset \overline{R_{\mathbf{J}_{cs}}^{-1}(\sigma(\Delta_{\mathbf{p}}) \cup \{0, 2\})} \\ &= R_{\mathbf{J}_{cs}}^{-1}(\sigma(\Delta_{\mathbf{p}})). \end{aligned} \quad \blacksquare$$

5. The one-dimensional path graphs case

In this section, we illustrate the results of the previous sections by focusing on one-dimensional path graphs. We apply the framework of Section 4 and start by addressing

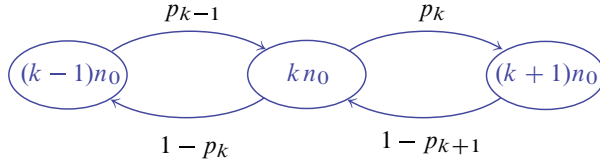


Figure 3. The directed path graph $G_p = (V(G_p), E(G_p))$.

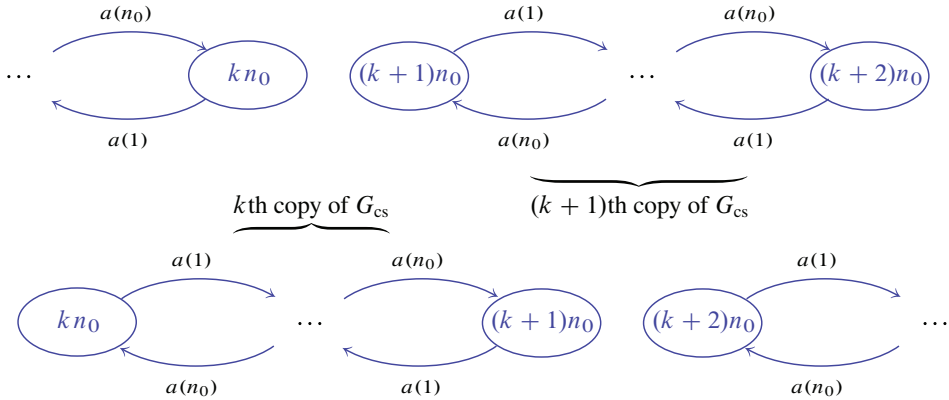


Figure 4. Constructing the graph G by substituting copies of G_{cs} between adjacent vertices in G_p .

the question concerning the existence of the Hilbert spaces and the isometry mapping in Assumption 4.4. Let $G_{cs} = (V(G_{cs}), E(G_{cs}))$ be defined as in Section 2.1. Suppose that G_{cs} consists of $n_0 + 1$ vertices for fixed $n_0 \geq 1$ and the associated weight matrix $\mathbf{J}_{cs} \in \mathcal{CSJ}$ is of the form (1). Next, we restrict the definition of $G_p = (V(G_p), E(G_p))$ as given in Section 2.2 to path graphs. We distinguish three cases, when G_p is a finite, semi-infinite, or infinite path graph. Accordingly, the set of vertices is given by

$$V(G_p) = \{0, n_0, \dots, k_0 n_0\}, \quad V(G_p) = n_0 \mathbb{Z}_+ \text{ or } V(G_p) = n_0 \mathbb{Z}.$$

The set of edges $E(G_p)$ is then given by

$$\begin{aligned} & \{(kn_0, kn_0 + n_0) \mid kn_0, (k + 1)n_0 \in V(G_p)\} \\ & \cup \{(kn_0 + n_0, kn_0) \mid kn_0, (k + 1)n_0 \in V(G_p)\}. \end{aligned}$$

We simplify the notation and set for the transition probabilities $p_k := p(kn_0, kn_0 + n_0)$. In particular, the third equation in conditions (2) implies that $p(kn_0, kn_0 - n_0) = 1 - p_k$, see Figure 3. Let $G = (V(G), E(G))$ be the constructed graph when substituting copies of G_{cs} between adjacent vertices in G_p as explained

in Section 2.3. Depending on G_p , we distinguish three cases, where G is a finite, semi-infinite or infinite path graph. Accordingly, the set of vertices is given by

$$V(G) = [0, n] \cap \mathbb{Z}_+, \quad V(G) = \mathbb{Z}_+ \text{ or } V(G) = \mathbb{Z},$$

where $n \in \mathbb{N}$, $n \geq 1$. In the finite graph case, we assume that n_0 is a divisor of n , i.e. $n = k_0 n_0$, and k_0 is the number of the copies of G_{cs} in G . We regard the vertices $\{kn_0, \dots, (k + 1)n_0\}$ as the vertices of the k th copy of G_{cs} , see Figure 4. The weight matrix associated with the graph G is a tridiagonal matrix, that is created by the substitution operator $\mathbf{J} = F_{G_p}(\Delta_p, \mathbf{J}_{cs})$. The operators Δ_p and \mathbf{J} are assumed to act on the Hilbert spaces

$$\begin{cases} \ell^2(G_p, d\pi_p) := \{f: V(G_p) \rightarrow \mathbb{C} \mid \sum_{x \in V(G_p)} |f(x)|^2 \pi_p(x) < \infty\}, \\ \langle f, g \rangle_p = \sum_{x \in V(G_p)} \overline{f(x)} g(x) \pi_p(x), \\ \ell^2(G, d\pi_J) := \{f: V(G) \rightarrow \mathbb{C} \mid \sum_{x \in V(G)} |f(x)|^2 \pi_J(x) < \infty\}, \\ \langle f, g \rangle_J = \sum_{x \in V(G)} \overline{f(x)} g(x) \pi_J(x), \end{cases}$$

respectively, where the set of vertices $V(G_p)$ and $V(G)$ are equipped with the following measures satisfying the Kolmogorov’s cycle condition [38, 43, 46, 47]:

$$\begin{cases} \pi_p(0) = 1, & \pi_p(kn_0) = \pi_p((k - 1)n_0) \frac{p_{k-1}}{p_k}, & kn_0 \in V(G_p) \setminus \{0\}, \\ \pi_J(0) = 1, & \pi_J(x) = \pi_J(x - 1) \frac{\mathbf{J}(x-1,x)}{\mathbf{J}(x,x-1)}, & x \in V(G). \end{cases} \tag{15}$$

Note that if we set $\mathbf{J}(x - 1, x) = \mathbf{J}(x, x - 1)$ for all $x \in \mathbb{Z}$ in the infinite graph case, we obtain $\ell^2(G, d\pi_J) = \ell^2(\mathbb{Z})$.

Proposition 5.1. *The operator \mathbf{J} (resp. Δ_p) is a bounded self-adjoint operator on $\ell^2(G, d\pi_J)$ (resp. $\ell^2(G_p, d\pi_p)$). Moreover, for $x \in V(G_p) \subset V(G)$, we have $\pi_p(x) = \pi_J(x)$.*

Proof. Let $W_n(f, g) := \pi_J(n) \mathbf{J}(n, n + 1)(f(n)g(n + 1) - f(n + 1)g(n))$ be the n -th Wronskian of f and g . Direct computation gives

$$\sum_{x=m}^n f(x) \mathbf{J} g(x) \pi_J(x) - \sum_{x=m}^n \mathbf{J} f(x) g(x) \pi_J(x) = W_n(f, g) - W_{m-1}(f, g).$$

For $f, g \in \ell^2(G, d\pi_J)$, we see that $\langle f, \mathbf{J} g \rangle_J - \langle \mathbf{J} f, g \rangle_J = \lim_{n \rightarrow \infty} W_n(f, g) - \lim_{m \rightarrow -\infty} W_{m-1}(f, g) = 0$. Similar computations for the semi-infinite graph case and the proof is identical for Δ_p . The second statement follows by (15) and the centrosymmetry assumption on \mathbf{J}_{cs} . ■

Using Proposition 5.1, we view $\ell^2(G_p, d\pi_p)$ as a subspace of $\ell^2(G, d\pi_J)$ via the identification

$$\ell^2(G_p, d\pi_p) \cong \{\psi \in \ell^2(G, d\pi_J) \mid \psi(x) = 0 \text{ for all } x \in V(G) \setminus V(G_p)\}.$$

In this sense, $U: \ell^2(G_p, d\pi_p) \rightarrow \ell^2(G, d\pi_J)$ is the inclusion operator.

Proposition 5.2. *Assume G_p is a finite path graph. Then*

$$\sigma(\mathbf{J}) = (R_{\mathbf{J}_{cs}}^{-1}(\sigma(\Delta_{\mathbf{p}})) \setminus \{0, 2\}) \cup \sigma(\mathbf{J}_{cs}).$$

Proof. The constant vector $(1, 1, 1, \dots)^\top$ is an eigenvector with the eigenvalue 0 and the alternating vector $(1, -1, 1, \dots)^\top$ is an eigenvector with the eigenvalue 2 for $\Delta_{\mathbf{p}}$. Hence, we have $\{0, 2\} \subset \sigma(\Delta_{\mathbf{p}}) \subset [0, 2]$. In particular, $|\sigma(\Delta_{\mathbf{p}}) \setminus \{0, 2\}| = k_0 - 1$. Note that $R_{\mathbf{J}_{cs}}(z)$ is as $P_{n_0}(z)$ a polynomial of degree n_0 . Theorem 3.6 implies

$$|R_{\mathbf{J}_{cs}}^{-1}(\sigma(\Delta_{\mathbf{p}}) \setminus \{0, 2\})| = n_0(k_0 - 1) = n_0k_0 - n_0.$$

Note that all the $n_0k_0 - n_0$ preimages are not in the exceptional set and therefore distinct eigenvalues of \mathbf{J} . Theorem 3.6 asserts $R_{\mathbf{J}_{cs}}^{-1}(\{0, 2\}) = \sigma(\mathbf{J}_{cs}) \cup \sigma(\mathbf{J}_{cs}^D)$. By excluding the exceptional points $\mathcal{E}_{\mathbf{J}_{cs}} = \sigma(\mathbf{J}_{cs}^D)$, we see that $R_{\mathbf{J}_{cs}}^{-1}(\{0, 2\})$ generates $n_0 + 1$ distinct eigenvalues of \mathbf{J} , namely the eigenvalues in $\sigma(\mathbf{J}_{cs})$. We generated $(n_0k_0 - n_0) + (n_0 + 1) = n_0k_0 + 1$ distinct eigenvalues, which shows with a dimension argument that we completely determined the spectrum $\sigma(\mathbf{J})$. ■

We now restrict our investigations to the case G_p is a finite path graph and use the substitution operator F_{G_p} to generate a multi-parameter family of self-similar probabilistic Laplacians. A key observation is that the centrosymmetric probabilistic Laplacians are invariant under the substitution operator in the sense that if $\Delta_{\mathbf{p}_1}, \Delta_{\mathbf{p}_2} \in \mathcal{CSJ}$ with $\Delta_{\mathbf{p}_1} \in \mathcal{L}_{G_p}$, then $F_{G_p}(\Delta_{\mathbf{p}_1}, \Delta_{\mathbf{p}_2}) \in \mathcal{CSJ} \cap \mathcal{L}_G$.

Definition 5.3. Let $\Delta_{\mathbf{p}}^{(1)} \in \mathcal{CSJ} \cap \mathcal{L}_{G_p}$ be given. We define the sequence

$$\{\Delta_{\mathbf{p}}^{(\ell)}\}_{\ell \in \mathbb{N}} \subset \mathcal{CSJ}$$

inductively by

$$\Delta_{\mathbf{p}}^{(\ell+1)} := F_{G_p}(\Delta_{\mathbf{p}}^{(1)}, \Delta_{\mathbf{p}}^{(\ell)}) \quad \text{for } \ell \geq 1.$$

We refer to $\{\Delta_{\mathbf{p}}^{(\ell)}\}_{\ell \in \mathbb{N}}$ as a *sequence of self-similar probabilistic Laplacians*.

If we initialize $\Delta_{\mathbf{p}}^{(1)} := \Delta_0$, then $\Delta_{\mathbf{p}}^{(\ell)}$ is a constant sequence, i.e., $\Delta_{\mathbf{p}}^{(\ell)} = \Delta_0$ for all $\ell \geq 1$. For $k_0 \geq 2$, $\mathbf{p} = \{p_0, p_1, \dots, p_{k_0}\}$ with $p_0 = 1$ and $p_{k_0} = 0$, we initialize $\Delta_{\mathbf{p}}^{(1)}$ as the following $(k_0 + 1) \times (k_0 + 1)$ -matrices:

$$\Delta_{\mathbf{p}}^{(1)} = \begin{pmatrix} 1 & -1 & 0 & \dots & 0 \\ p_1 - 1 & 1 & -p_1 & \dots & 0 \\ 0 & p_2 - 1 & 1 & \ddots & \vdots \\ \vdots & \vdots & \ddots & \ddots & p_1 - 1 \\ 0 & 0 & 0 & -1 & 1 \end{pmatrix}, \tag{16a}$$

$$\Delta_{\mathbf{p}}^{(1),D} = \begin{pmatrix} 1 & -p_1 & \dots & 0 \\ p_2 - 1 & 1 & \ddots & \vdots \\ \vdots & \ddots & \ddots & p_2 - 1 \\ 0 & 0 & -p_1 & 1 \end{pmatrix}. \tag{16b}$$

Note that the centrosymmetry assumption impose $p_1 = 1 - p_{k_0-1}$, $p_2 = 1 - p_{k_0-2}$, and so on. Proposition 4.6 implies that $\Delta_{\mathbf{p}}^{(1)}$ is spectrally similar to Δ_0 with the functions $R_{\Delta_{\mathbf{p}}^{(1)}}$ and $\phi_{\Delta_{\mathbf{p}}^{(1)}}$ given by

$$R_{\Delta_{\mathbf{p}}^{(1)}}(z) = 1 - (-1)^{k_0} \frac{P_{k_0}(z)}{\prod_{i=0}^{k_0-1} p_i}, \quad \phi_{\Delta_{\mathbf{p}}^{(1)}}(z) = (-1)^{k_0+1} \frac{\prod_{i=0}^{k_0-1} p_i}{P_{k_0-1}^D(z)}, \tag{17}$$

where the polynomial P_{k_0} (resp. $P_{k_0-1}^D$) is defined by the recurrence relation (6) corresponding to the matrix $\Delta_{\mathbf{p}}^{(1)}$ (resp. by the recurrence relation (7) corresponding to the matrix $\Delta_{\mathbf{p}}^{(1),D}$).

Note that in the special case of a symmetric random walk, i.e., $p_k = \frac{1}{2}$ for $k = 1, \dots, k_0 - 1$, we refer to $\Delta_{\mathbf{p}}^{(1)}$ as a *standard probabilistic Laplacian*. A direct computation shows that the spectral decimation function corresponding to a standard probabilistic Laplacian can be derived from a Chebyshev polynomial. Recall that the Chebyshev polynomials of the first kind satisfy the recurrence relations $\text{Cheb}_0(z) = 1$, $\text{Cheb}_1(z) = z$, $\text{Cheb}_k(z) = 2z \text{Cheb}_{k-1}(z) - \text{Cheb}_{k-2}(z)$, where $k \in \{2, \dots, k_0\}$. If $\Delta_{\mathbf{p}}^{(1)}$ is a standard probabilistic Laplacian, i.e., given by (16) and $p_k = \frac{1}{2}$ for $k = 1, \dots, k_0 - 1$, then the corresponding spectral decimation function in (17) is $R_{\Delta_{\mathbf{p}}^{(1)}}(z) = 1 - (-1)^{k_0} \text{Cheb}_{k_0}(z - 1)$. This is discussed in detail in [20, Section 4]. It is evident that for $k_0 = 2$ the 3×3 standard probabilistic Laplacian is the only possible centrosymmetric probabilistic Laplacian of this size.

When $k_0 = 3$, then $\Delta_{\mathbf{p}}^{(1)}$ is of size 4×4 with $\mathbf{p} = \{1, p_1, p_2, 0\}$. Imposing the centrosymmetry assumption on the transition probabilities gives $p_2 = 1 - p_1$. Hence, we obtain a one-parameter family of centrosymmetric probabilistic Laplacians and

it is not difficult to see that this type of probabilistic Laplacians was already studied in [83] under the terminology of a *pq-model*, see also [16, 30] and more recent [56, Proposition 2.3].

5.1. One-parameter family of Laplacians with $k_0 = 4$

Now, we consider the case $k_0 = 4$, i.e., a centrosymmetric probabilistic Laplacian $\Delta_{\mathbf{p}}^{(1)}$ of size 5×5 with $\mathbf{p} = \{1, p_1, p_2, p_3, 0\}$. Imposing the centrosymmetry assumption on the transition probabilities gives $p_3 = 1 - p_1$ and $p_2 = 1 - p_2$. We obtain again a one-parameter family of centrosymmetric probabilistic Laplacians whose matrices are given by

$$\Delta_{\mathbf{p}}^{(1)} = \begin{pmatrix} 1 & -1 & 0 & 0 & 0 \\ p-1 & 1 & -p & 0 & 0 \\ 0 & -\frac{1}{2} & 1 & -\frac{1}{2} & 0 \\ 0 & 0 & -p & 1 & p-1 \\ 0 & 0 & 0 & -1 & 1 \end{pmatrix}, \quad \Delta_{\mathbf{p}}^{(1),D} = \begin{pmatrix} 1 & -p & 0 \\ -\frac{1}{2} & 1 & -\frac{1}{2} \\ 0 & -p & 1 \end{pmatrix} \tag{18}$$

where we set $p_1 = p$ for some $p \in (0, 1)$. Note that this type of probabilistic Laplacians is related to the graph Laplacians studied in [41]. Direct computation gives

$$\begin{cases} \sigma(\Delta_{\mathbf{p}}^{(1)}) = \{0, 1 - \sqrt{1-p}, 1, 1 + \sqrt{1-p}, 2\}, \\ \sigma(\Delta_{\mathbf{p}}^{(1),D}) = \{1 - \sqrt{p}, 1, 1 + \sqrt{p}\}. \end{cases}$$

We compute the spectral decimation function using the formula in (17),

$$R_{\Delta_{\mathbf{p}}^{(1)}}(z) = \frac{2z(2-z)(z-1)^2}{p(1-p)}. \tag{19}$$

We obtain for the set of the preimages

$$\begin{cases} R_{\Delta_{\mathbf{p}}^{(1)}}^{-1}(0) = \{0, 1, 2\}, \\ R_{\Delta_{\mathbf{p}}^{(1)}}^{-1}(2) = \{1 - \sqrt{1-p}, 1 - \sqrt{p}, 1 + \sqrt{p}, 1 + \sqrt{1-p}\}. \end{cases} \tag{20}$$

Figure 5 (top) shows the preimages in (20) using the cutoffs $y = 0$ and $y = 2$. The sequence of self-similar probabilistic Laplacians $\Delta_{\mathbf{p}}^{(\ell)}$ is then constructed as in Definition 5.3, where $\Delta_{\mathbf{p}}^{(1)}$ is initialized by (18). Figure 5 (bottom) shows how the spectrum of $\Delta_{\mathbf{p}}^{(\ell)}$, $\ell = 6$ changes when varying the parameter $p \in (0, 1)$.

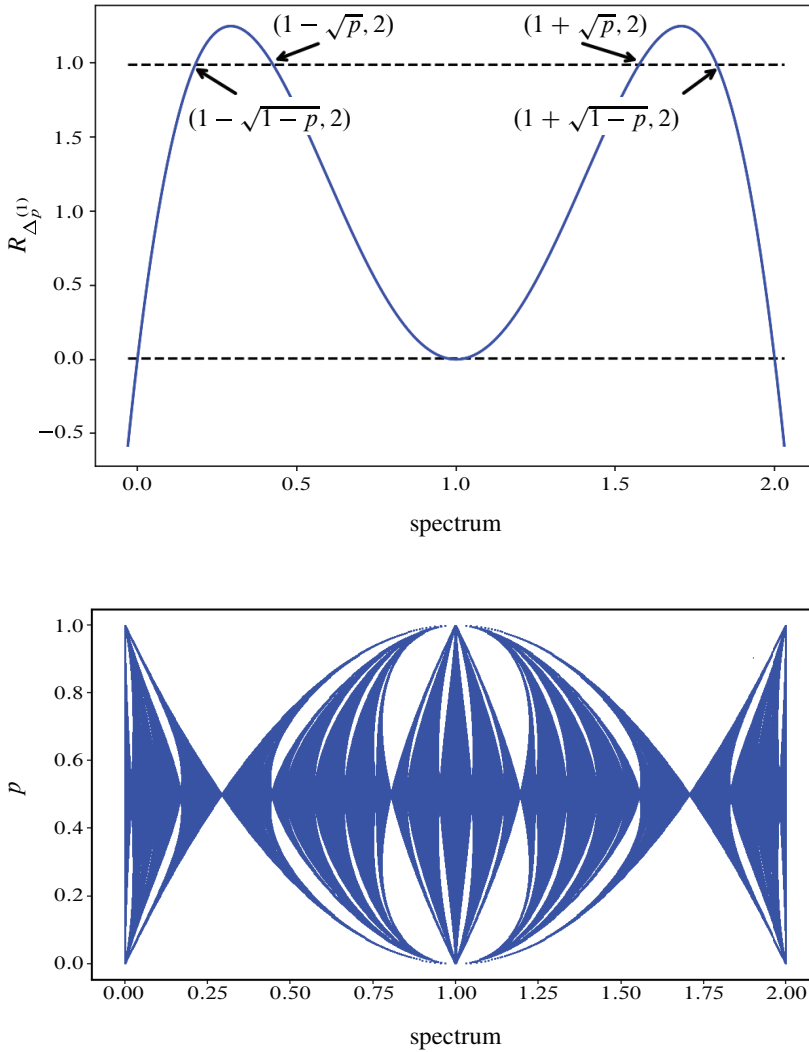


Figure 5. Top. The spectral decimation function (19) corresponding to the probabilistic Laplacians (18). The preimages in (20) are indicated using the cutoffs $y = 0$ and $y = 2$. Bottom. The spectrum of $\Delta_{\mathbf{p}}^{(\ell)}$ for $\ell = 6$ (x-axis) is plotted for $p \in (0, 1)$ (y-axis).

5.2. Two-parameter family of Laplacians with $k_0 = 5$

Now, we consider the case $k_0 = 5$, i.e. a centrosymmetric probabilistic Laplacian $\Delta_{\mathbf{p}}^{(\ell)}$ of size 6×6 with $\mathbf{p} = \{1, p_1, p_2, p_3, p_4, 0\}$. Imposing the centrosymmetry assumption

on the transition probabilities gives $p_4 = 1 - p_1$ and $p_3 = 1 - p_2$. We obtain in this case a two-parameter family of centrosymmetric probabilistic Laplacians whose matrices are given by

$$\Delta_{\mathbf{p}}^{(1)} = \begin{pmatrix} 1 & -1 & 0 & 0 & 0 & 0 \\ p_1 - 1 & 1 & -p_1 & 0 & 0 & 0 \\ 0 & p_2 - 1 & 1 & -p_2 & 0 & 0 \\ 0 & 0 & -p_2 & 1 & p_2 - 1 & 0 \\ 0 & 0 & 0 & -p_1 & 1 & p_1 - 1 \\ 0 & 0 & 0 & 0 & -1 & 1 \end{pmatrix}, \quad (21a)$$

$$\Delta_{\mathbf{p}}^{(1),D} = \begin{pmatrix} 1 & -p_1 & 0 & 0 \\ p_2 - 1 & 1 & -p_2 & 0 \\ 0 & -p_2 & 1 & p_2 - 1 \\ 0 & 0 & -p_1 & 1 \end{pmatrix}. \quad (21b)$$

We compute the spectral decimation function using the formula in (17),

$$R_{\Delta_{\mathbf{p}}^{(1)}}(z) = \frac{z}{p_1 p_2 (p_1 - 1)(p_2 - 1)} (z^2 + z(p_2 - 3) + p_1 p_2 - 2p_2 + 2) \\ \times (z^2 - z(p_2 + 2) + p_1 p_2 - p_1 + p_2 + 1)$$

For the convenience of the notation, we fix $p_1 = \frac{2}{3}$ and compute the eigenvalues as functions of the parameter p_2 ,

$$\sigma(\Delta_{\mathbf{p}}^{(1)}) = \{\lambda_1, \lambda_2, \lambda_3, \lambda_4, \lambda_5, \lambda_6\}, \quad \sigma(\Delta_{\mathbf{p}}^{(1),D}) = \{\lambda_1^D, \lambda_2^D, \lambda_3^D, \lambda_4^D\}. \quad (22)$$

The formulas for eigenvalues are given by

$$\begin{aligned} \lambda_1 &= 0, \\ \lambda_2 &= \frac{1 + p_2}{2} - \frac{\sqrt{9p_2^2 - 6p_2 + 9}}{6}, \\ \lambda_3 &= \frac{1 + p_2}{2} + \frac{\sqrt{9p_2^2 - 6p_2 + 9}}{6}, \\ \lambda_4 &= \frac{3 - p_2}{2} - \frac{\sqrt{9p_2^2 - 6p_2 + 9}}{6}, \\ \lambda_5 &= \frac{3 - p_2}{2} + \frac{\sqrt{9p_2^2 - 6p_2 + 9}}{6}, \\ \lambda_6 &= 2, \end{aligned}$$

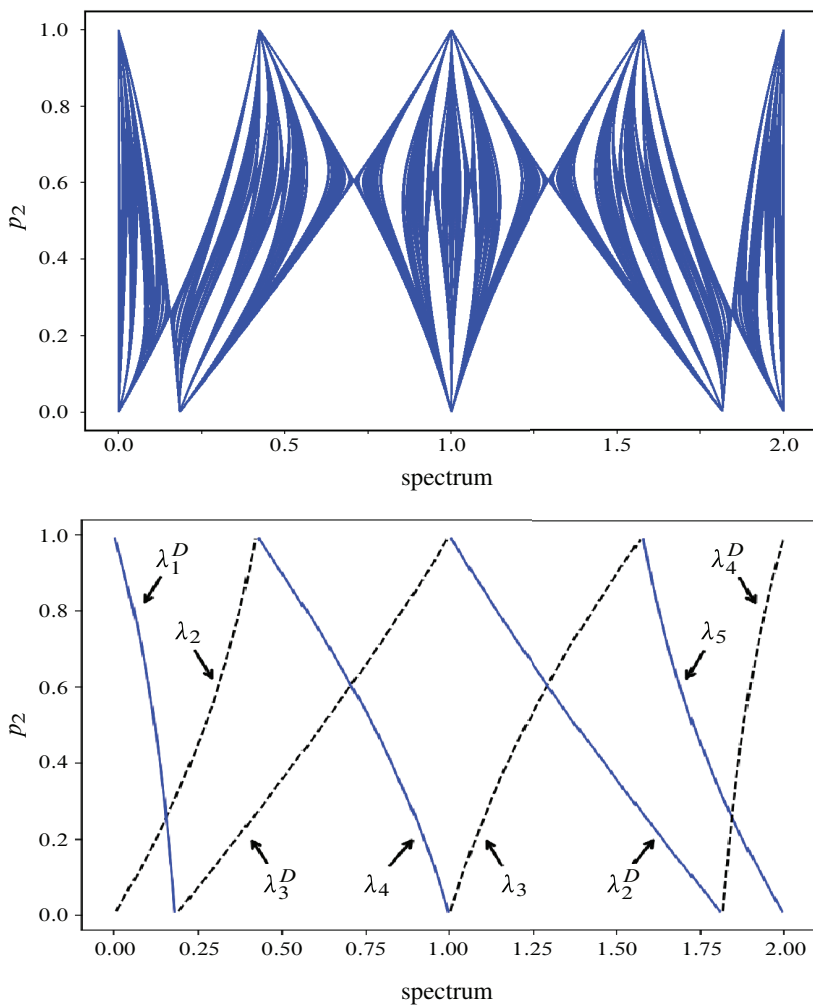


Figure 6. (Top) The spectrum of $\Delta_{\mathbf{p}}^{(\ell)}$ for $\ell = 5$ is plotted on the x-axis for $p_2 \in (0, 1)$ (y-axis), while $p_1 = \frac{2}{3}$ is fixed. (Bottom) Plotting the eigenvalues as functions of p_2 reproduces the contour of the spectra.

and

$$\lambda_1^D = \frac{2 - p_2}{2} - \frac{\sqrt{9p_2^2 - 24p_2 + 24}}{6}, \quad \lambda_2^D = \frac{2 - p_2}{2} + \frac{\sqrt{9p_2^2 - 24p_2 + 24}}{6},$$

$$\lambda_3^D = \frac{2 + p_2}{2} - \frac{\sqrt{9p_2^2 - 24p_2 + 24}}{6}, \quad \lambda_4^D = \frac{2 + p_2}{2} + \frac{\sqrt{9p_2^2 - 24p_2 + 24}}{6}.$$

Now, we construct the sequence of self-similar probabilistic Laplacians $\Delta_{\mathbf{p}}^{(\ell)}$ as in Definition 5.3, where $\Delta_{\mathbf{p}}^{(1)}$ is initialized by (21). Figure 6 (top) shows how the spectrum of $\Delta_{\mathbf{p}}^{(\ell)}$, $\ell = 5$ changes when varying the parameter $p_2 \in (0, 1)$ and fixing $p_1 = \frac{2}{3}$. Plotting the eigenvalues (22) as functions of p_2 reproduces the contour of the spectra in Figure 6 (top). Using the eigenvalue-formulas, we can for example determine when the spectral gap between λ_1^D and λ_2 closes, namely by reducing the problem to solving the equation $\lambda_1^D = \lambda_2$, see Figure 6 (bottom).

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